International Union of Crystallography

Commission on Mathematical and Theoretical Crystallography

Symmetry Relationships between Crystal Structures with Applications to Structural and Magnetic Phase Transitions

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CRYSTALLOGRAPHIC POINT GROUPS II
(further developments)

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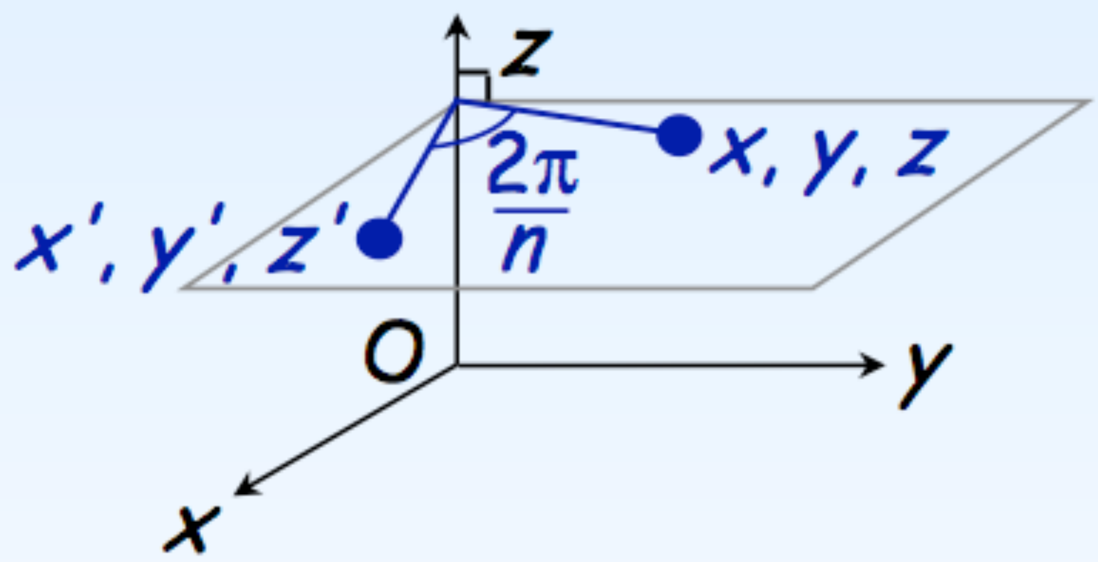
CRYSTALLOGRAPHIC POINT GROUPS

(brief overview)

Symmetry operations in 3D
Rotations

Rotation (around an axis)

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



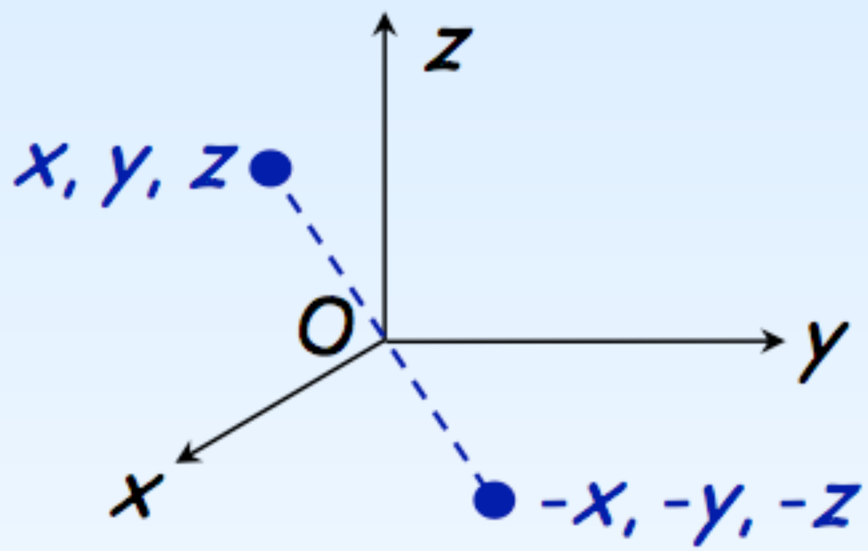
n

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

Det = +1

Symmetry operations in 3D
Rotoinvertions

Inversion (through a point)



$\bar{1}$

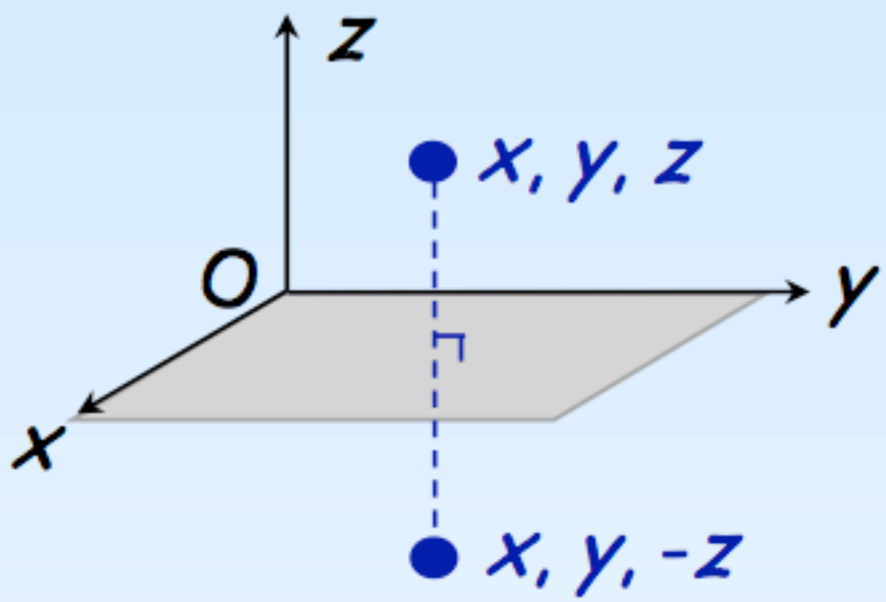
a crystal which has the inversion symmetry is called centrosymmetrical.

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

Det = -1

Symmetry operations in 3D
Rotoinvertions

Reflection (through a mirror plane)



m

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

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

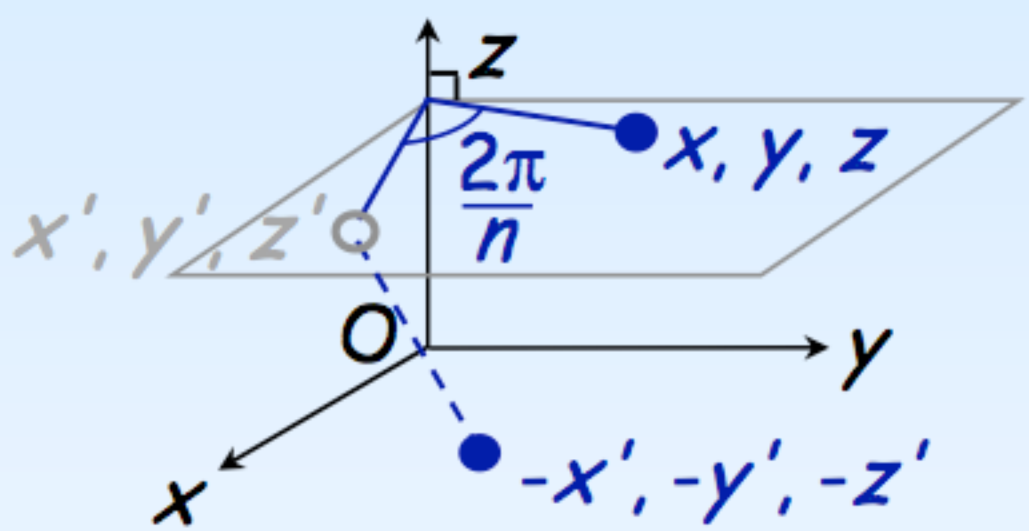
Det = -1

Symmetry operations in 3D
Rotoinversions

Roto-inversion

(around an axis and through a point)

Rotation followed by an inversion



$\bar{n}$

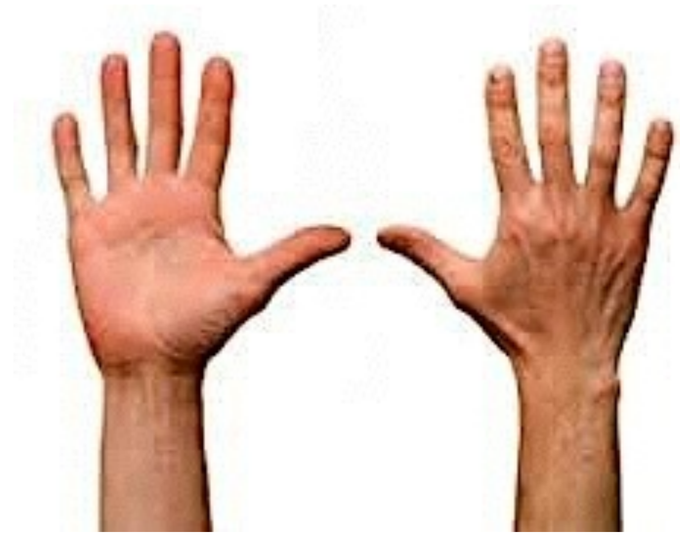
$$\alpha(\bar{n}) = \begin{pmatrix} -\cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det = -1

Crystallographic Point Groups in 3D

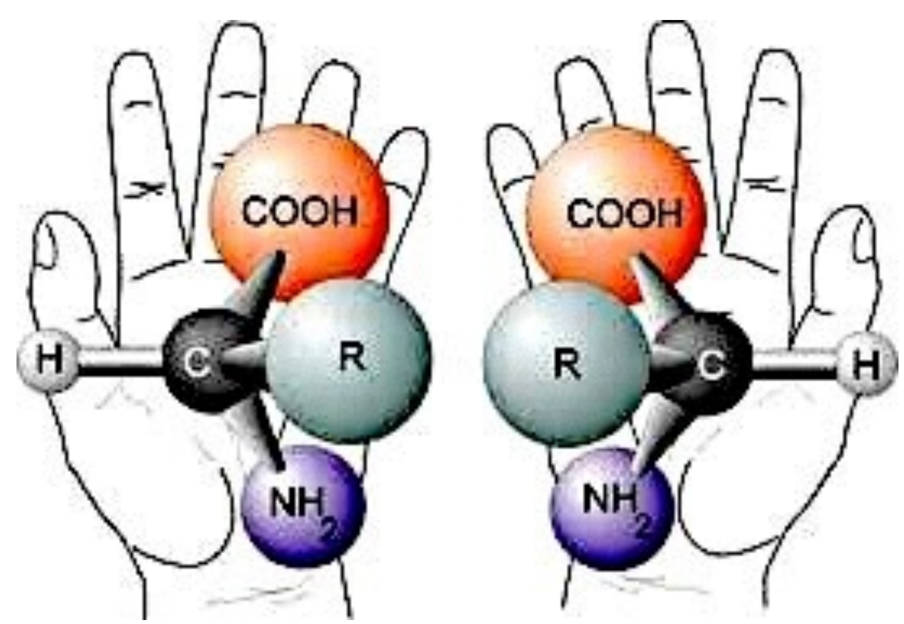
Proper rotations: det =+1: 1 2 3 4 6

chirality preserving



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

chirality non-preserving



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

-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, *mm*2, *mmm*	$\alpha = \beta = \gamma = 90°$	[100]	[010]	[001]
Tetragonal	4, $\bar{4}$, 4/*m* 422, 4*mm*, $\bar{4}2m$, 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, $\bar{4}3m$, $m\bar{3}m$	$a = b = c$ $\alpha = \beta = \gamma = 90°$	$\{[100], [010], [001]\}$	$\{[111], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]\}$	$\{[1\bar{1}0], [110], [01\bar{1}], [011], [\bar{1}01], [101]\}$

Crystallographic Point Groups in 3D

System used in this volume	Point group International symbol Short	 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

Crystallographic point groups as abstract groups

Symbol	order	HM symbols
$\mathcal{C}_1$	1	1
$\mathcal{C}_2$	2	2, m, $\overline{1}$
$\mathcal{C}_3$	3	3
$\mathcal{C}_4$	4	4, $\overline{4}$
$\mathcal{C}_6 \equiv \mathcal{C}_3 \times \mathcal{C}_2$	6	$\overline{3}$, 6, $\overline{6}$
$\mathcal{D}_2 \equiv \mathcal{C}_2 \times \mathcal{C}_2$	4	$2/m$, 222, $mm2$
$\mathcal{D}_3$	6	32, $3m$
$\mathcal{D}_4$	8	422, $4mm$, $\overline{4}2m$
$\mathcal{D}_6 \equiv \mathcal{D}_3 \times \mathcal{C}_2$	12	$\overline{3}m$, 622, $6mm$, $\overline{6}2m$
$\mathcal{D}_{2h} \equiv \mathcal{C}_2 \times \mathcal{C}_2 \times \mathcal{C}_2$	8	mmm
$\mathcal{C}_{4h} \equiv \mathcal{C}_4 \times \mathcal{C}_2$	8	$4/m$
$\mathcal{C}_{6h} \equiv \mathcal{C}_6 \times \mathcal{C}_2$	12	$6/m$
$\mathcal{D}_{4h} \equiv \mathcal{D}_4 \times \mathcal{C}_2$	16	$4/mmm$
$\mathcal{D}_{6h} \equiv \mathcal{D}_6 \times \mathcal{C}_2$	24	$6/mmm$
$\mathcal{T}$	12	23
$\mathcal{T}_h \equiv \mathcal{T} \times \mathcal{C}_2$	24	$m\overline{3}$
$\mathcal{O}$	24	432, $\overline{4}3m$
$\mathcal{O}_h \equiv \mathcal{O} \times \mathcal{C}_2$	48	$m\overline{3}m$

Crystallographic point groups and abstract groups

Abstract groups →

- Cyclic groups
- Abelian non-cyclic groups
- Non-Abelian groups
- Direct products of non-Abelian groups with cyclic groups of order 2

Crystal classes —Affine equivalence→ Abstract groups

32 → 18

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: $(g_1,g_2)\ (g'_1,g'_2) = (g_1 g'_1, g_2 g'_2)$.

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

Properties of $G_1 \otimes G_2$

(i) $G_1 \otimes G_2 \triangleright \{(g_1,e_2), g_1 \in G_1\} \cong G_1$

$G_1 \otimes G_2 \triangleright \{(e_1,g_2), g_2 \in G_2\} \cong G_2$

(ii) $\{(g_1,e_2), g_1 \in G_1\} \cap \{(e_1,g_2), g_2 \in G_1\} = \{(e_1,e_2)\}$

(iii) $\forall\ (g_1,g_2) \in G_1 \otimes G_2 :\ (g_1,g_2) = (g_1,e_2)\ (e_1,g_2)$

Examples: Direct product groups

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

$G_1 = \{1, 2_z\}$ $G_2 = \{1, m_x\}$

$G_1 \otimes G_2 = \{1.1,\ 2_z.1,\ 1.m_x,\ 2_z m_x = m_y\}$

Centro-symmetrical groups

G_1: rotational groups

$G_2 = \{1, \bar{1}\}$ group of inversion

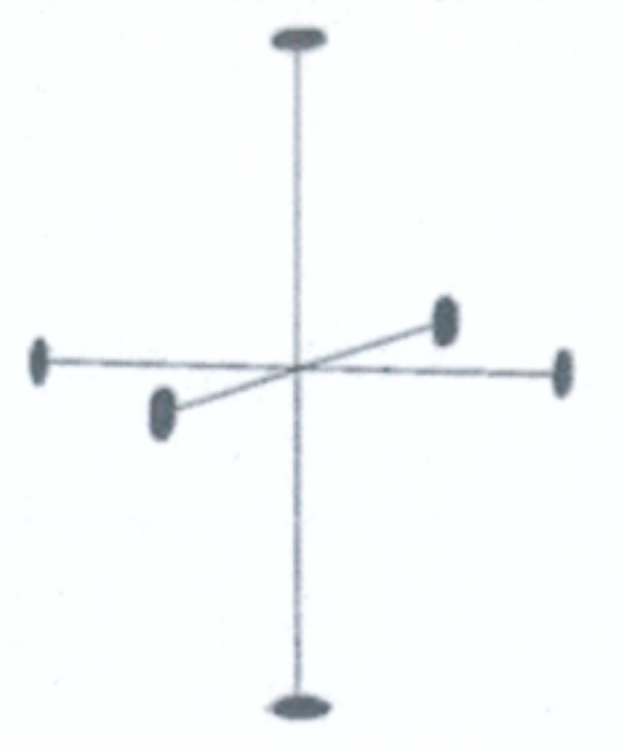
$G_1 \otimes \{1, \bar{1}\} = G_1 + \bar{1}.G_1$

Rotation Crystallographic Point Groups in 3D

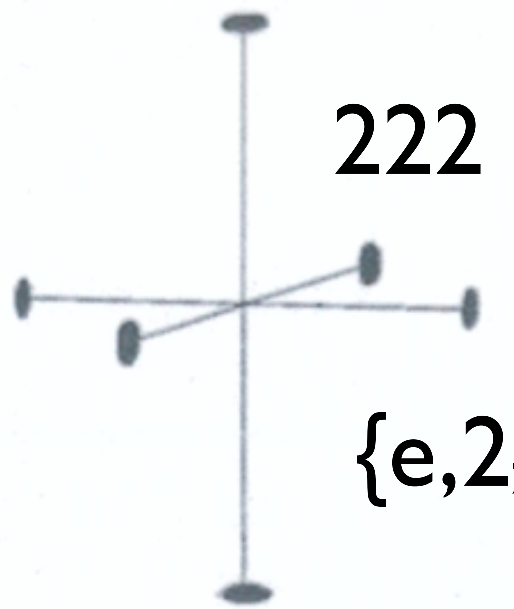
Cyclic: 1(C_1), 2(C_2), 3(C_3), 4(C_4), 6(C_6)

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

Cubic: 23 (T), 432 (O)

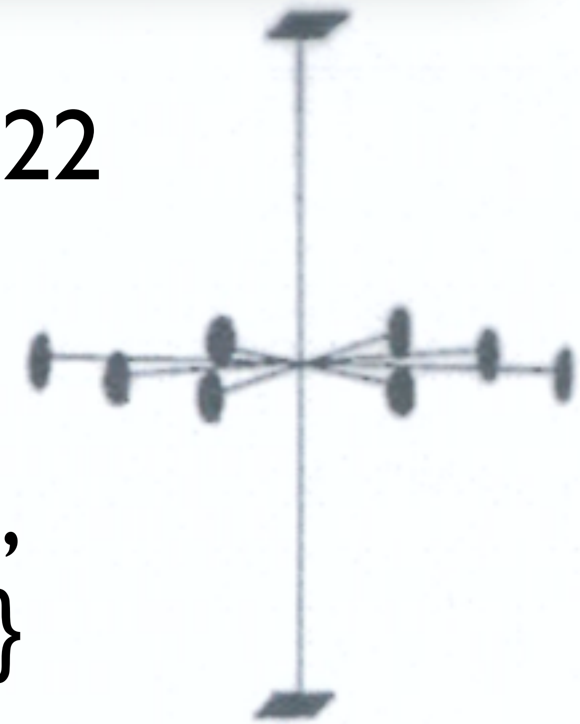


Dihedral Point Groups



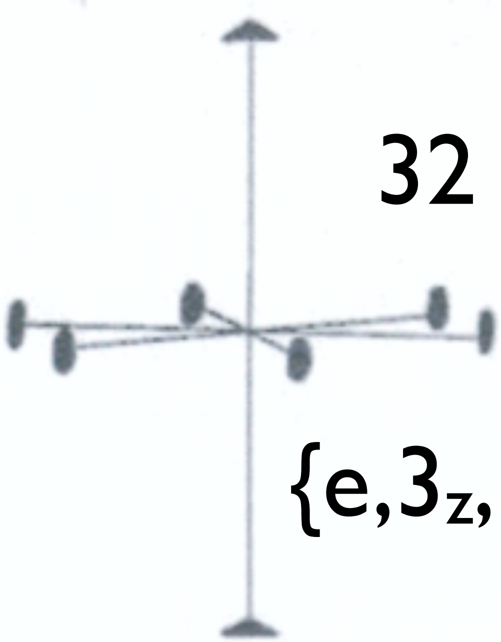
222

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



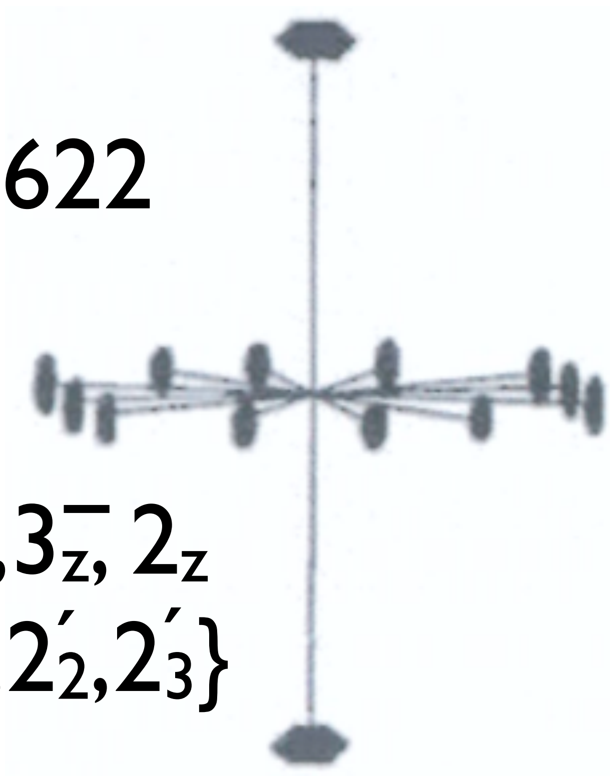
422

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



32

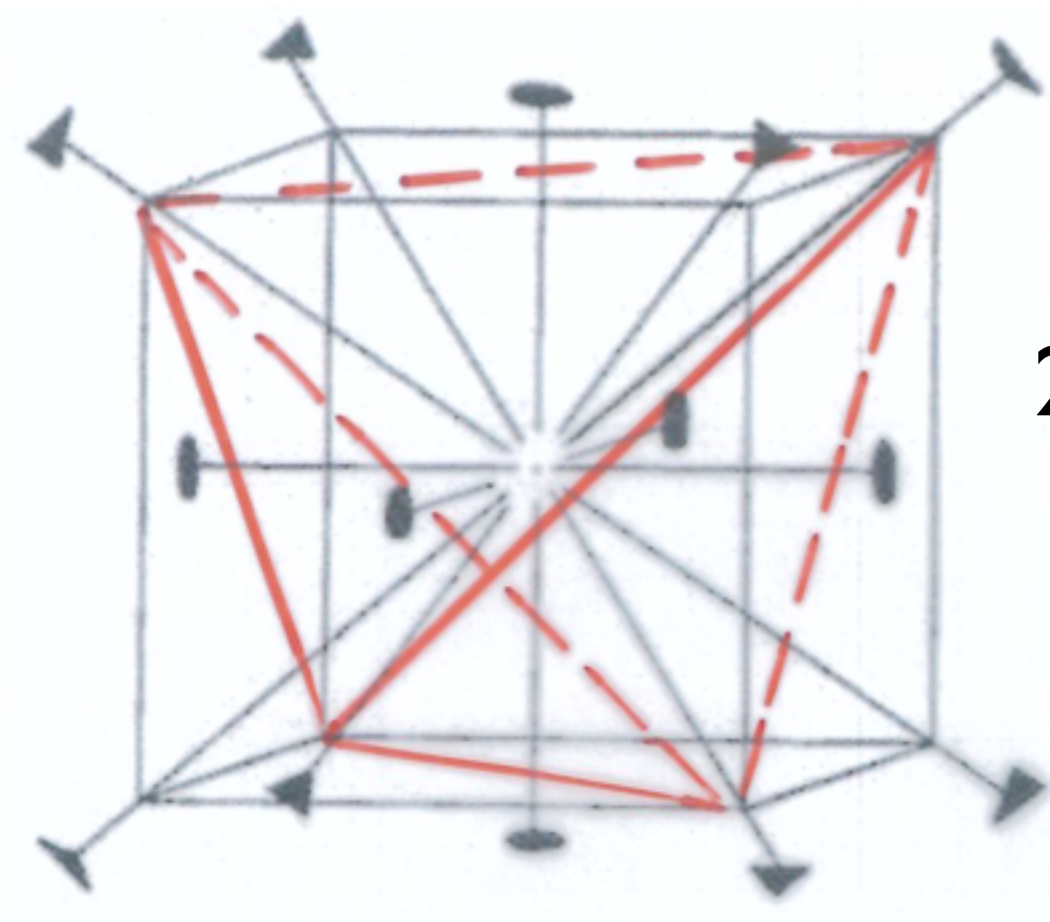
$\{e, 3_z, 3_z^{-}, 2_1, 2_2, 2_3\}$



622

$\{e, 6_z, 6_z^{-}, 3_z, 3_z^{-}, 2_z\ 2_1, 2_2, 2_3, 2_1', 2_2', 2_3'\}$

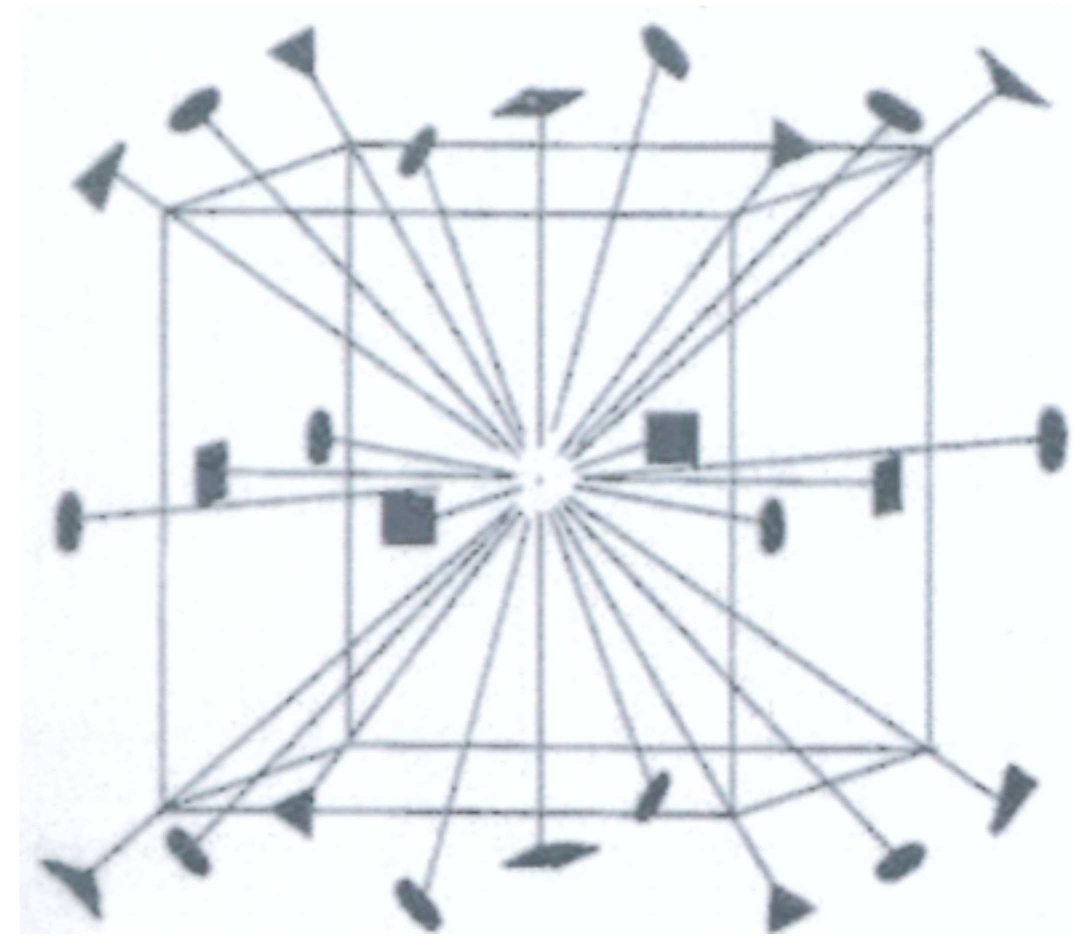
Cubic Rotational Point Groups



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)



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

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})

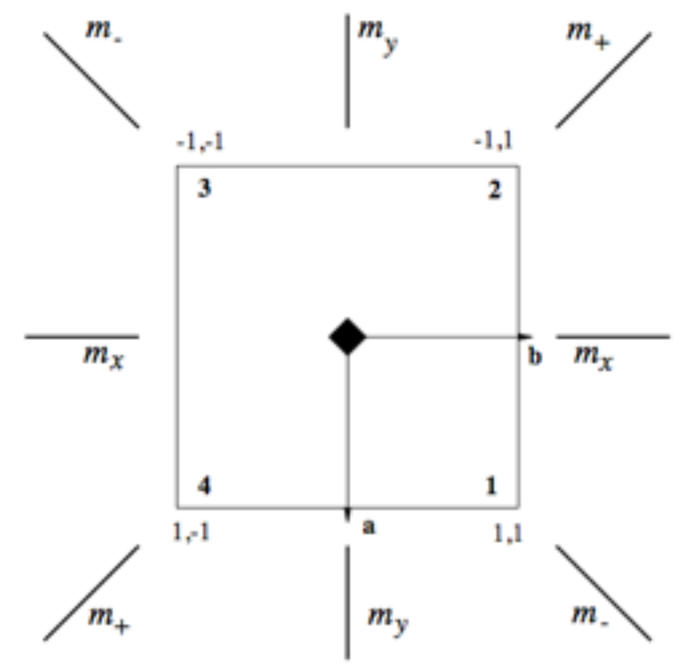
Crystallographic Point Groups

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)

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	$2_+ 2_-$

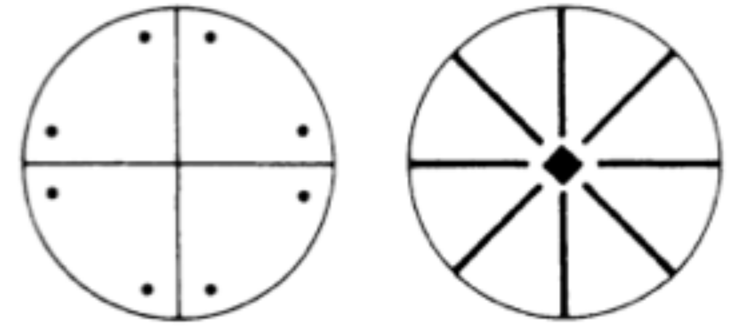


Groups isomorphic to 622

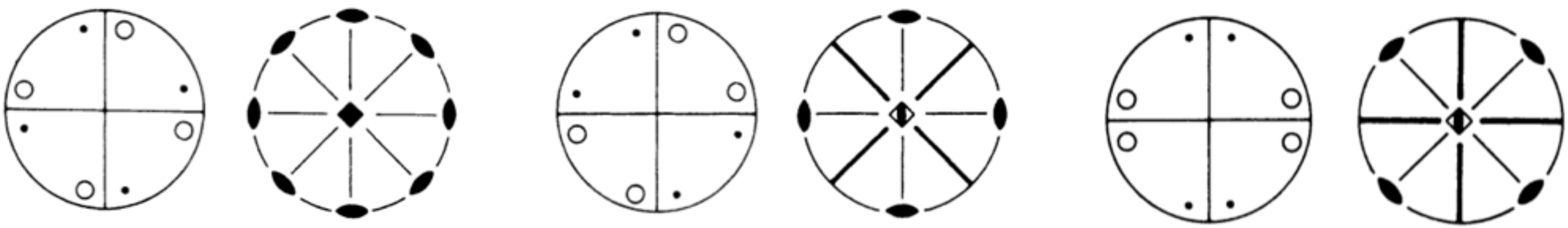
622	e	$6_z 6_z^{-}$	$3_z 3_z^{-}$	2_z	$2_1 2_2 2_3$	$2'_1 2'_2 2'_3$
6mm	e	$6_z 6_z^{-}$	$3_z 3_z^{-}$	2_z	$m_1 m_2 m_3$	$m'_1 m'_2 m'_3$
$\bar{6}2m$	e	$\bar{6}_z \bar{6}_z^{-}$	$3_z 3_z^{-}$	m_z	$2_1 2_2 2_3$	$m'_1 m'_2 m'_3$
$\bar{6}m2$	e	$\bar{6}_z \bar{6}_z^{-}$	$3_z 3_z^{-}$	m_z	$m_1 m_2 m_3$	$2'_1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

Problem 2.11

4mm



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



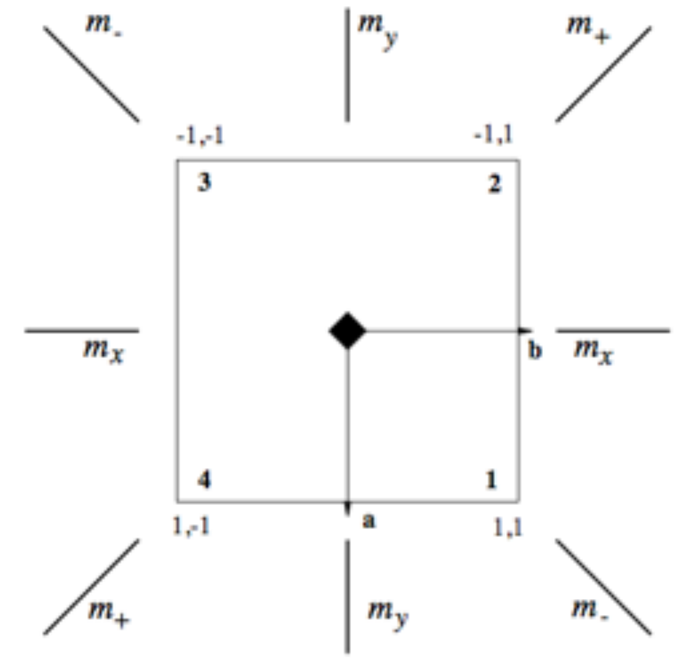
(i) Determine those point groups by indicating their symbols, symmetry operations and possible sets of generators;
(ii) Construct the corresponding multiplication tables;
(iii) For each of the isomorphic point groups indicate the one-to-one correspondence with the symmetry operations of ***4mm***.

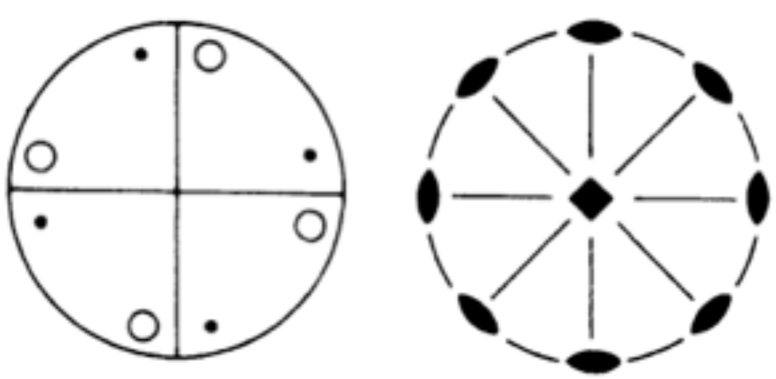
Problem 2.11

SOLUTION

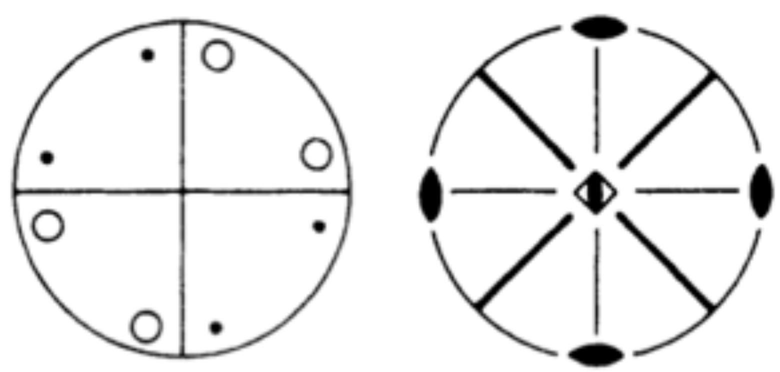
Groups isomorphic to 4mm

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

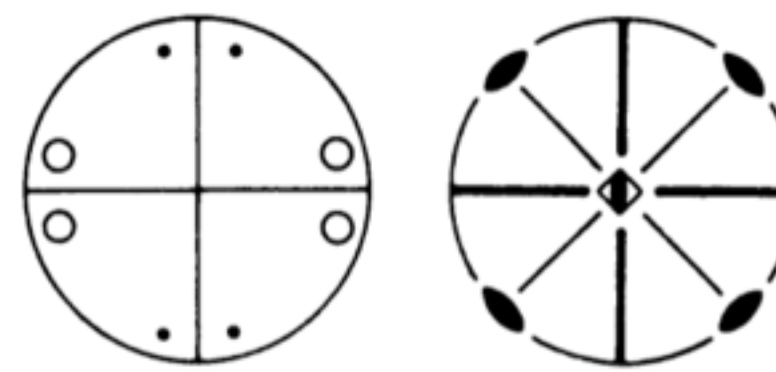




422



$\bar{4}2m$



$\bar{4}m2$

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, ... - generate the rest of elements

Example

Generation of the group of the square

Composition series: $\mathbf{1} \overset{2_z}{\underset{[2]}{\lhd}} \mathbf{2} \overset{4_z}{\underset{[2]}{\lhd}} \mathbf{4} \overset{m_x}{\underset{[2]}{\lhd}} \mathbf{4mm}$

Step 1:

$\mathbf{1} = \{1\}$

Step 2:

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

Step 3:

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

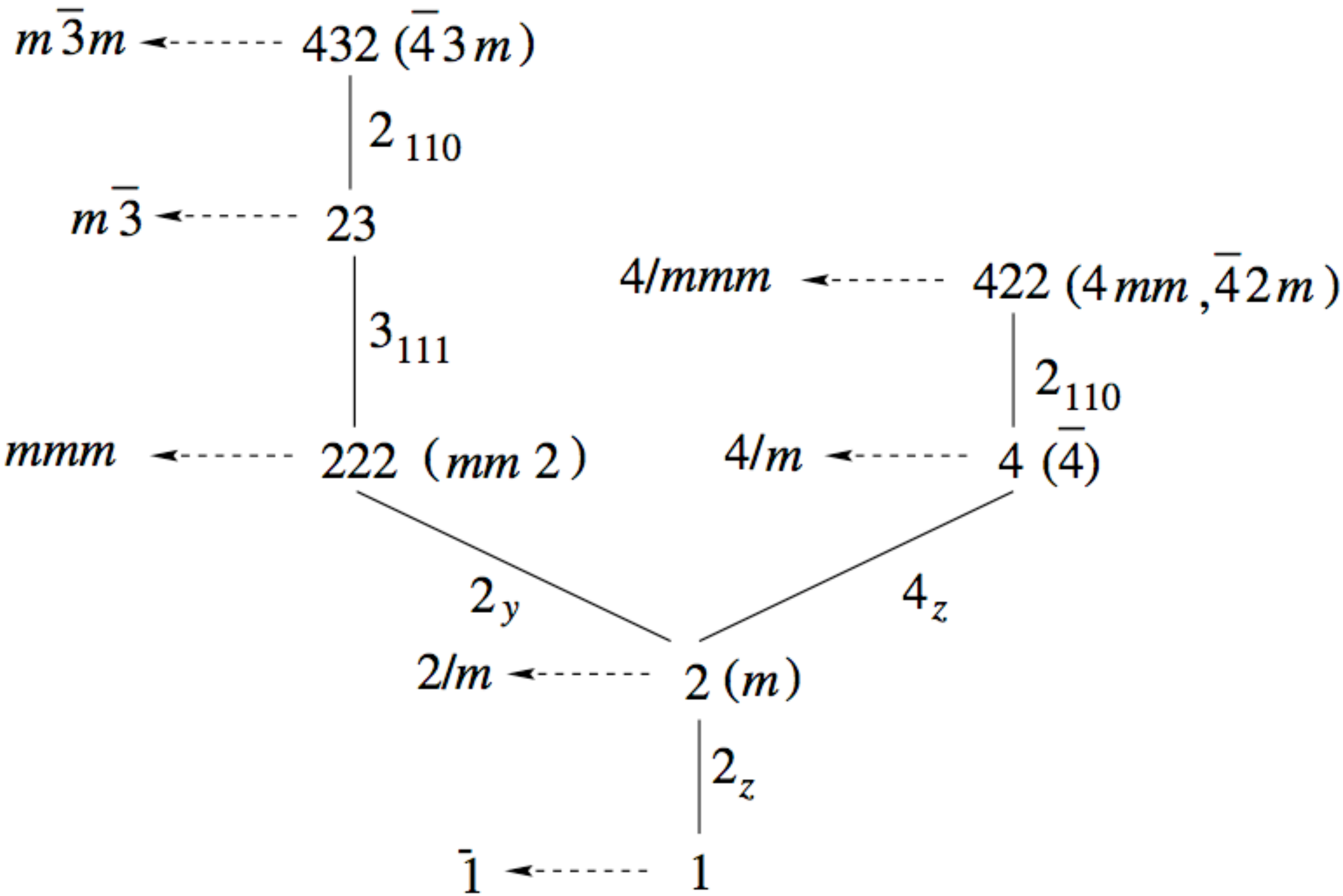
Step 4:

$\mathbf{4mm} = \mathbf{4} + m_x \mathbf{4}$

	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
1	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
2	2	1	4^{-1}	4	m_y	m_-	m_x	m_+
4	4	4^{-1}	2	1	m_+	m_y	m_-	m_x
4^{-1}	4^{-1}	4	1	2	m_-	m_x	m_+	m_y
m_x	m_x	m_y	m_-	m_+	1	4^{-1}	2	4
m_+	m_+	m_-	m_x	m_y	4	1	4^{-1}	2
m_y	m_y	m_x	m_+	m_-	2	4	1	4^{-1}
m_-	m_-	m_+	m_y	m_x	4^{-1}	2	4	1

Multiplication table of $4mm$

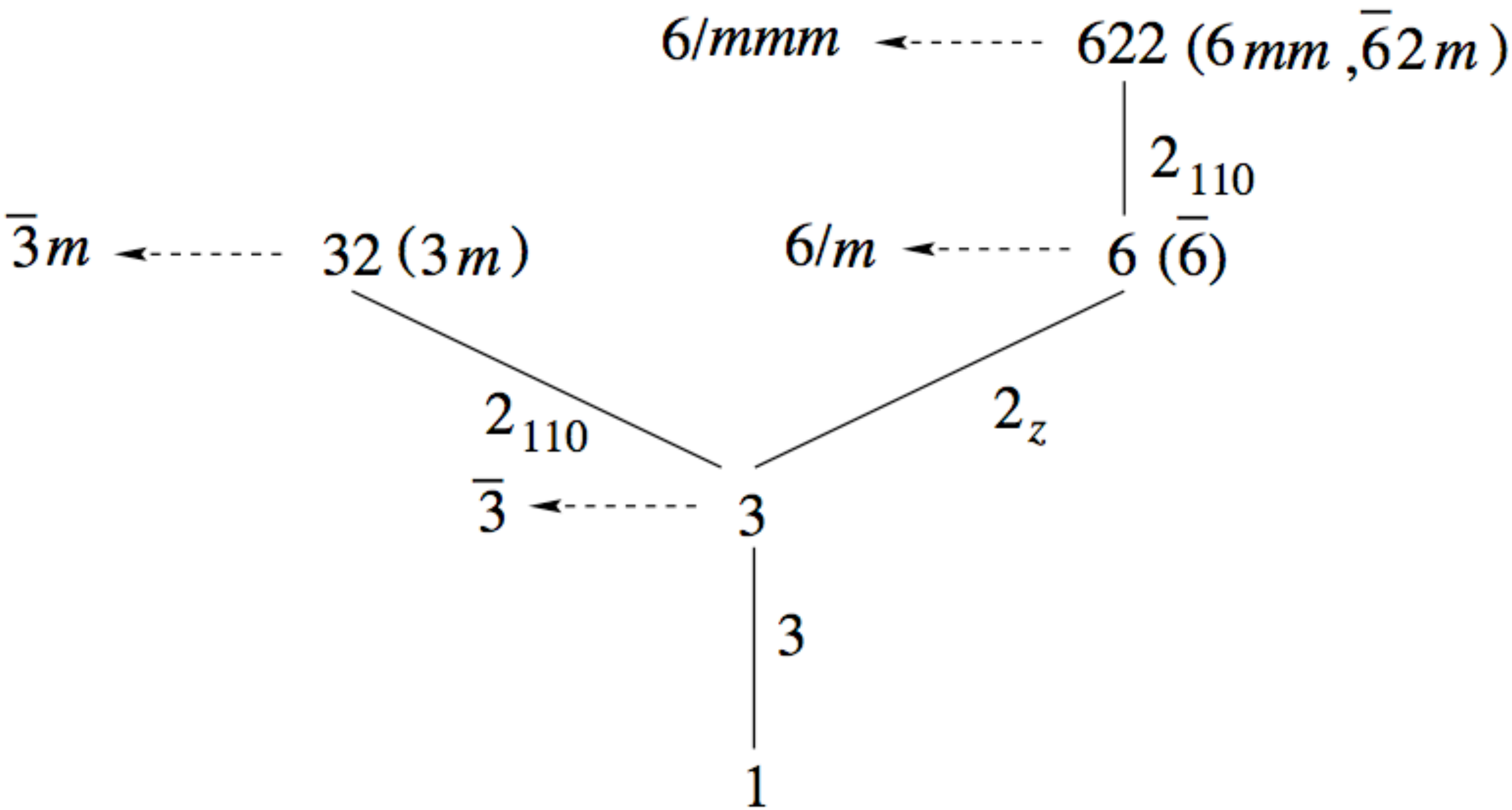
Generation of sub-cubic point groups



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.