CRYSTALLOGRAPHY ONLINE Workshop

on the use and applications of the structural and magnetic tools of the

BILBAO CRYSTALLOGRAPHIC SERVER

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OVERVIEW OF CRYSTALLOGRAPHIC POINT SYMMETRY

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GROUP THEORY
(few basic facts)

1. Crystallographic symmetry operations

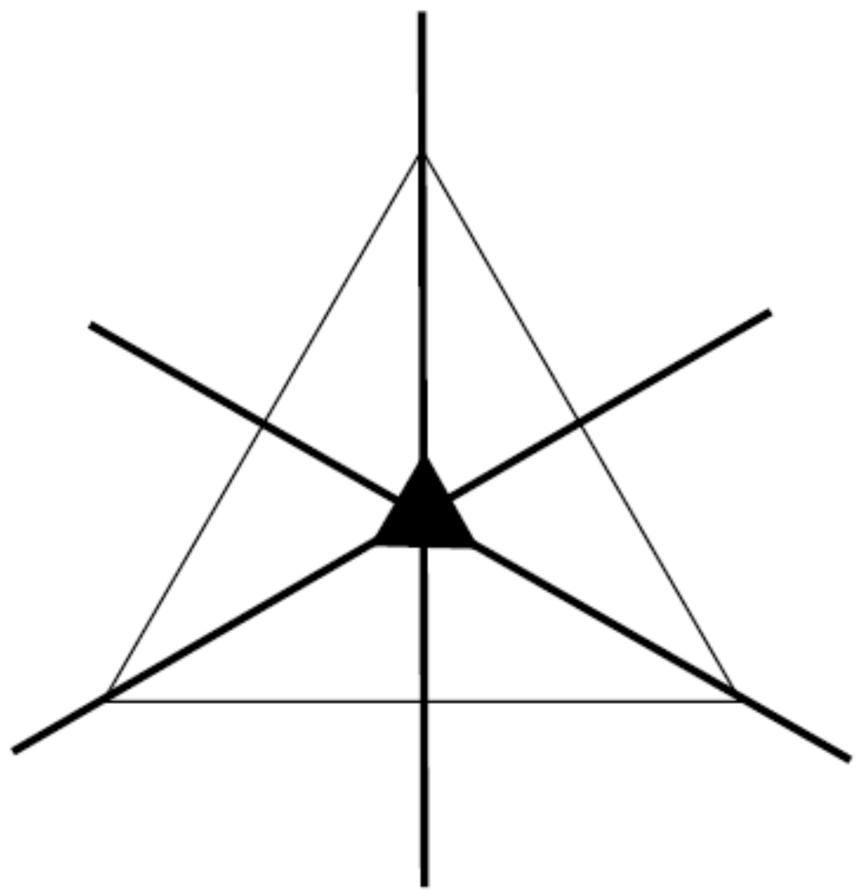
Symmetry operations of an object

The symmetry operations are *isometries, i.e.* they are special kind of *mappings* between an object and its image that leave all distances and angles invariant.

The isometries which map the object onto itself are called *symmetry operations of this object*. The *symmetry* of the object is the set of all its symmetry operations.

Crystallographic symmetry operations

If the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.

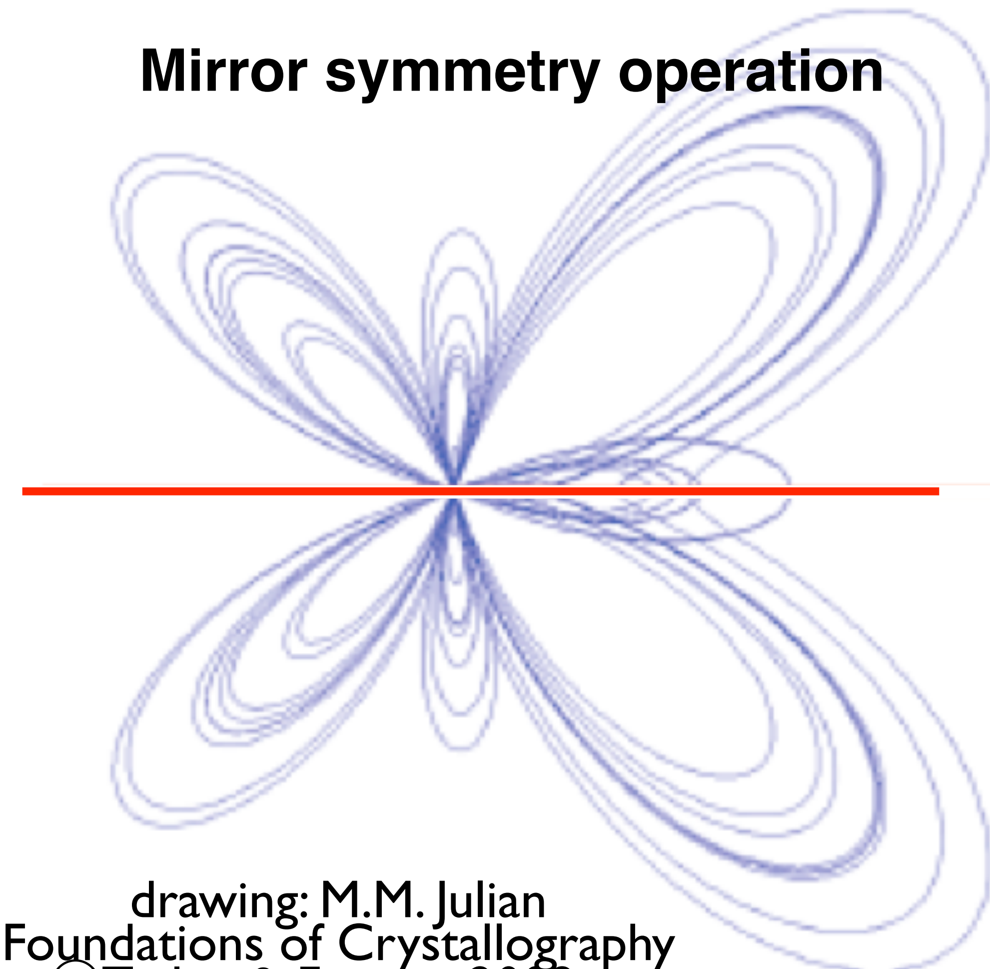


Symmetry operations?

The equilateral triangle allows **six** symmetry operations: **rotations** by 120 and 240 around its centre, **reflections** through the three thick lines intersecting the centre, and the identity operation.

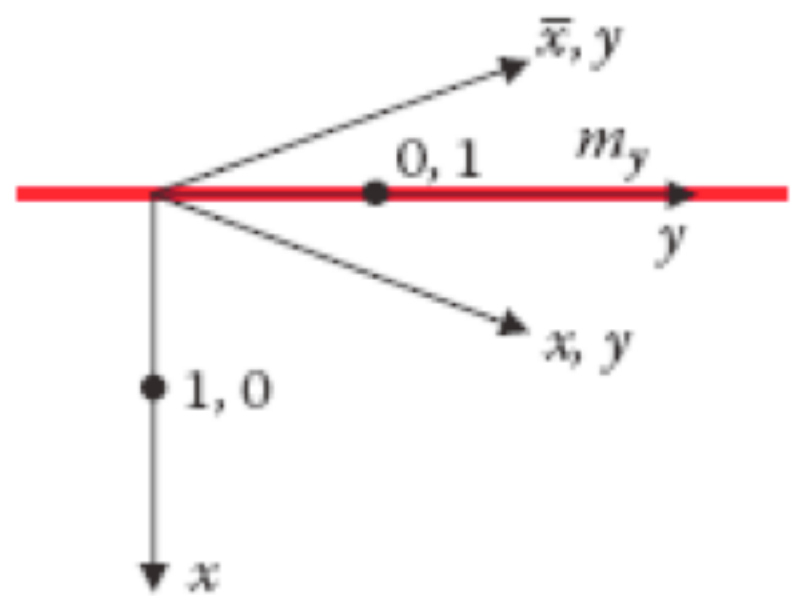
Symmetry operations in the plane
Matrix representations

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Fixed points

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

Matrix representation

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

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

Geometric element and symmetry element

2. Group axioms

DEFINITION. The symmmetry operations of an object constitute its symmetry group.

DEFINITION. A group is a set $G = \{e, g_1, g_2, g_3 \ldots\}$ together with a product $\circ$, such that

i) G is "closed under $\circ$": if g_1 and g_2 are any two members of G then so are $g_1 \circ g_2$ and $g_2 \circ g_1$;

ii) G contains an identity e: for any g in G, $e \circ g = g \circ e = g$;

iii) $\circ$ is associative: $(g_1 \circ g_2) \circ g_3 = g_1 \circ (g_2 \circ g_3)$;

iv) Each g in G has an inverse g^{-1} that is also in G: $g \circ g^{-1} = g^{-1} \circ g = e$.

Group properties

1. **Order of a group $|G|$:** number of elements

crystallographic point groups: $1 \leq |G| \leq 48$

space groups: $|G| = \infty$

2. **Abelian group G:**

$g_i \cdot g_j = g_j \cdot g_i \quad \forall g_i, g_j \in G$

3. **Cyclic group G:**

$G = \{g, g^2, g^3, \ldots, g^n\}$

finite: $|G| = n$, $g^n = e$

infinite: $G = \langle g, g^{-1} \rangle$

order of a group element: $g^n = e$

4. How to define a group

Multiplication table

	E	A	B
E	E	A	B
A	A	B	E
B	B	E	A

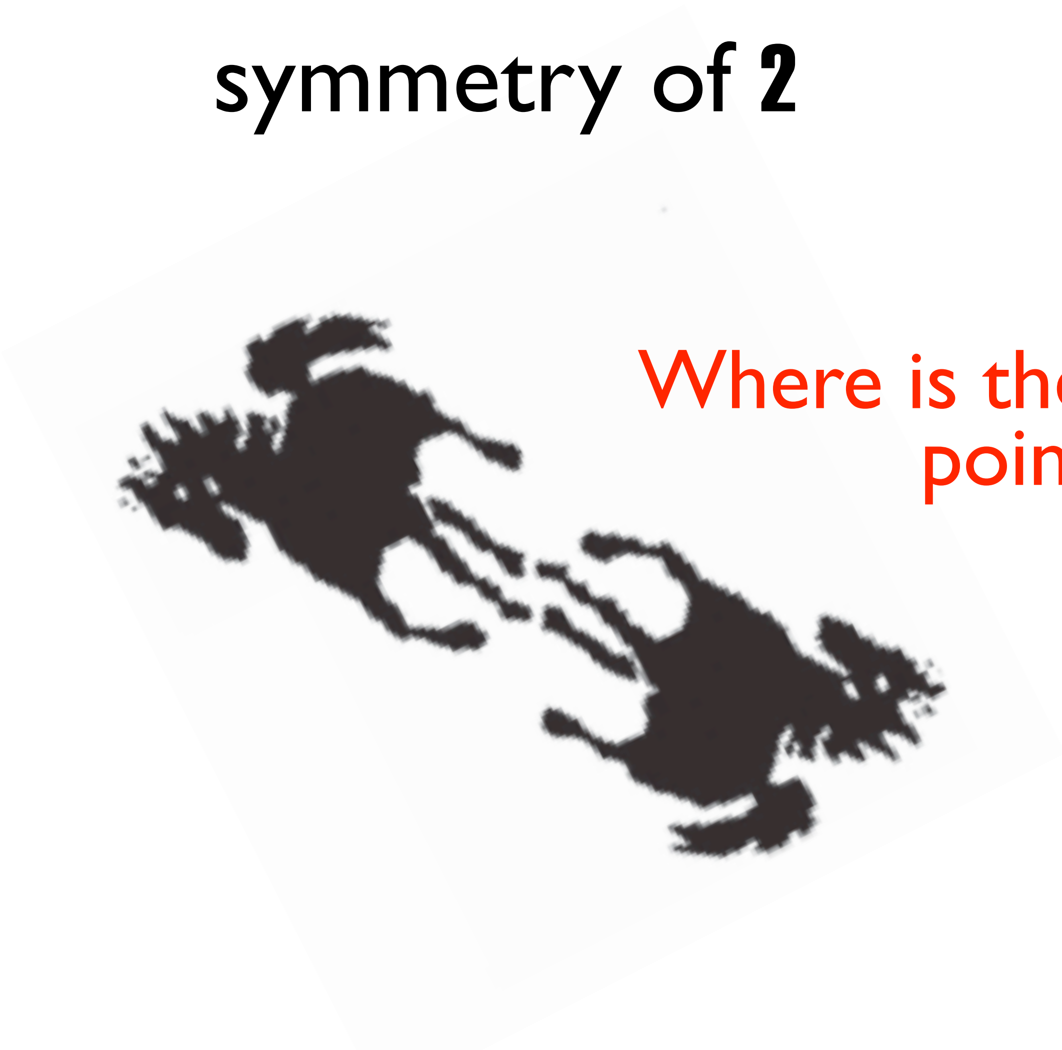
Group generators

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

Crystallographic Point Groups in 2D

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

Motif with symmetry of **2**



Where is the two-fold point?

drawing: M.M. Julian
Foundations of Crystallography
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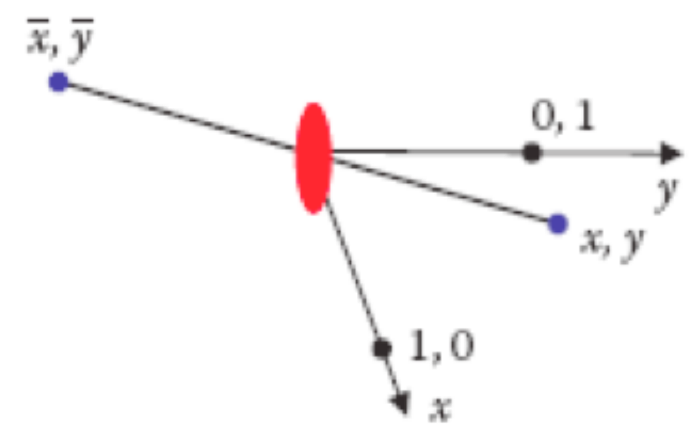


$$2_z \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ -y \end{pmatrix} = \begin{pmatrix} -1 & \\ & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

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

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

Crystallographic Point Groups in 2D

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

Motif with symmetry of **2**

drawing: M.M. Julian
Foundations of Crystallography

-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**?

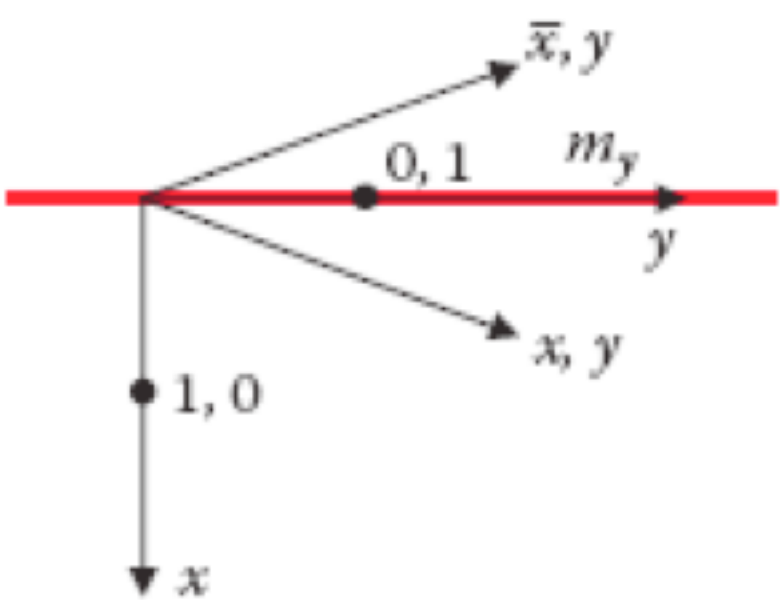
Crystallographic symmetry operations in the plane

Mirror symmetry operation

Where is the mirror line?

drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Matrix representation

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

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

Crystallographic Point Groups in 2D

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

Motif with symmetry of **m**

drawing: M.M. Julian
Foundations of Crystallography

-group axioms?

$$m \times m = \begin{array}{|c|c|}\hline -1 & \\ \hline & 1 \\ \hline \end{array} \times \begin{array}{|c|c|}\hline -1 & \\ \hline & 1 \\ \hline \end{array} = \begin{array}{|c|c|}\hline 1 & \\ \hline & 1 \\ \hline \end{array}$$

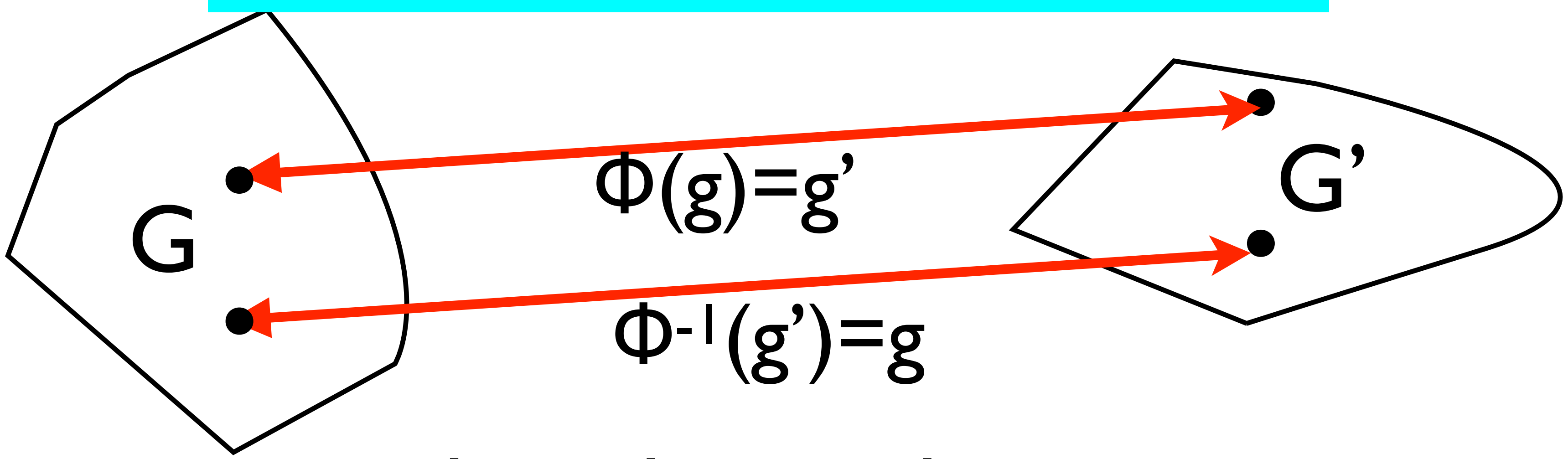
-order of **m**?

-multiplication table

$\times$	1	m_y
1	1	m_y
m_y	m_y	1

-generators of **m**?

Isomorphic groups



$$\Phi(g_1)\Phi(g_2) = \Phi(g_1\ g_2)$$

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

×	1	2
1	1	2
2	2	1

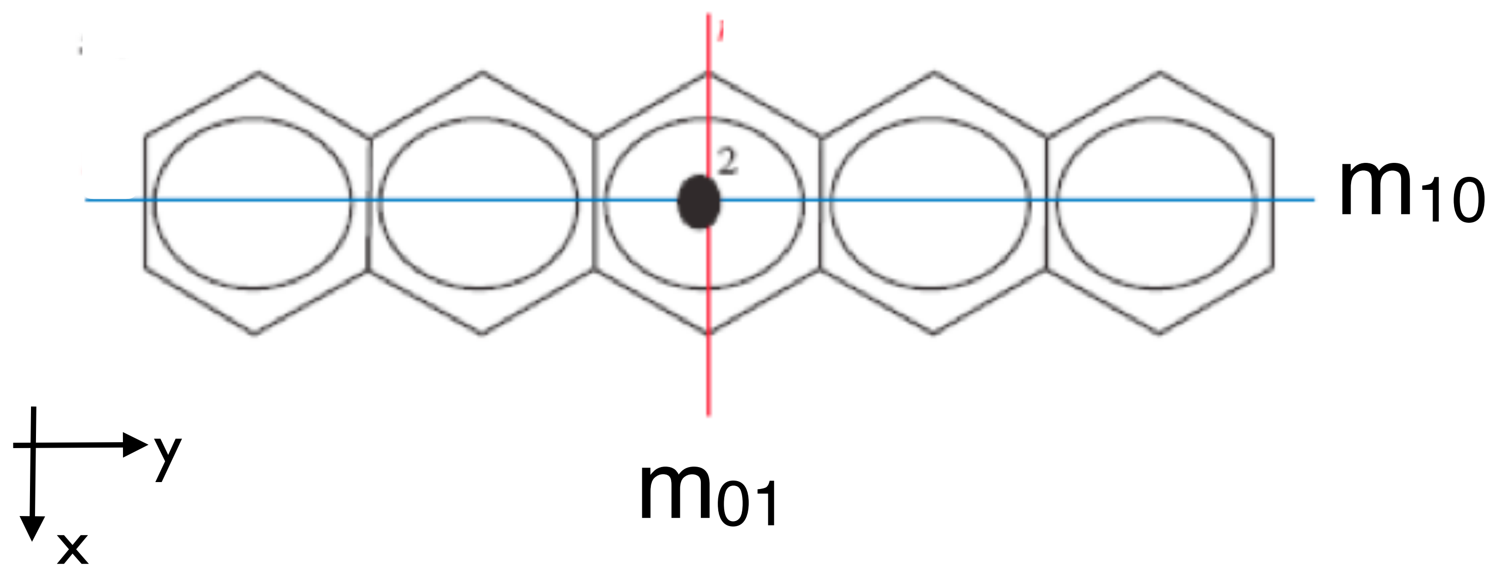
Point group **m** = {1,m}

×	1	m_y
1	1	m_y
m_y	m_y	1

-groups with the same multiplication table

Example (Problem 1.6.1.1)

Consider the model of the molecule of the organic semiconductor pentacene ($C_{22}H_{14}$):



Determine:

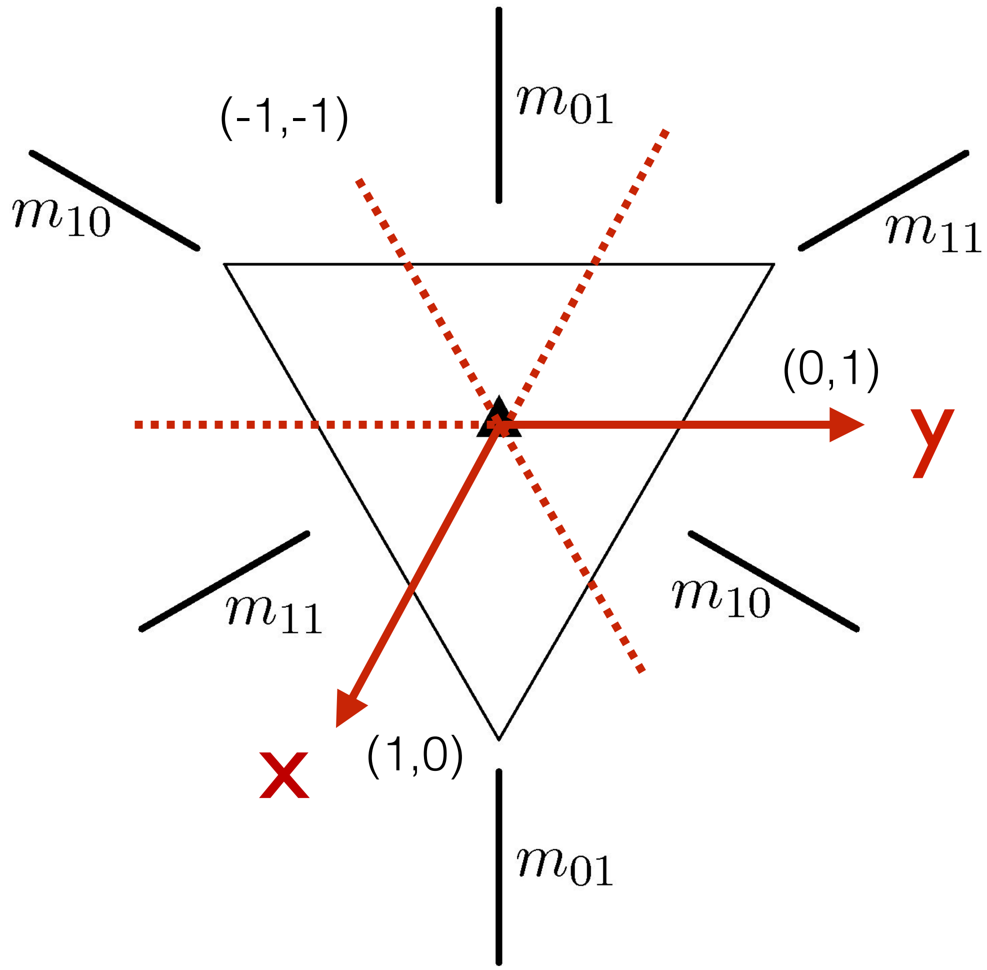
-symmetry operations:
 matrix and (x,y) presentation

-generators

-multiplication table

Exercise 1.6.1.3

Consider the symmetry group of the equilateral triangle. Determine:



-symmetry operations: matrix and (x,y) presentation

-generators

-multiplication table

SEITZ SYMBOLS FOR SYMMETRY OPERATIONS

point-group symmetry operation

- specify the type and the order of the symmetry operation

1 and $\bar{1}$	identity and inversion
m	reflections
2, 3, 4 and 6	rotations
$\bar{3}$, $\bar{4}$ and $\bar{6}$	rotoinversions

- orientation of the symmetry element by the direction of the axis for rotations and rotoinversions, or the direction of the normal to reflection planes.

SHORT-HAND NOTATION OF SYMMETRY OPERATIONS

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = R \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\left| \begin{array}{l} x' = R_{11}x + R_{12}y \\ y' = R_{21}x + R_{22}y \end{array} \right.$$

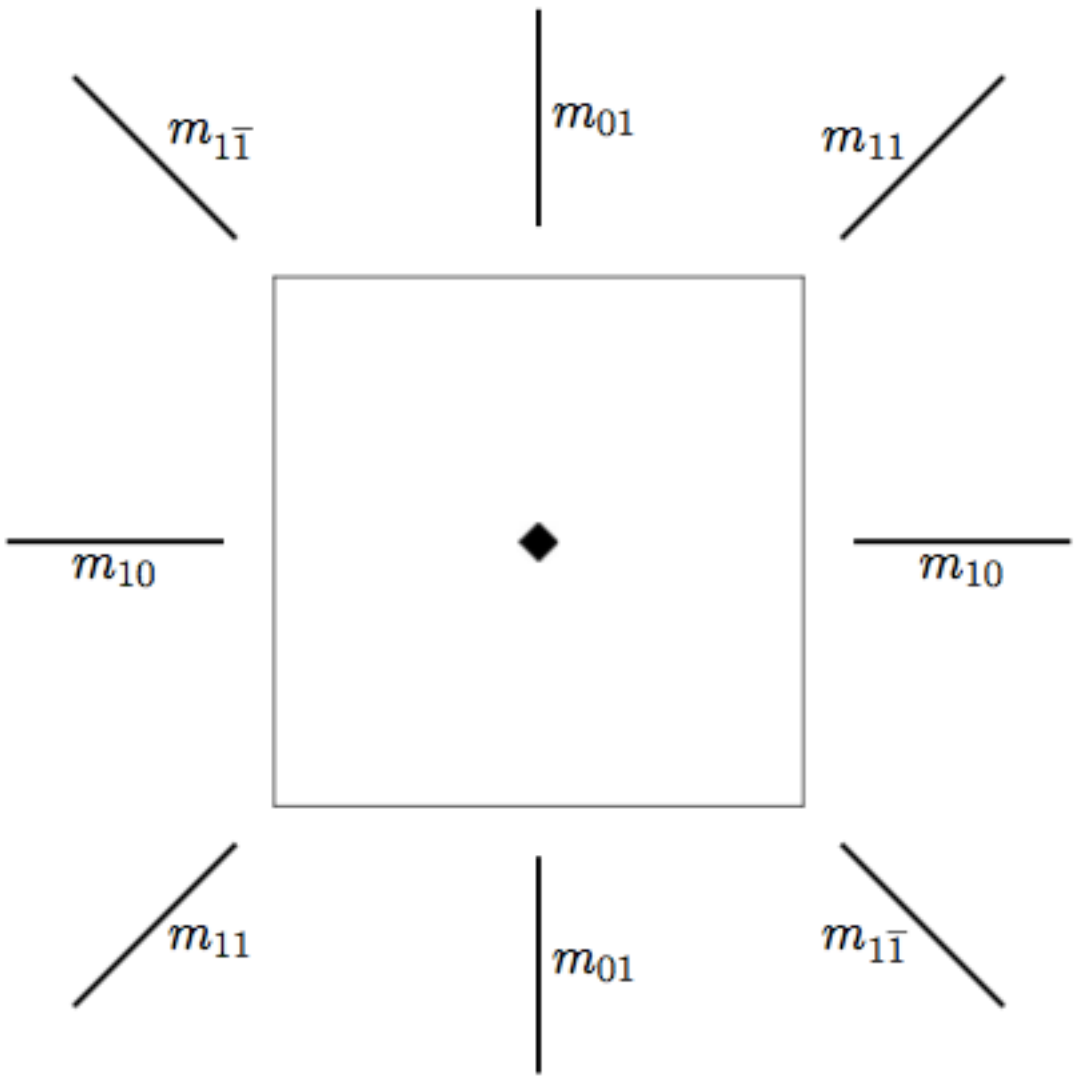
notation:

-left-hand side: omitted
-coefficients 0, +1, -1
-different rows in one line, separated by commas

$$\begin{pmatrix} 0 & -1 \\ -1 & 1 \end{pmatrix} \longrightarrow \left\{ \begin{array}{l} -y, -x+y \\ \bar{y}, \bar{x}+y \end{array} \right.$$

Problem 1.6.1.2

Consider the symmetry group of the square. Determine:



symmetry operations: matrix and (x,y) presentation

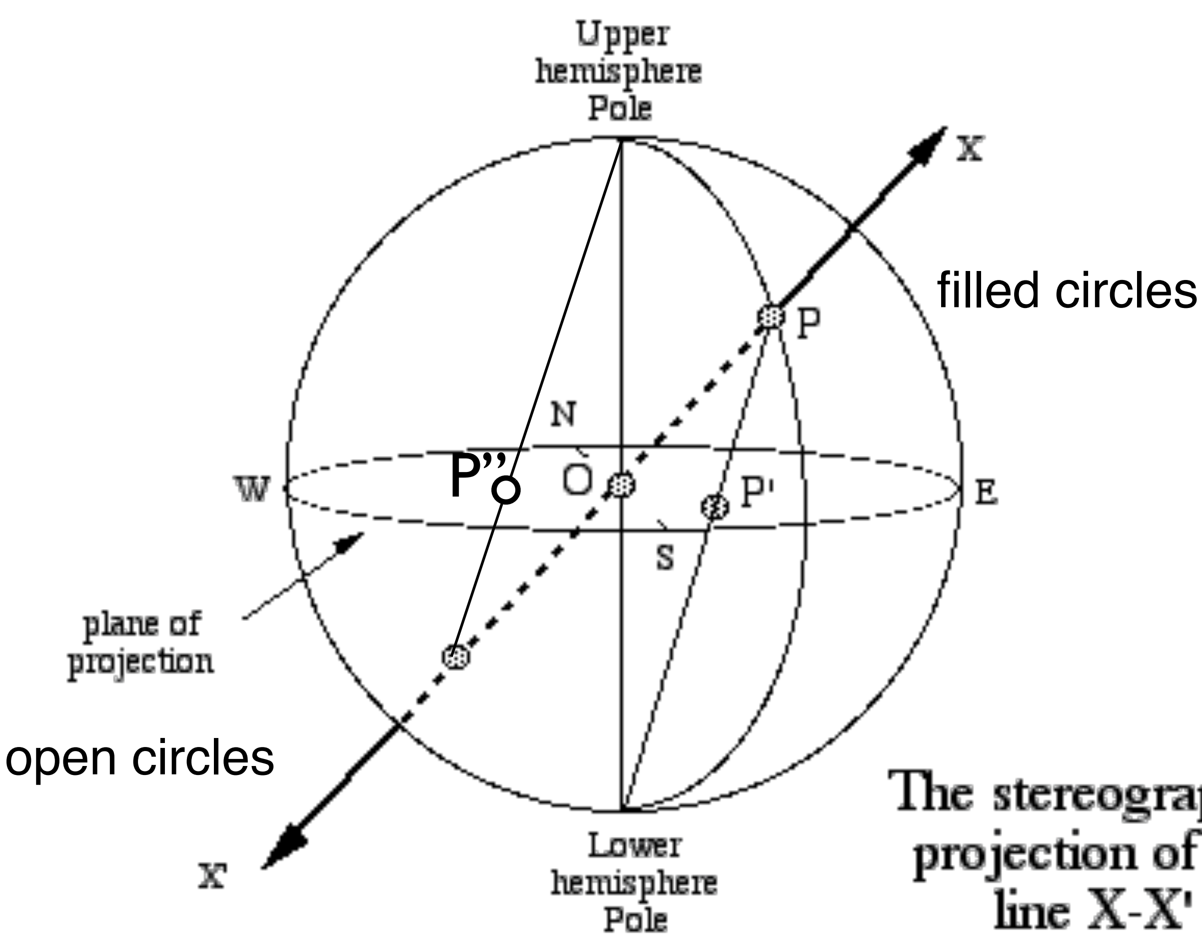
generators

multiplication table

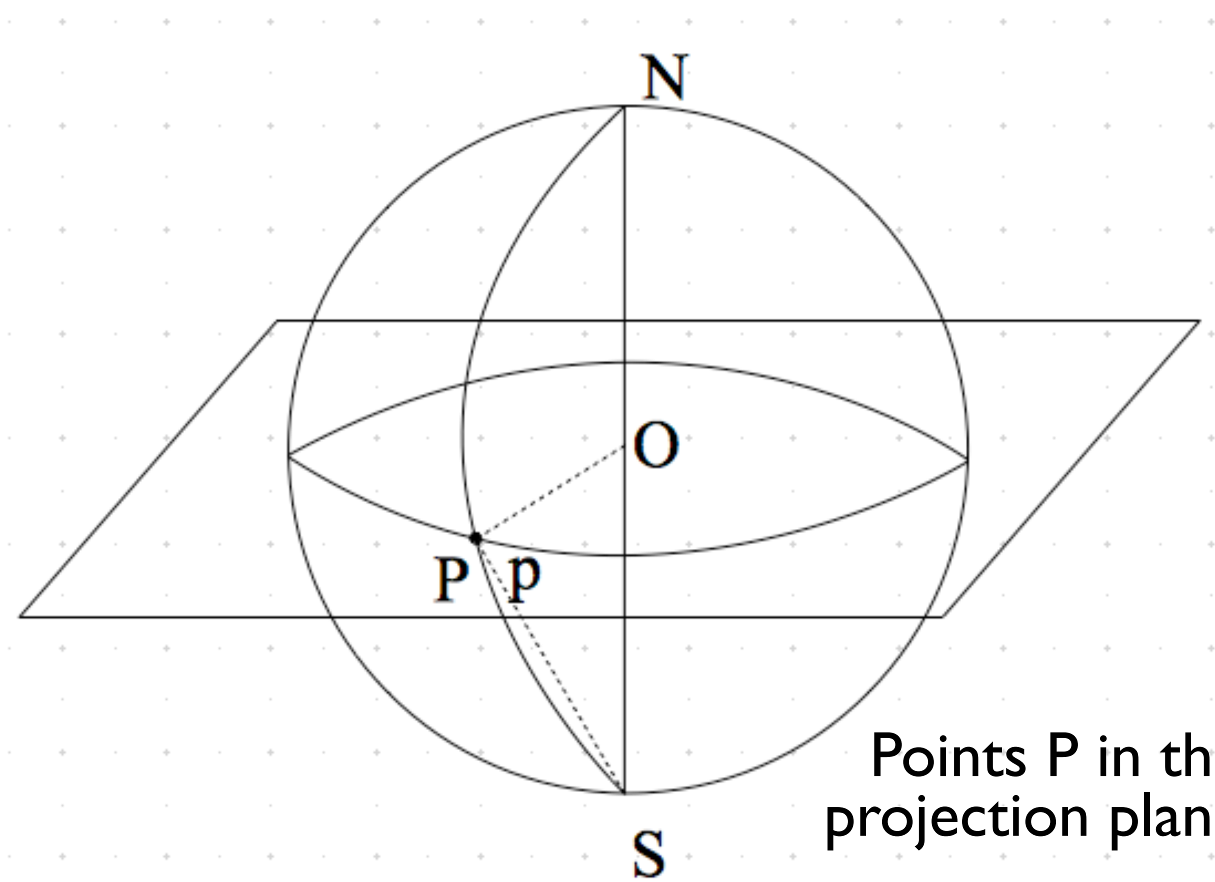
Visualization of Crystallographic Point Groups (3D)

- general position diagram
- symmetry elements diagram

Stereographic Projections



The stereographic projection of the line X-X'



Points P in the projection plane

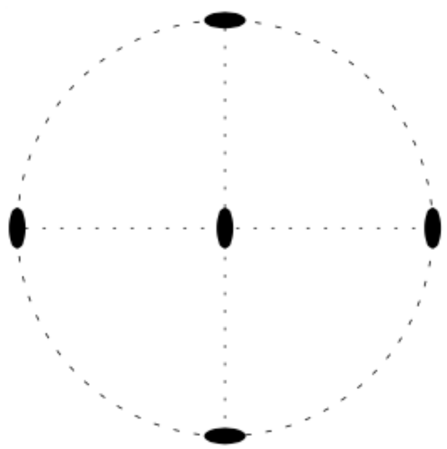
Symmetry-elements diagrams

-symmetry point of the point group is placed in the centre of the sphere

-intersections of the upper hemisphere of the symmetry elements of the point group (rotation axes, mirror planes) are projected on the stereonet plane

Rotation axes

-are lines which intersect the upper hemisphere as points



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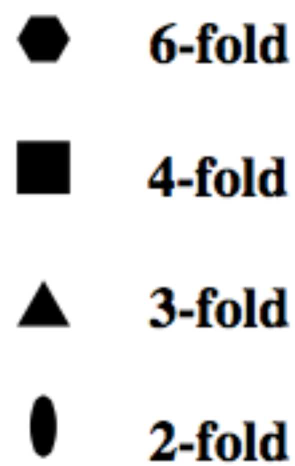
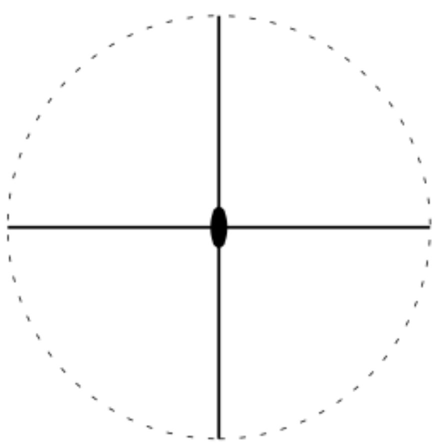


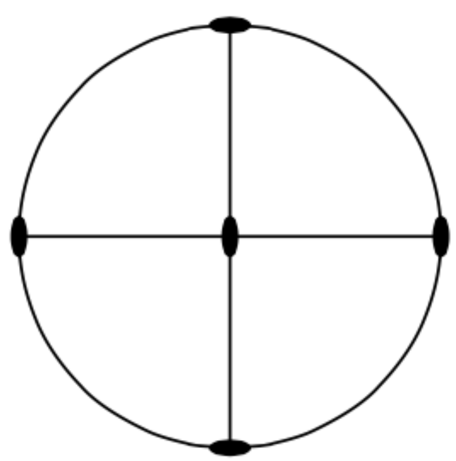
filled polygons with the same number of sides as the foldness of the axes

Mirror planes

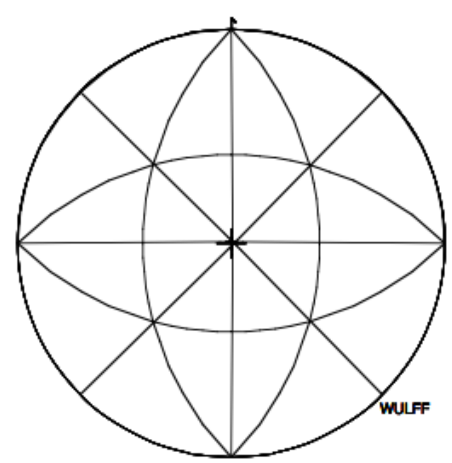
-intersect the upper hemisphere as great circles: horizontal and vertical mirror planes



2mm



2/m 2/m 2/m



Combinations of symmetry elements

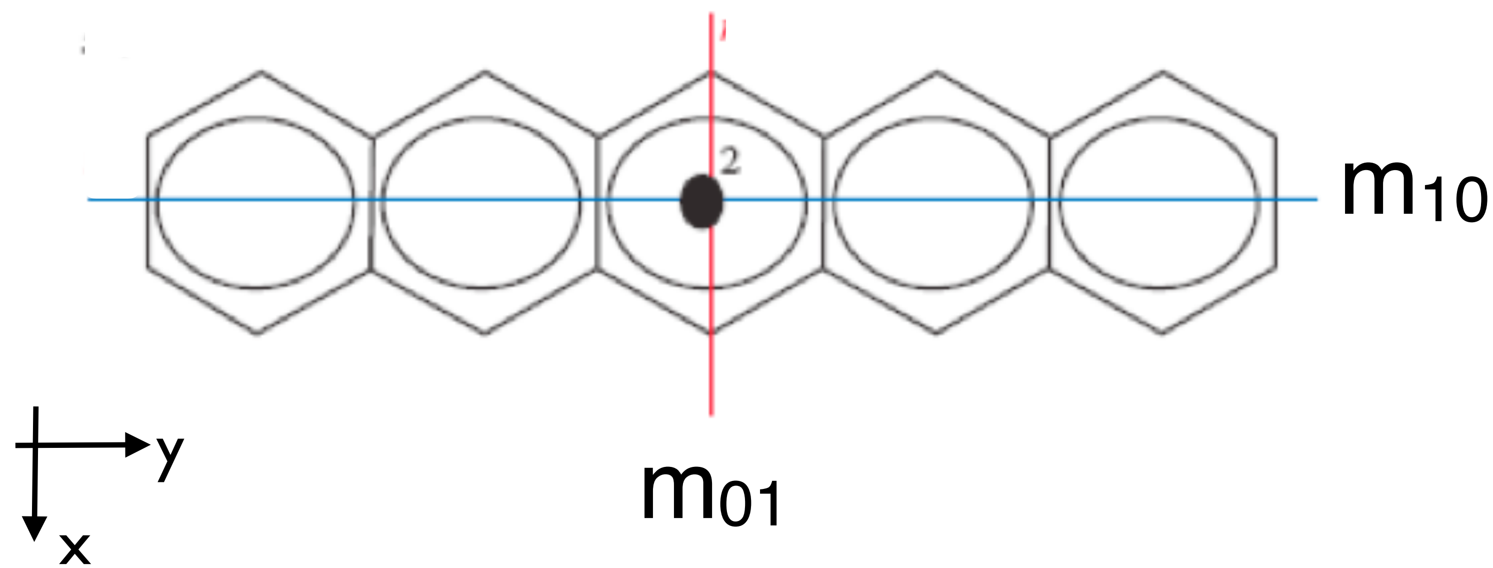
- **line of intersection of any two mirror planes must be a rotation axis**.

EXAMPLE

Stereographic Projections of ***mm2*** **(3D)**

Point group **mm2** $= \{1, 2, m_{10}, m_{01}\}$

Molecule of pentacene



Stereographic projections diagrams

general position

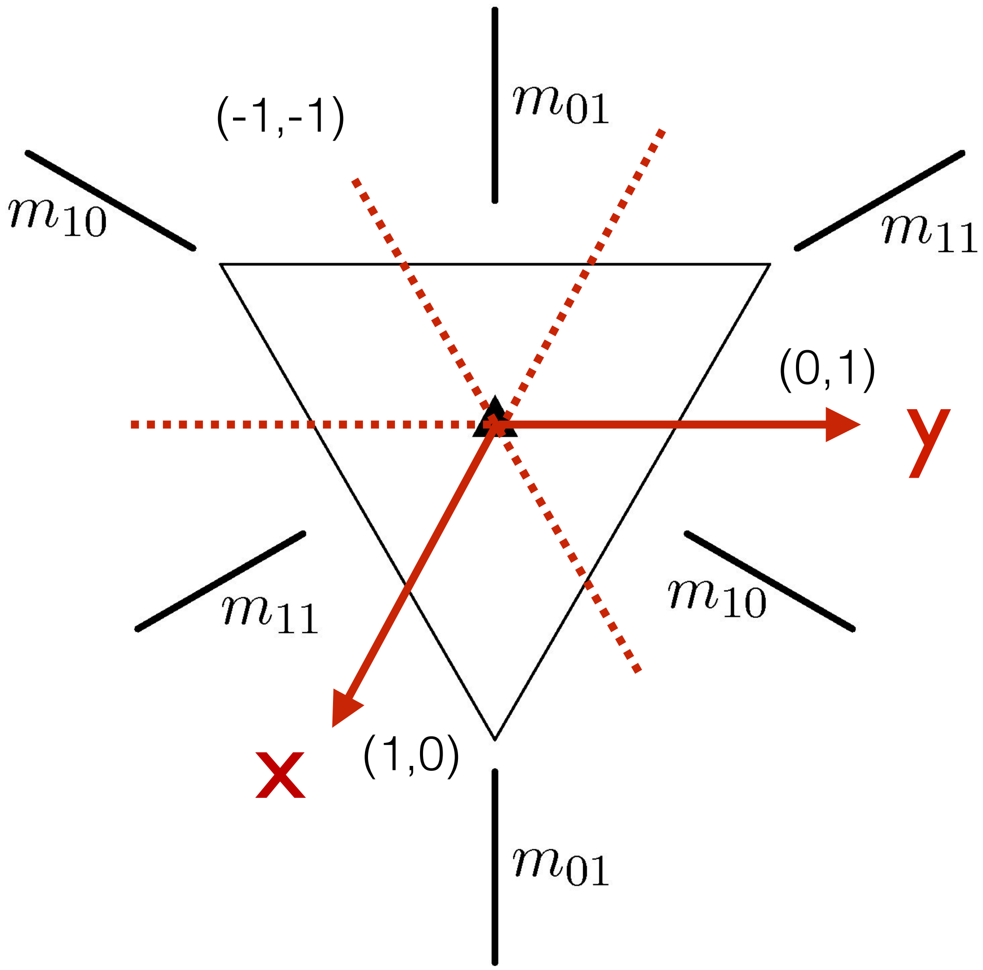
?

symmetry elements

?

EXAMPLE

Stereographic Projections of *3m* (3D)



Point group **3m** =

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

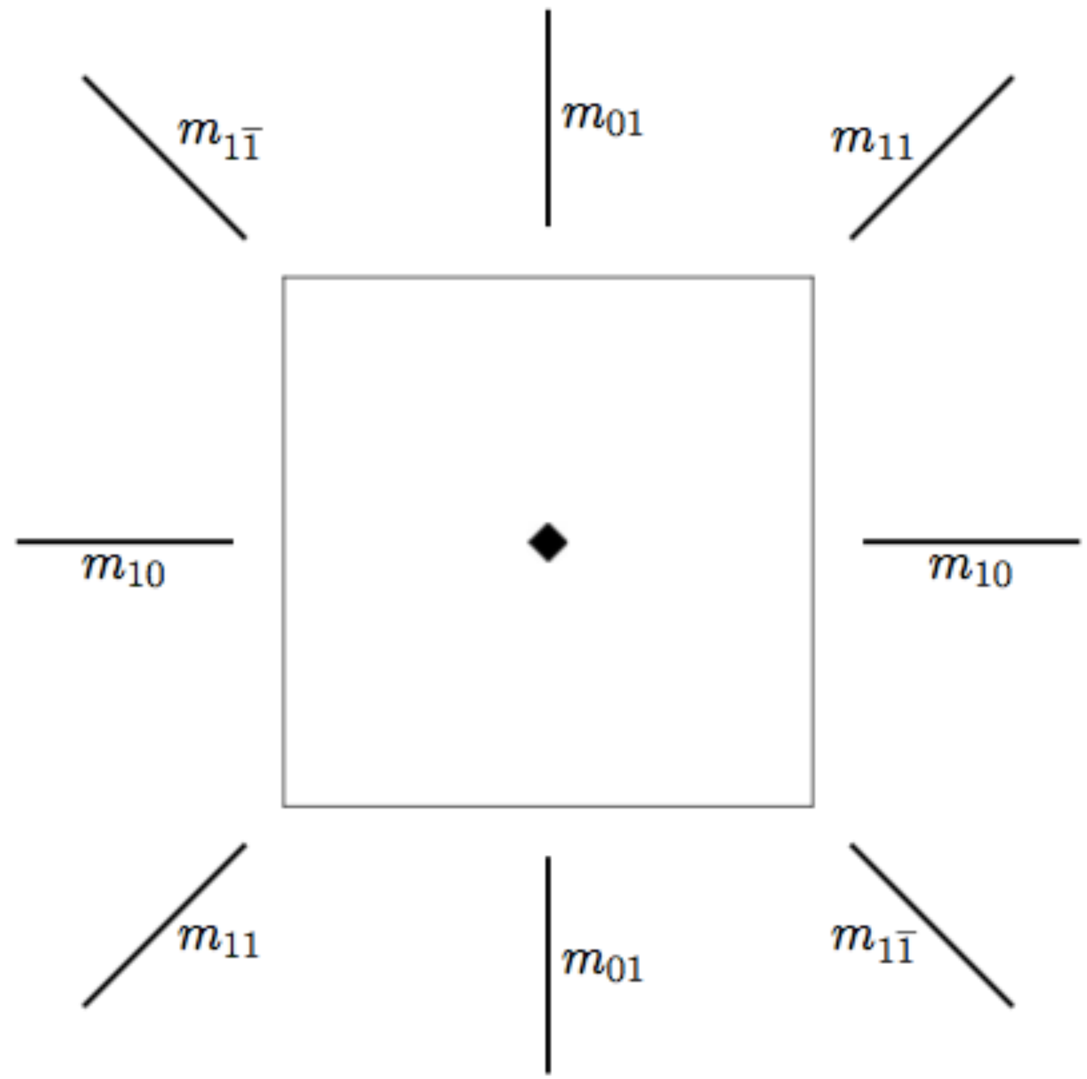
Stereographic projections diagrams

general position **?**

? symmetry elements

Problem 1.6.1.2 (cont.)

Stereographic Projections of ***4mm***



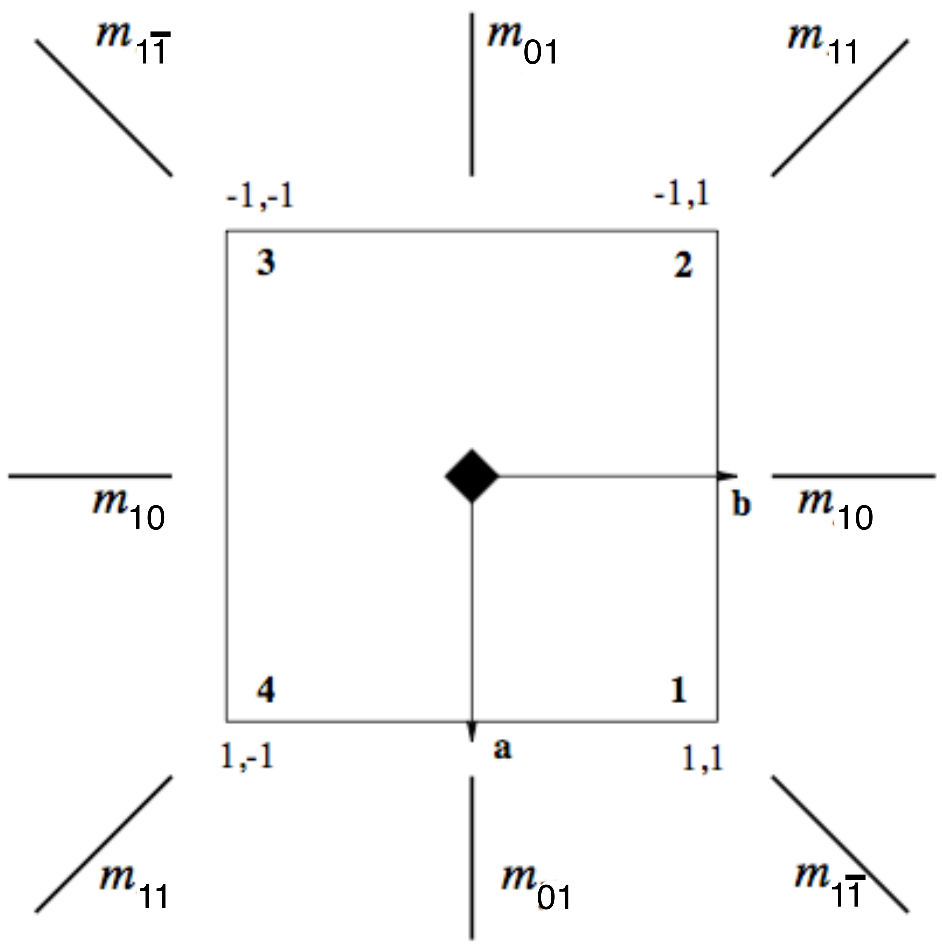
general position diagram

?

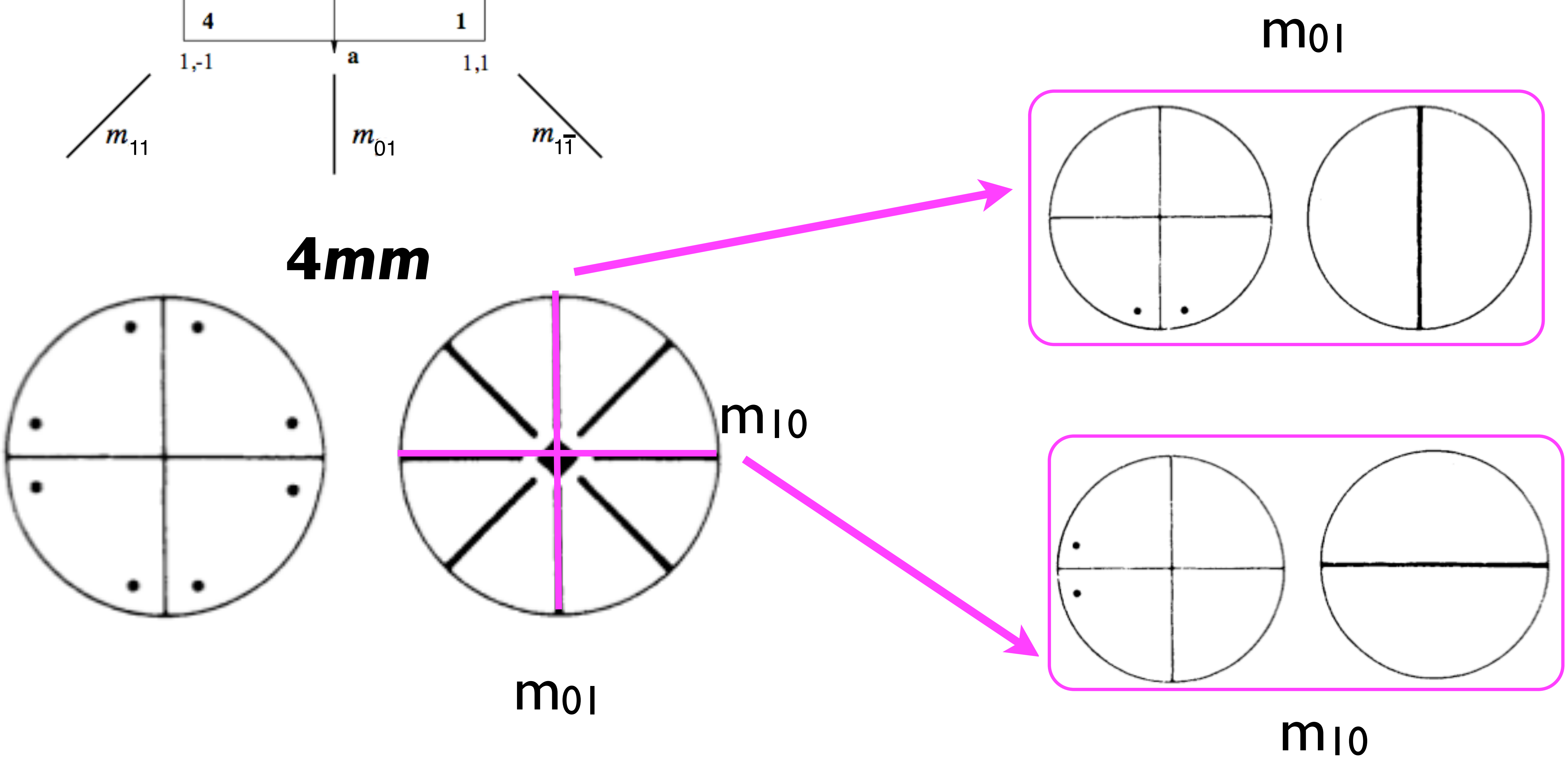
symmetry elements diagram

?

Conjugate elements



$$m_{10} \overset{4^{+}}{\sim} m_{01}$$



Conjugate elements

Conjugate elements

$g_i \sim g_k$ if $\exists\, g$: $g^{-1} g_i g = g_k$,
where $g, g_i, g_k, \in G$

Classes of conjugate elements

$L(g_i)=\{g_j |\ g^{-1} g_i g = g_j,\ g \in G\}$

Conjugation-properties

(i) $L(g_i) \cap L(g_j) = \{\varnothing\}$, if $g_i \notin L(g_j)$

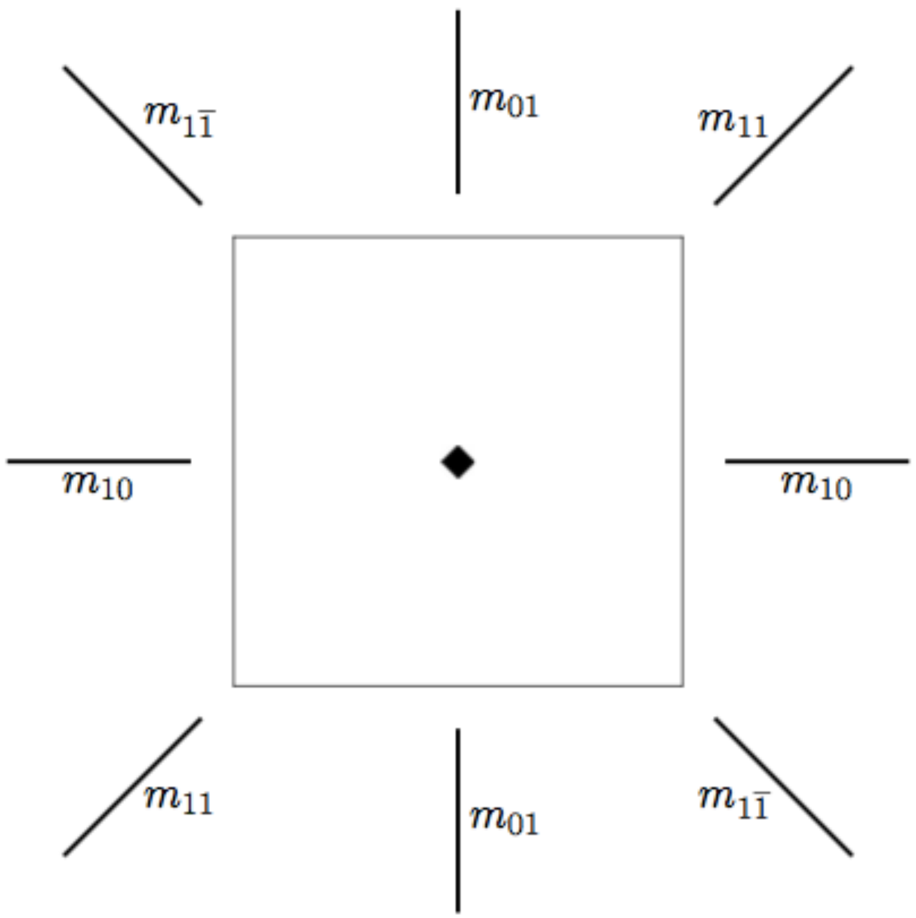
(ii) $|L(g_i)|$ is a divisor of $|G|$ (iii) $L(e)=\{e\}$

(iv) if $g_i, g_j \in L$, then $(g_i)^k=(g_j)^k= e$

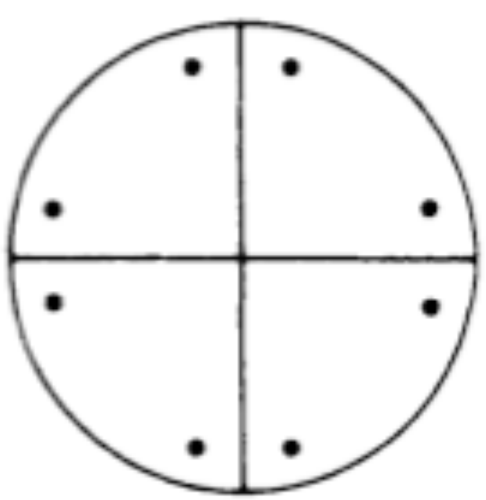
Problem 1.6.1.2 (cont.)

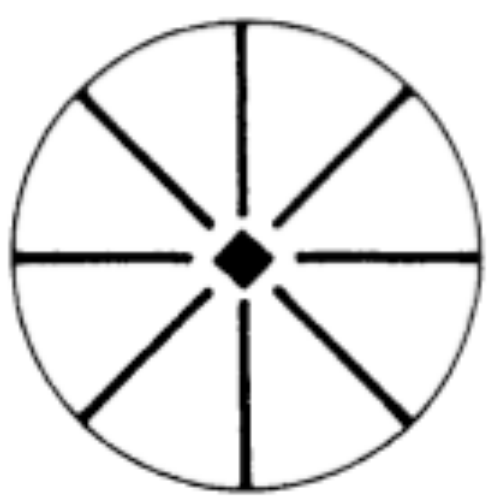
Classes of conjugate elements

Distribute the symmetry operations of the group of the square ***4mm*** into classes of conjugate elements



	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



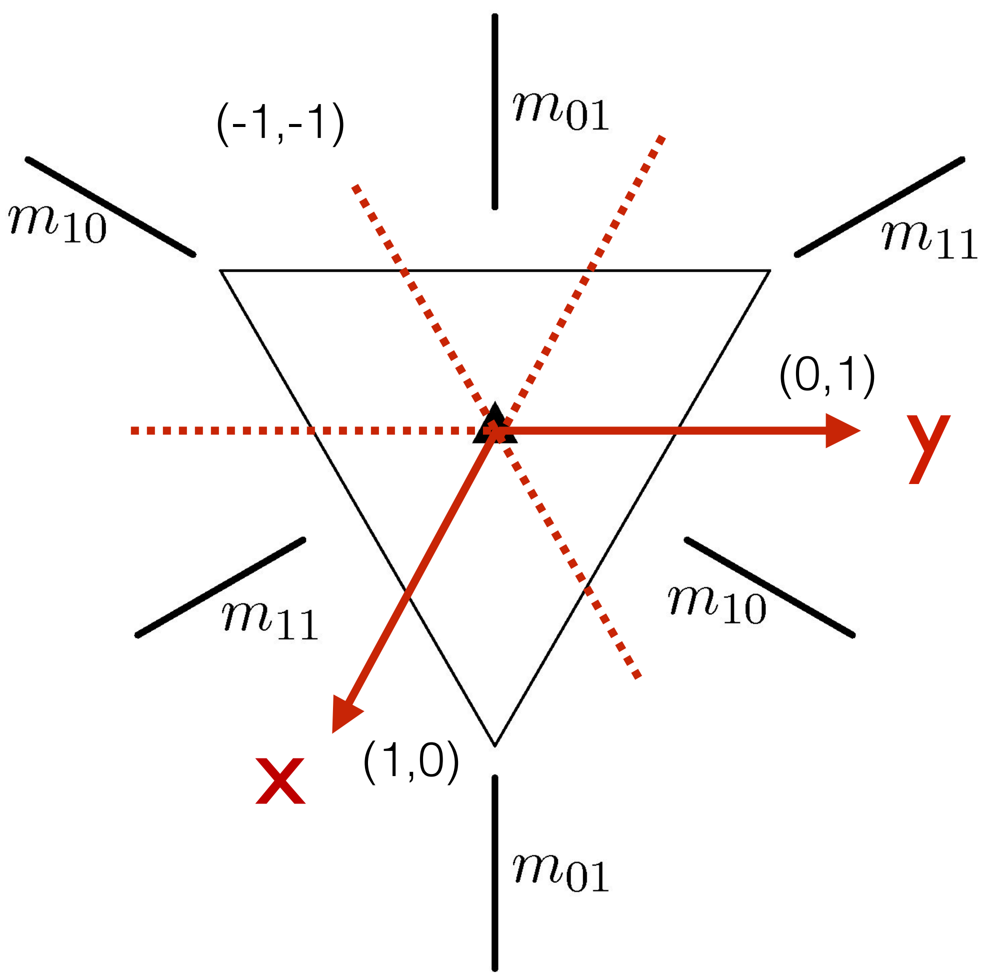


Hint: $g_i \sim g_k$ if $\exists\ g$: $g^{-1} g_i g = g_k$

Example (Problem 1.6.1.3 (cont.))

Classes of conjugate elements

Distribute the symmetry operations of the group of the equilateral triangle 3***m*** into classes of conjugate elements



Point group **3m** =

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

Multiplication table of **3m**

	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

GROUP-SUBGROUP RELATIONS

I. Subgroups: index, coset decomposition and normal subgroups

II. Conjugate subgroups

III. Group-subgroup graphs

Subgroups: Some basic results (summary)

Subgroup H < G

1. $H=\{e,h_1,h_2,\ldots,h_k\} \subset G$
2. H satisfies the group axioms of G

Proper subgroups H < G, and
trivial subgroup: {e}, G

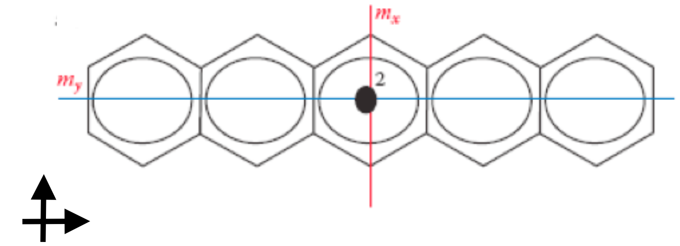
Index of the subgroup H in G: [i]=|G|/|H|
(order of G)/(order of H)

Maximal subgroup H of G
NO subgroup Z exists such that:
H < Z < G

Example

Subgroups of point groups

Molecule of pentacene



Subgroups of **mm2**

$\{1,2,m_{10},m_{01}\}$

$\{1, 2\}$ $\{2, m_{10}\}$ $\{1, m_{10}\}$

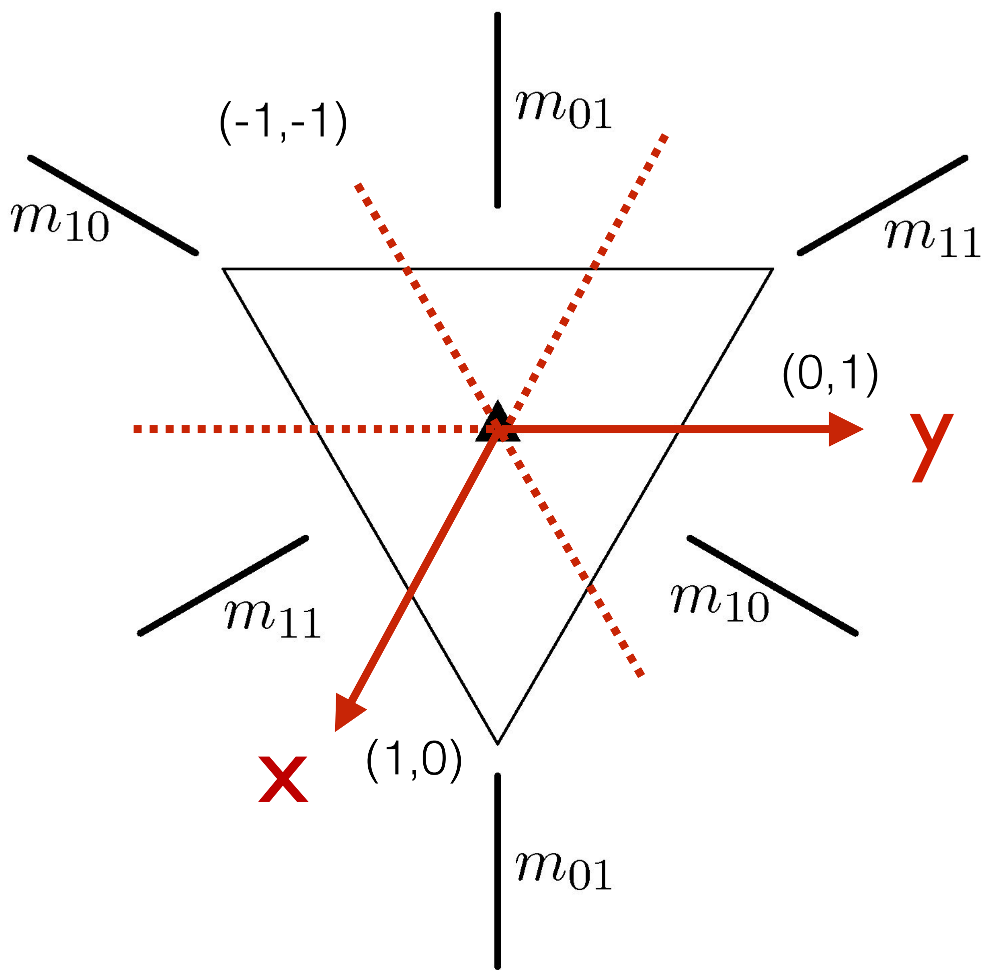
Subgroup graph

				Index
4		**mm2** $= \{1,2,m_{10},m_{01}\}$		1
2	$\{1, 2\}$	$\{1,m_{10}\}$	$\{1,m_{01}\}$	2
1		$\{1\}$		4

Problem 1.6.1.5

(i) Consider the group of the equilateral triangle and determine its subgroups;

(ii) Construct the maximal subgroup graph of 3m



	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

Multiplication table of **3m**

Coset decomposition G:H

Group-subgroup pair H < G

left coset decomposition: $G = H + g_2 H + \ldots + g_m H$, $g_i \notin H$, m=index of H in G

right coset decomposition: $G = H + H g_2 + \ldots + H g_m$, $g_i \notin H$ m=index of H in G

Coset decomposition-properties

(i) $g_i H \cap g_j H = \{\varnothing\}$, if $g_i \notin g_j H$

(ii) $|g_i H| = |H|$

(iii) $g_i H = g_j H$, $g_i \in g_j H$

Coset decomposition G:H

Normal subgroups

$Hg_j = g_jH$, for all $g_j = 1, ..., [i]$

Theorem of Lagrange

group G of order |G|
subgroup H<G of order |H|

then

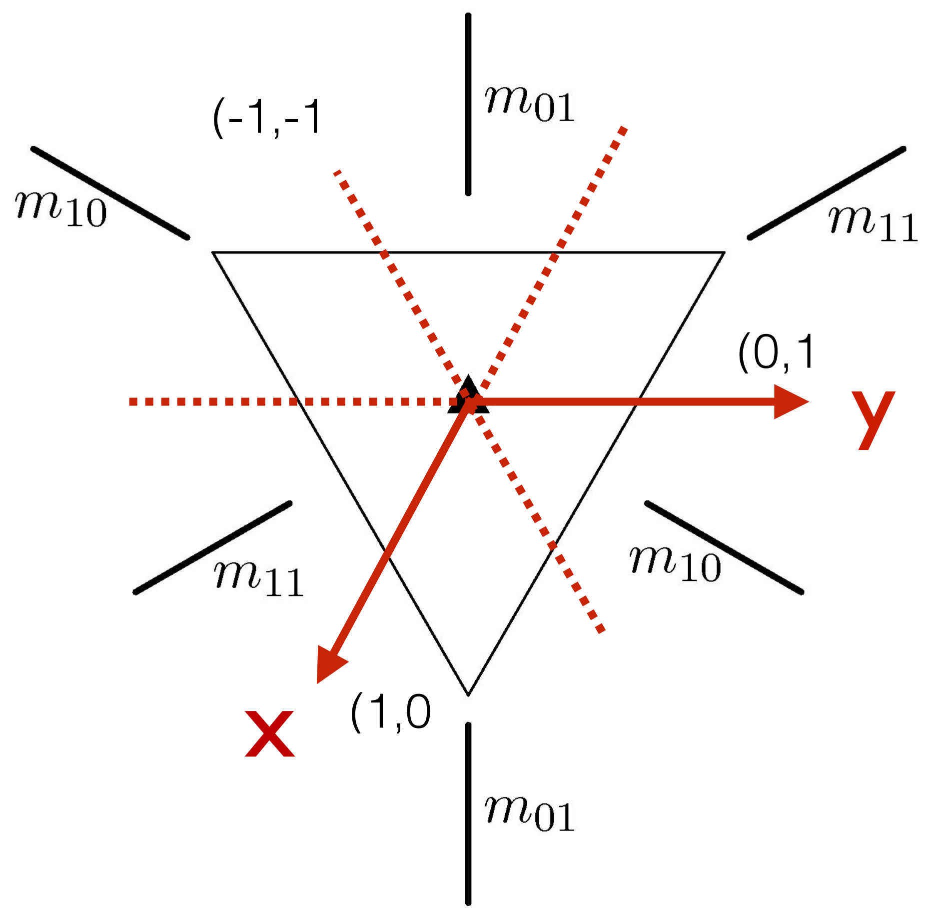
|H| is a divisor of |G|
and [i]=|G:H|

Corollary

The order *k* of any element of G, $g^k=e$, is a divisor of |G|

Example:

Coset decompositions of *3m*



	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

Multiplication table of *3m*

Consider the subgroup $\{1, m_{10}\}$ of *3m* of index *3*. Write down and compare the right and left coset decompositions of *3m* with respect to $\{1, m_{10}\}$.

Problem 1.6.1.7

Demonstrate that H is always a normal subgroup if |G:H|=2.

Conjugate subgroups

Conjugate subgroups

Let $H_1 < G$, $H_2 < G$

then, $H_1 \sim H_2$, if $\exists\, g \in G$: $g^{-1} H_1 g = H_2$

(i) Classes of conjugate subgroups: $L(H)$

(ii) If $H_1 \sim H_2$, then $H_1 \cong H_2$

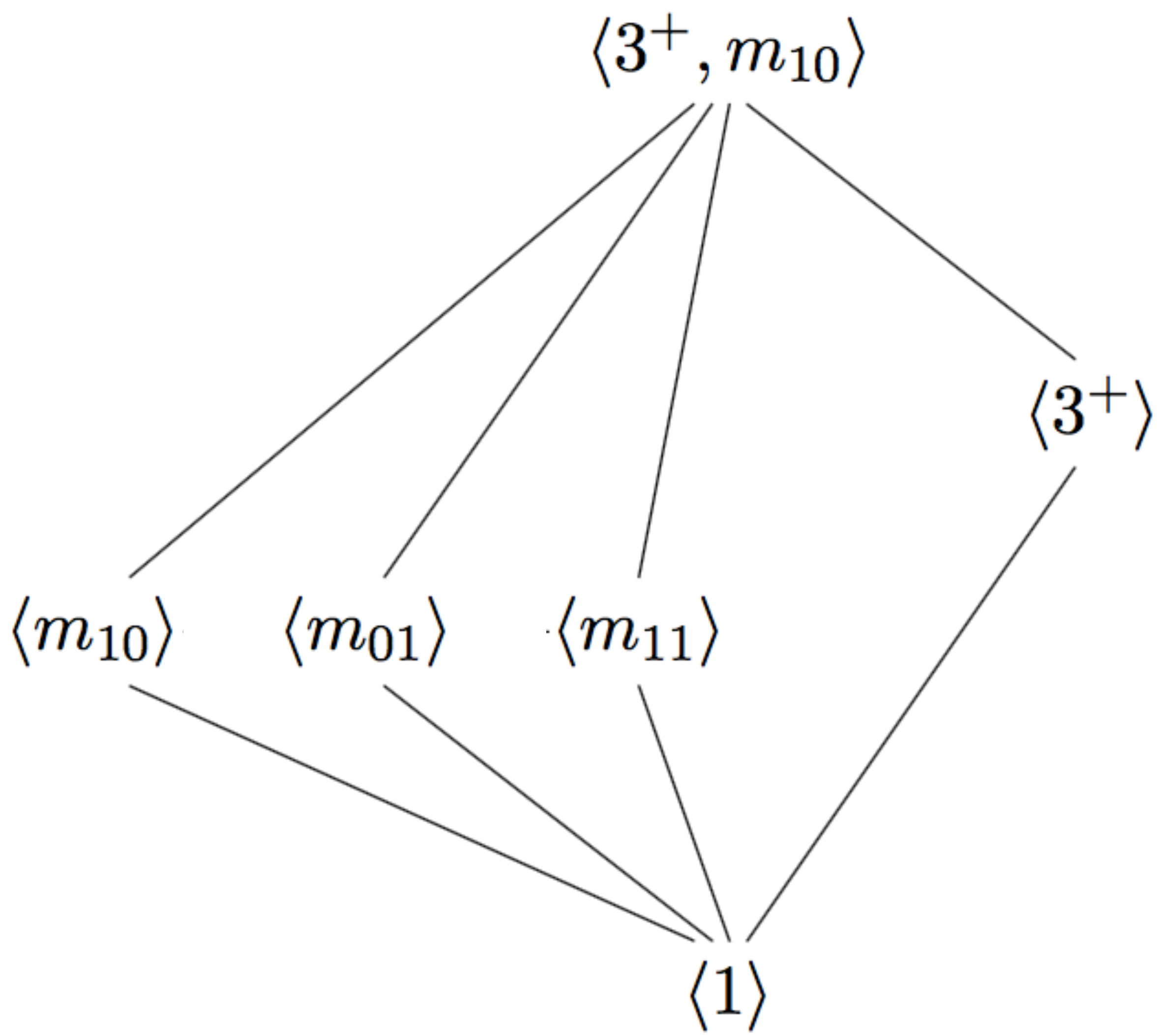
(iii) $|L(H)|$ is a divisor of $|G|/|H|$

Normal subgroup

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

Problem 1.6.1.5 (cont.)

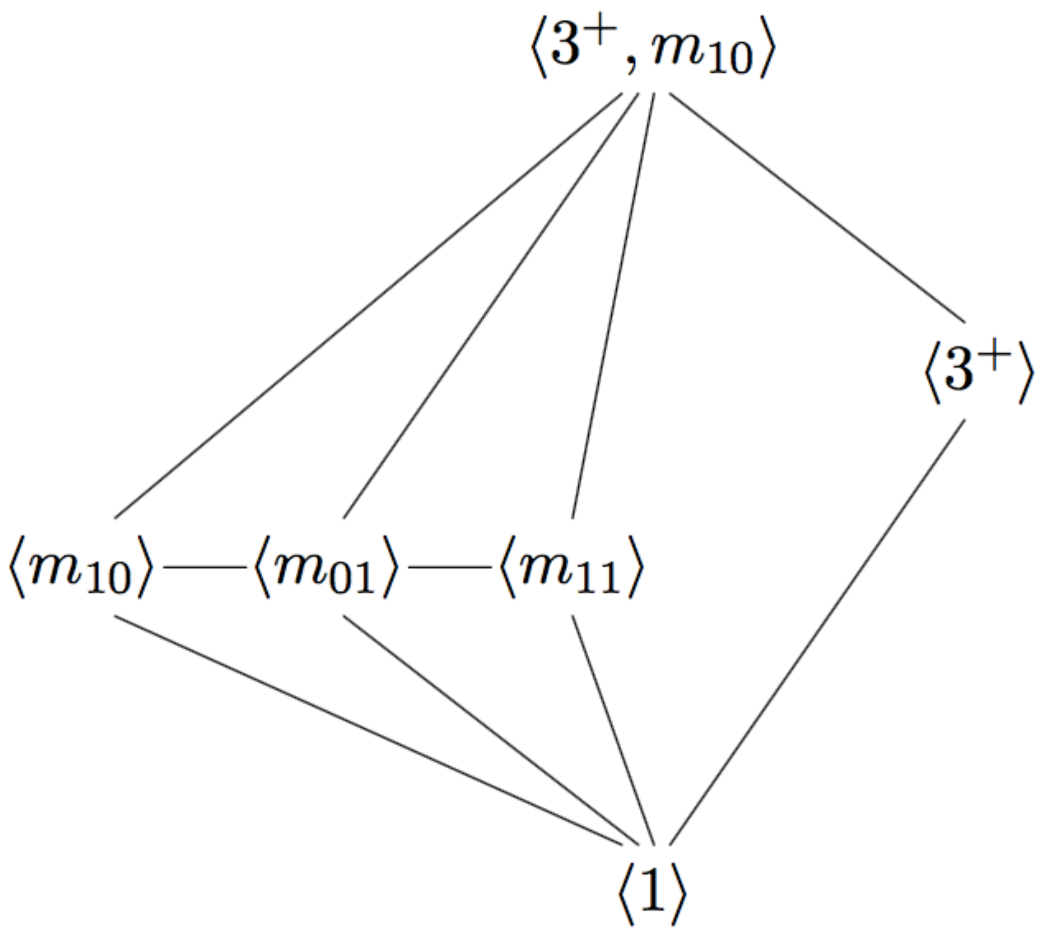
Consider the subgroups of 3m and distribute them into classes of conjugate subgroups



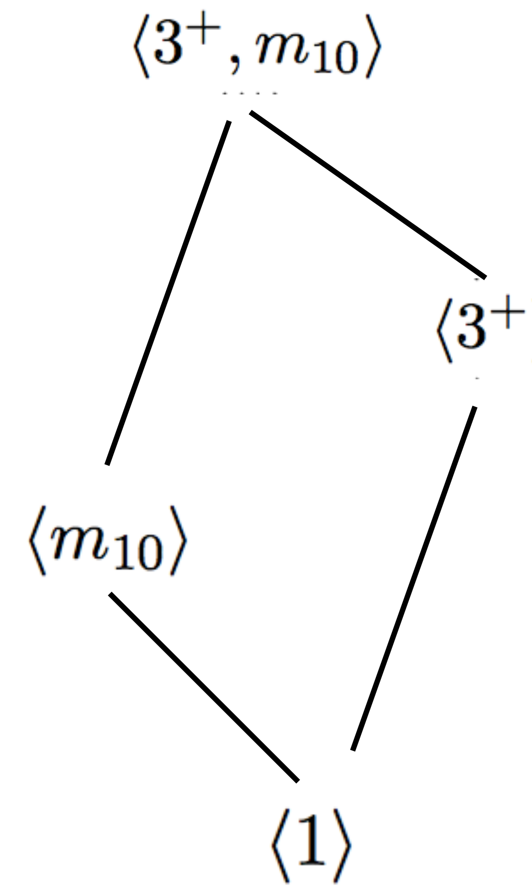
	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

Multiplication table of *3m*

Complete and contracted group-subgroup graphs



Complete graph of maximal subgroups



Contracted graph of maximal subgroups

International Tables for Crystallography, Vol. A, Chapter 3.2

Group-subgroup relations of point groups

Hahn and Klapper

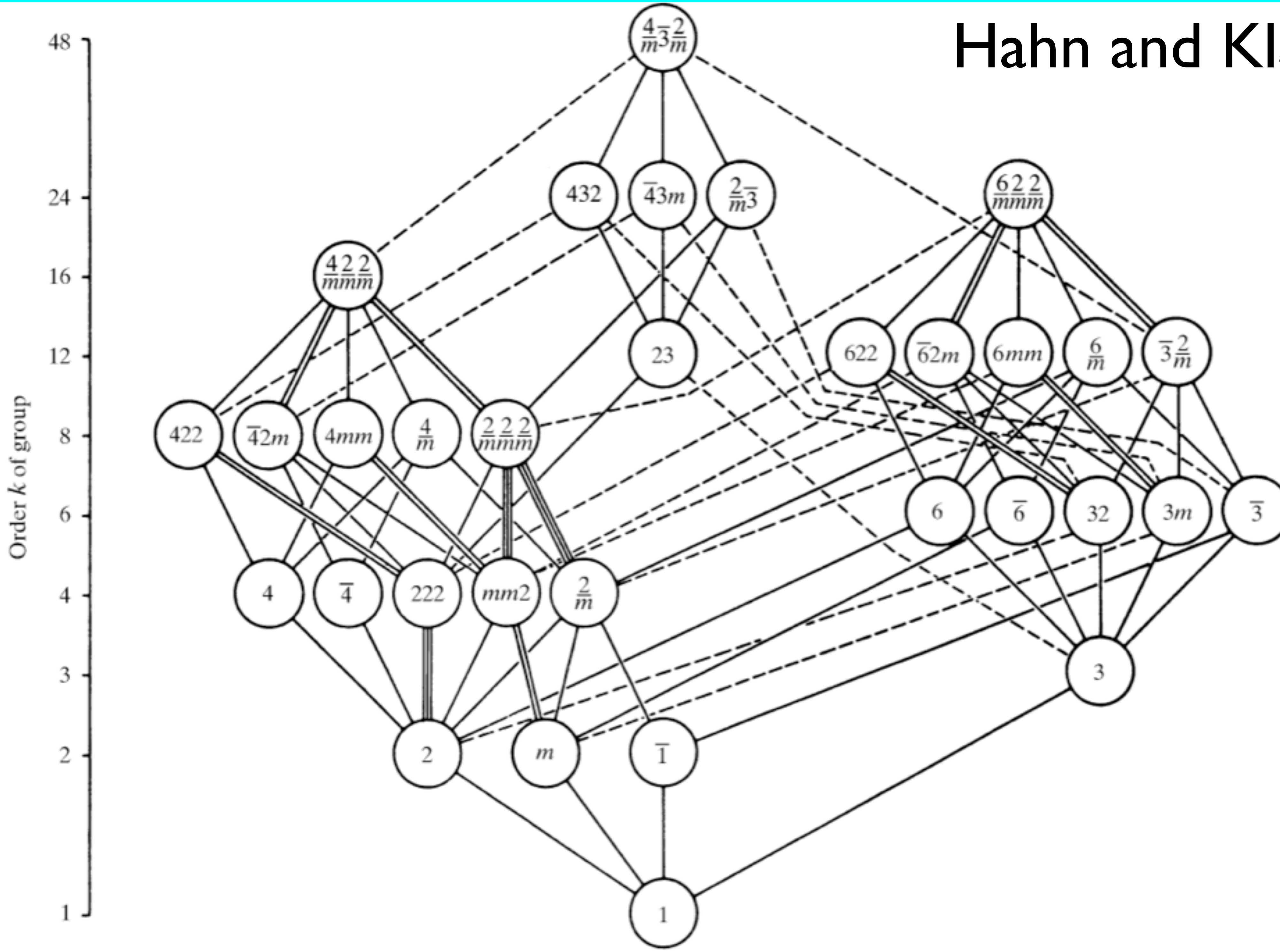
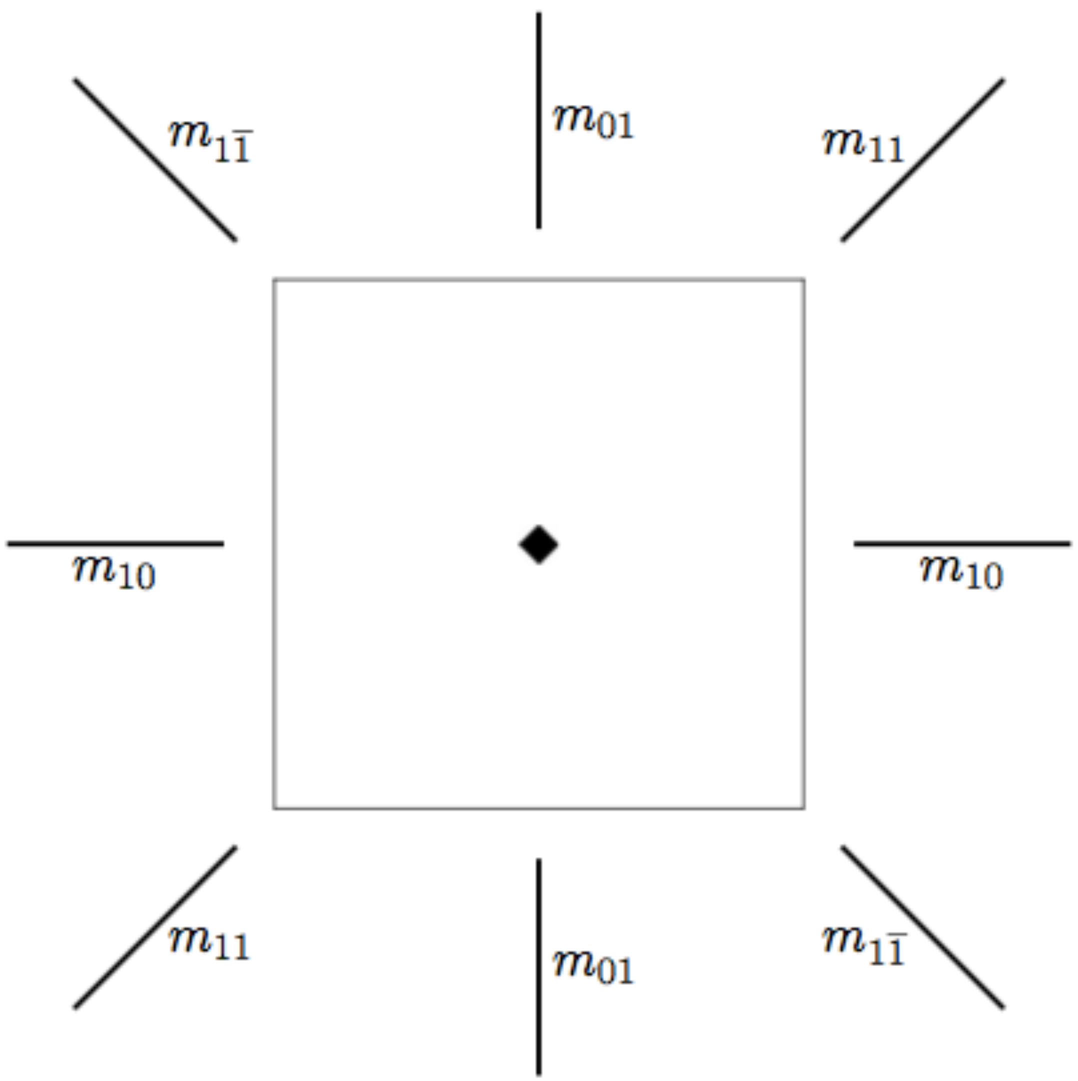


Fig. 10.1.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann–Mauguin symbols are used.

EXERCISES

Problem 1.6.1.4

Consider the group of the square and determine its subgroups



	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

Multiplication table of ***4mm***

FACTOR GROUP

Factor group

product of sets: $G=\{e, g_2, ..., g_p\}$ $\begin{cases} K_j=\{g_{j1},g_{j2},...,g_{jn}\} \\ K_k=\{g_{k1},g_{k2},...,g_{km}\} \end{cases}$

$K_j\ K_k=\{\ g_{jp}g_{kq}=g_r \mid g_{jp} \in K_j, g_{kq} \in K_k\}$

Each element g_r is taken only once in the product $K_j\ K_k$

factor group G/H: $H \triangleleft G$

$G=H+g_2H+...+g_mH,\ g_i \notin H,$

$G/H=\{H, g_2H, ..., g_mH\}$

group axioms:

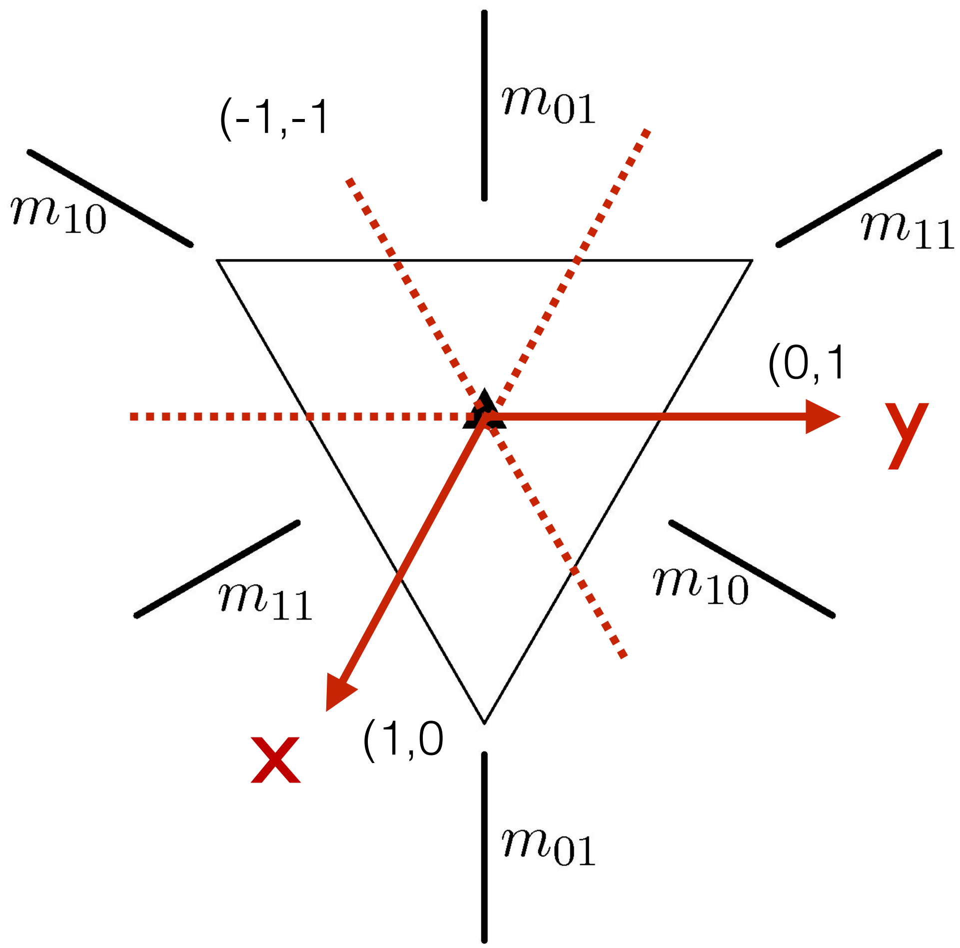
(i) $(g_iH)(g_jH) = g_{ij}H$

(ii) $(g_iH)H = H(g_iH) = g_iH$

(iii) $(g_iH)^{-1} = (g_i^{-1})H$

Example:

Factor group 3m/3



	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

Multiplication table of *3m*

(i) coset decomposition

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

E A

(ii) factor group and multiplication table

	E	**A**
E	E	A
A	A	E

Problem 1.6.1.6

Consider the normal subgroup {e,2} of 4*mm*, of index 4, and the coset decomposition 4*mm*: {e,2}:

(3) Show that the cosets of the decomposition 4*mm*:{e,2} fulfill the group axioms and form a factor group

(4) Multiplication table of the factor group

(5) A crystallographic point group isomorphic to the factor group?

GENERAL AND SPECIAL WYCKOFF POSITIONS

General and special Wyckoff positions

Orbit of a point X_o under P: $P(X_o)=\{W\ X_o, W \in P\}$

Multiplicity

Site-symmetry group $S_o=\{W\}$ of a point X_o

$$WX_o = X_o$$

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}$$

Multiplicity: $|P|/|S_o|$

General position X_o

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

Multiplicity: $|P|$

Special position X_o

$S_o>\mathbf{1}=\{1,...,\}$

Multiplicity: $|P|/|S_o|$

Site-symmetry groups: oriented symbols

Example

General and special Wyckoff positions

Point group $\mathbf{2} = \{1, 2_{001}\}$

Site-symmetry group $S_o=\{W\}$ of a point $X_o=(0,0,z)$

$S_o = \mathbf{2}$

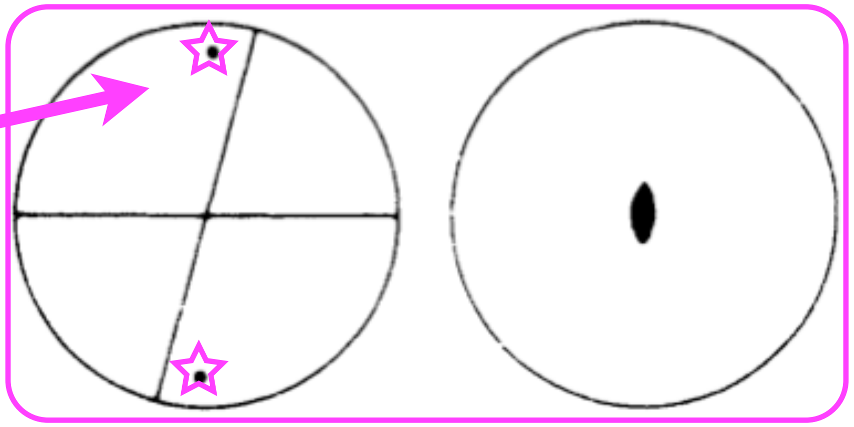
$WX_o = X_o$

$$2_{001}: \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$$

Multiplicity: $|P|/|S_o|$

2 b 1 (x,y,z) (-x,-y,z)

1 a 2 (0,0,z)



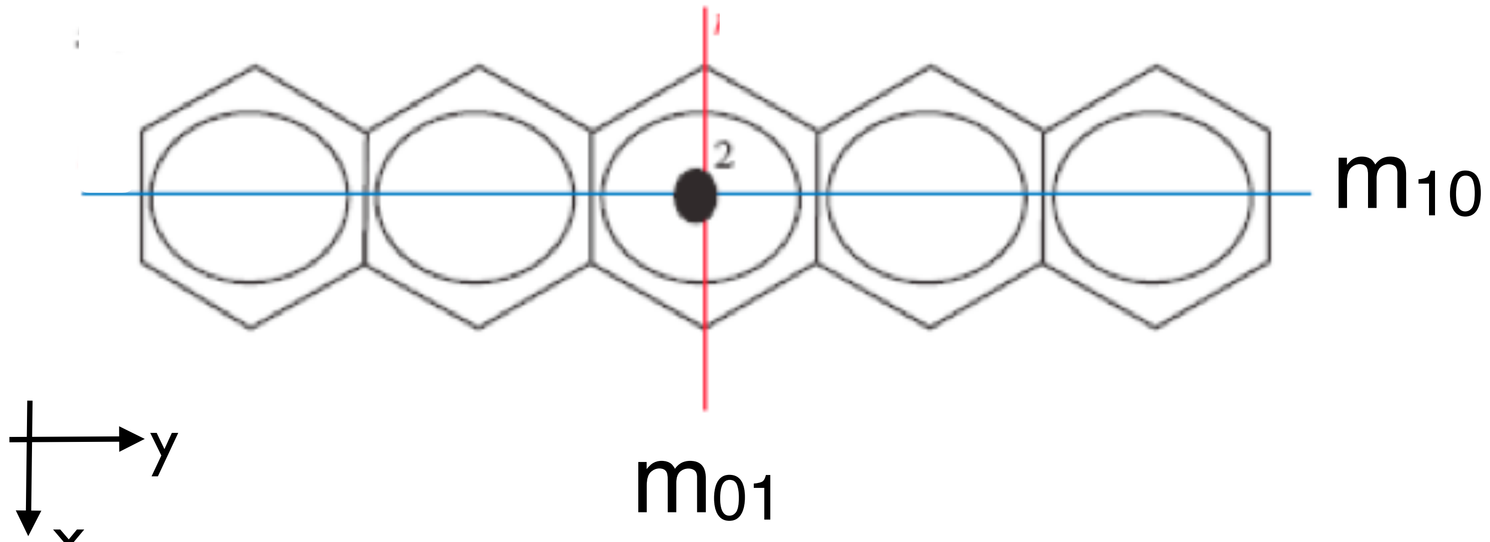
Problem 1.6.1.8

General and special Wyckoff positions

Determine the general and special Wyckoff positions of the group **mm2**

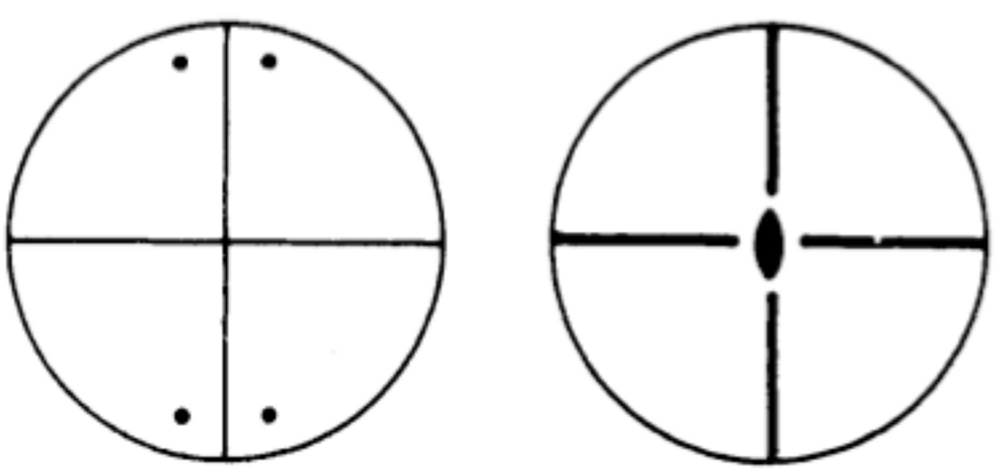
Point group **mm2** = $\{1,2,m_{10},m_{01}\}$

Molecule of pentacene



Stereographic projections diagrams

general position



symmetry elements

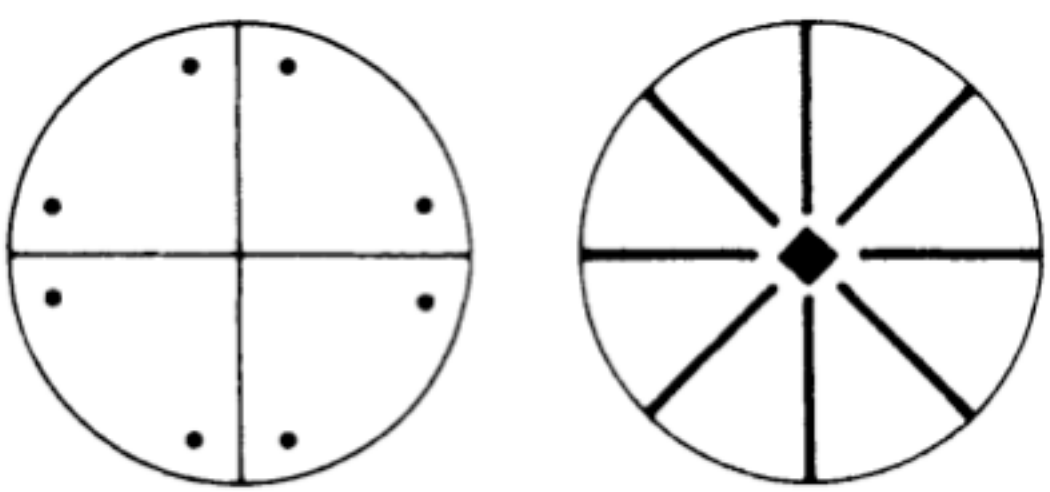
EXERCISES

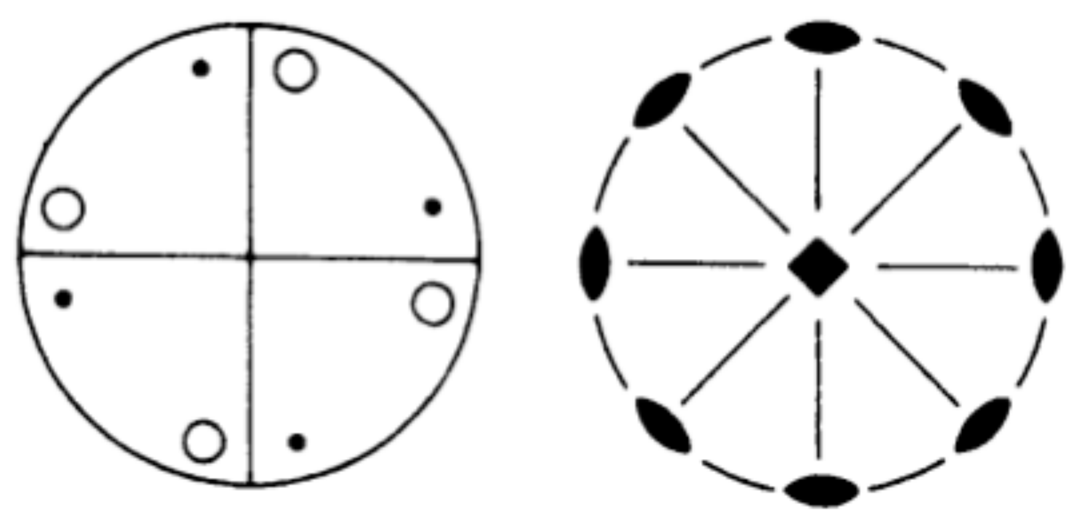
Problem 1.6.1.9

Consider the symmetry group of the square **4mm** and the point group **422** that is isomorphic to it.

Determine the general and special Wyckoff positions of the two groups.

Hint: The stereographic projections could be rather helpful





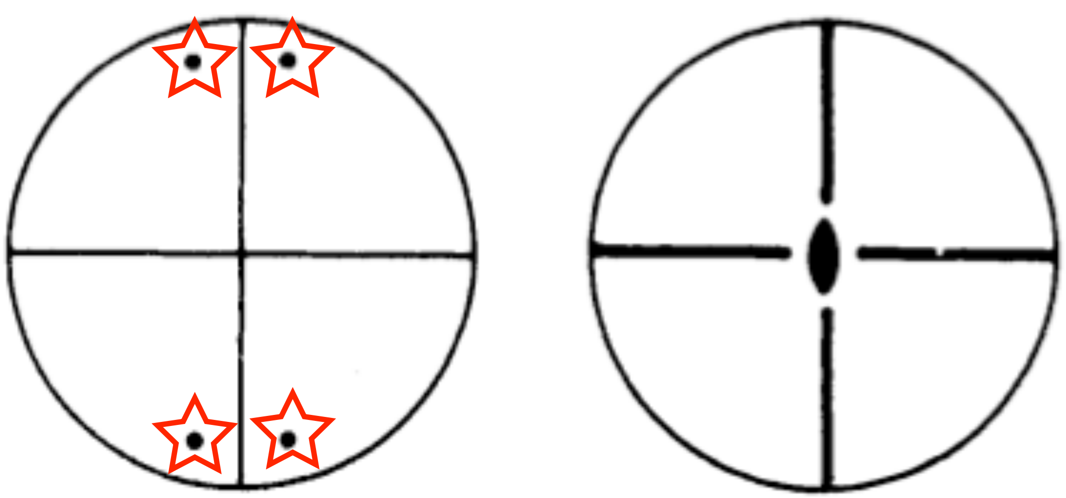
Problem 1.6.1.10

Group-subgroup relations

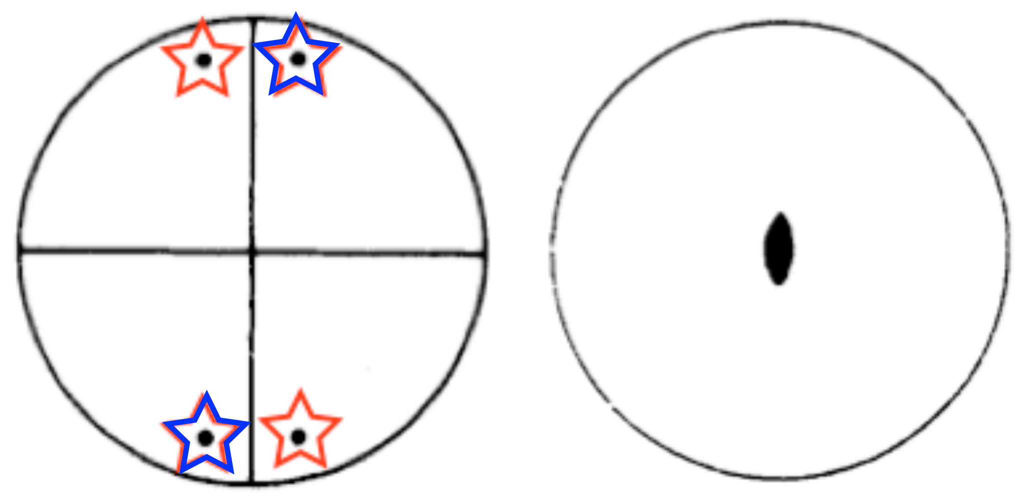
Wyckoff positions splitting schemes

Group-subgroup pair *mm2* >2, [i]=2

mm2



2



4 d 1 (x,y,z) (-x,-y,z) (x,-y,z) (-x,y,z)

$x,y,z = x_1,y_1,z_1$ 2 b 1
$-x,-y,z = -x_1,-y_1,z_1$

$x,-y,z = x_2,y_2,z_2$ 2 b 1
$-x,y,z = -x_2,-y_2,z_2$

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)

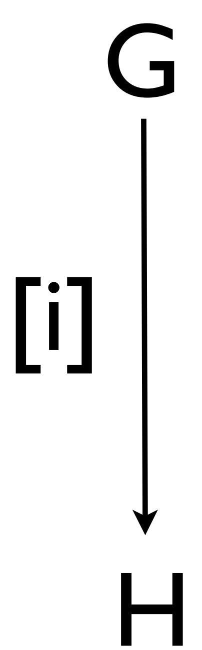
Minimal supergroups G of H

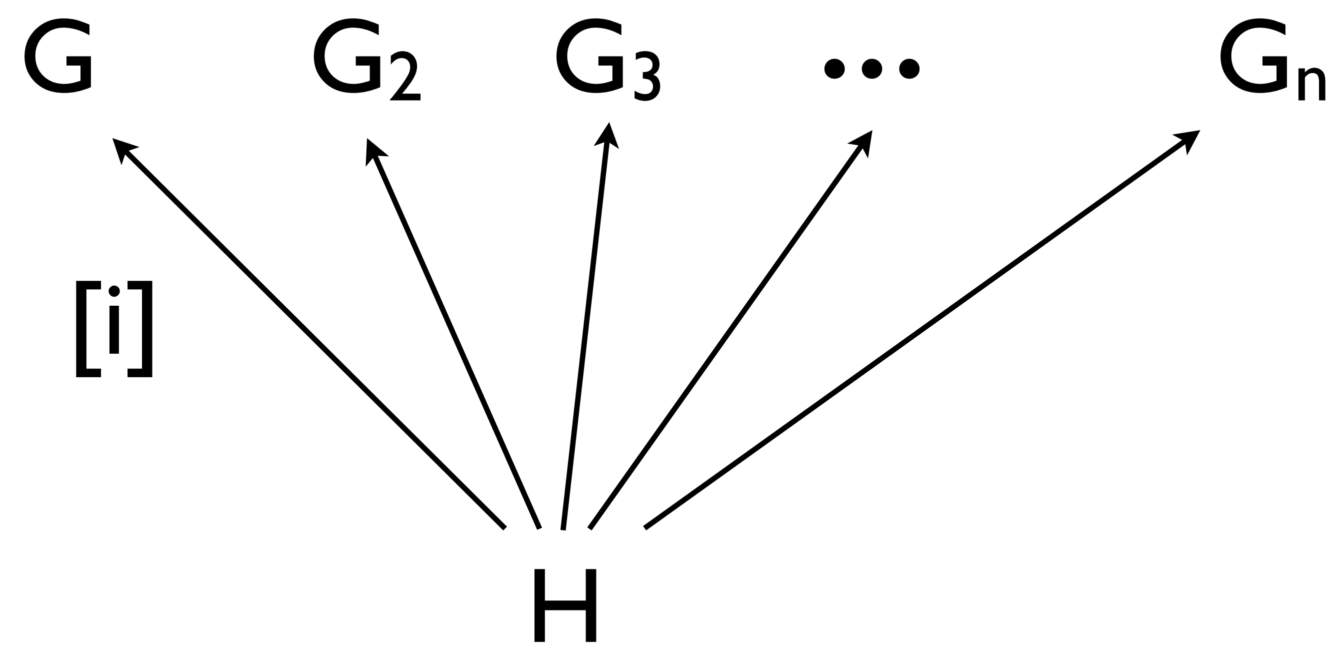
NO subgroup Z exists such that:
$H < Z < G$

The Supergroup Problem

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

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



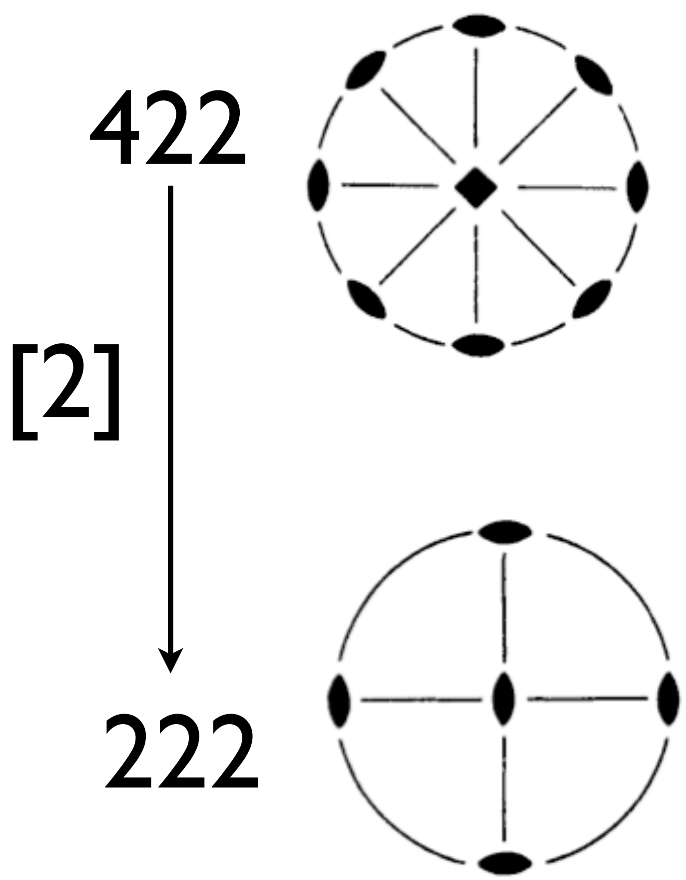


all G_k>H contain H as subgroup

$G_k = H + g_2 H + \ldots + g_{ik} H$

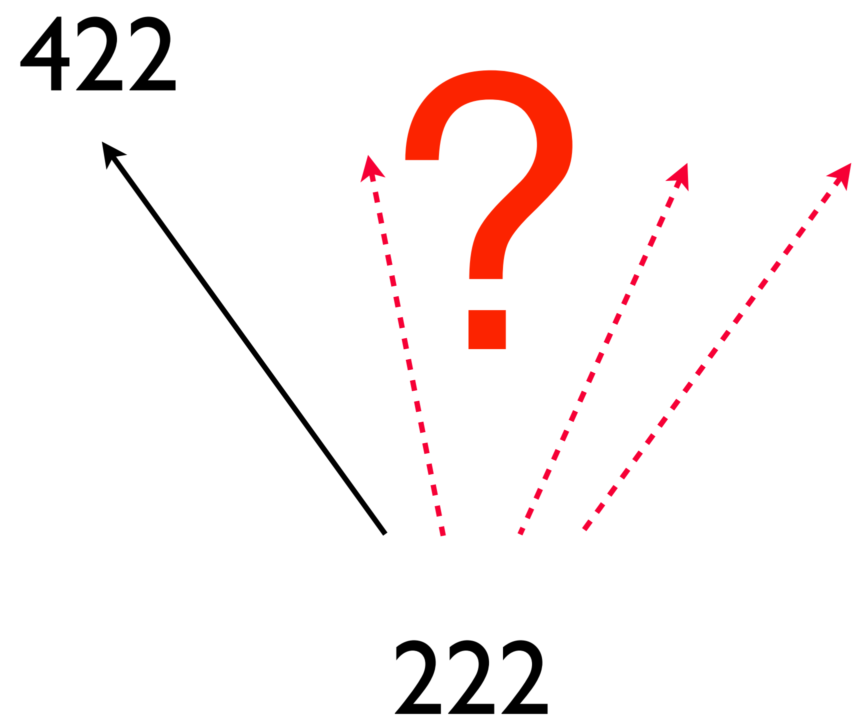
Example: Supergroup problem

Group-subgroup pair 422>222



How many are the subgroups 222 of 422?

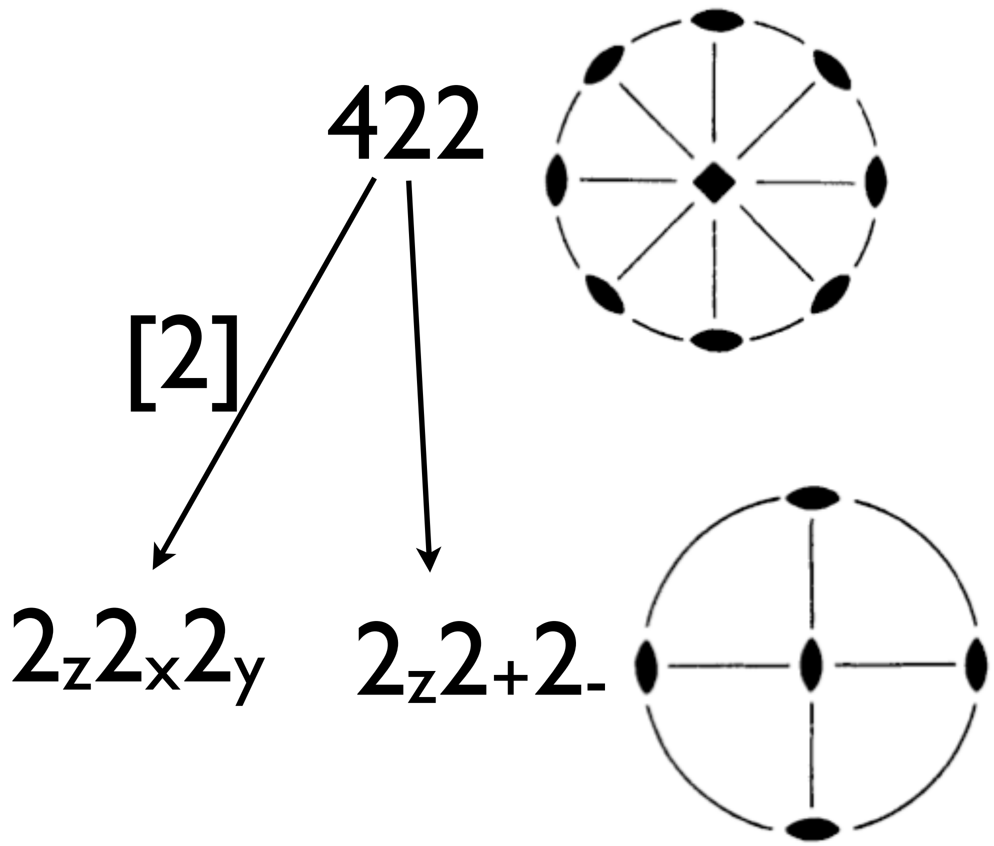
Supergroups 422 of the group 222



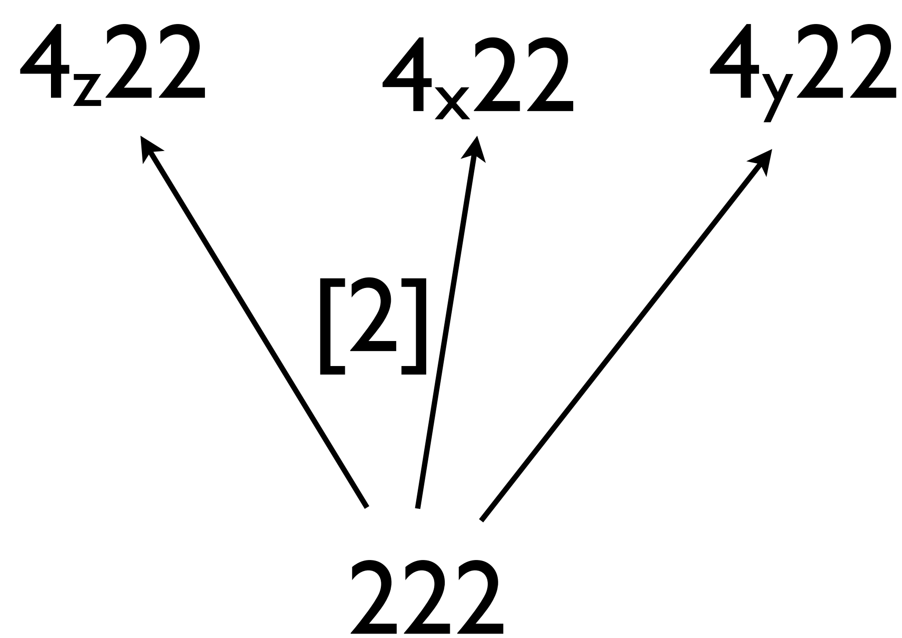
How many are the supergroups 422 of 222?

Example: Supergroup problem

Group-subgroup pair 422>222



Supergroups 422 of the group 222



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

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

$4_z22 = 222 + 4_z222$

$4_y22 = 222 + 4_y222$

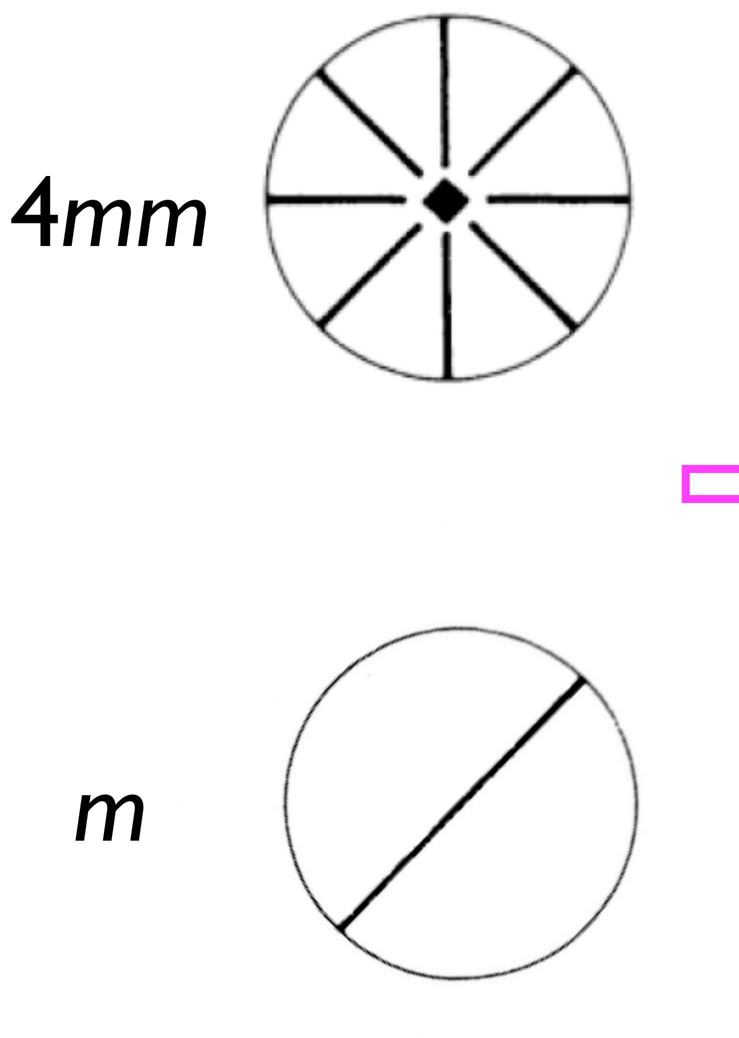
$4_x22 = 222 + 4_x222$

NORMALIZERS

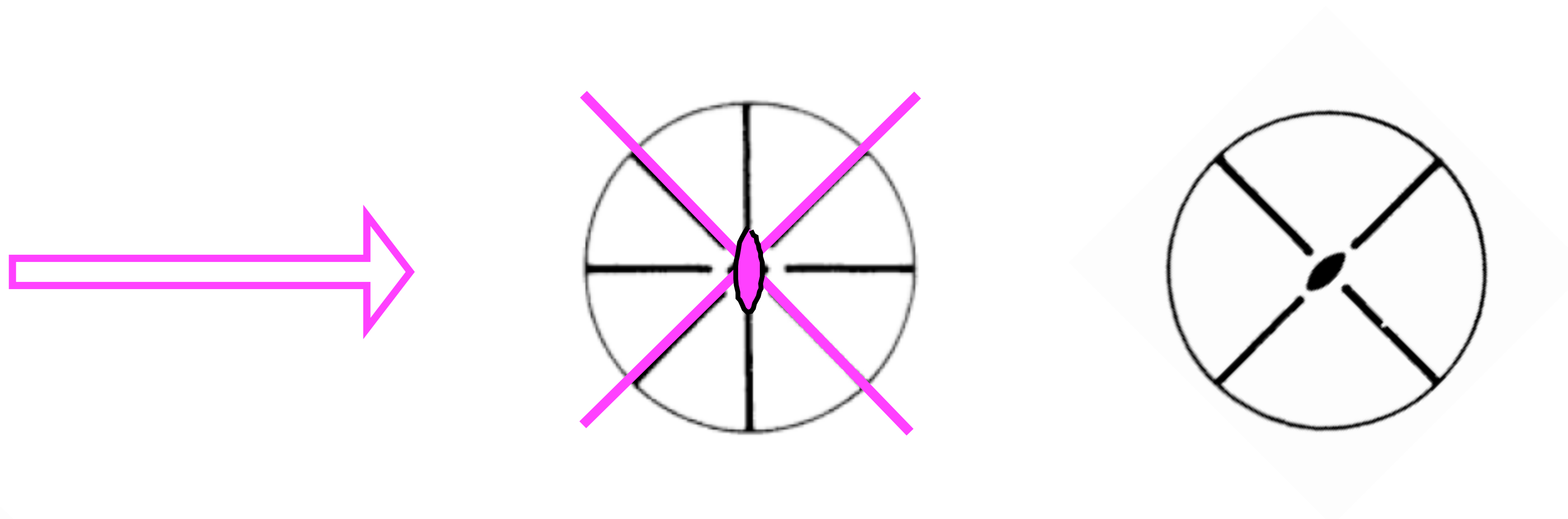
Normalizer of H < G

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

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



$\{1,m_+\}$



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

Normalizer of H in G

Normal subgroup

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

Normalizer of H in G, H<G

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

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

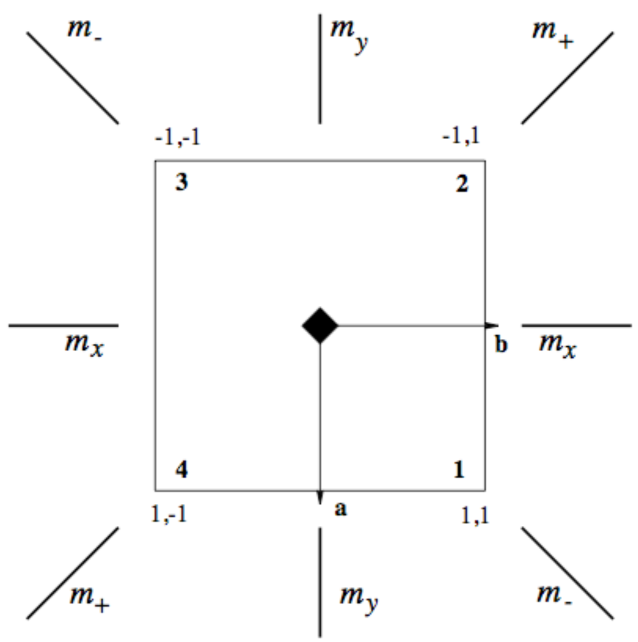
What is the normalizer $N_G(H)$ if $H \triangleleft G$?

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

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

Problem 1.6.1.15

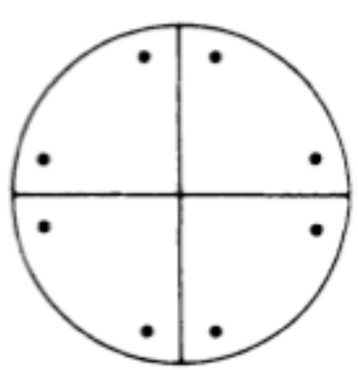
Consider the group 4*mm* and its subgroups of index 4. Determine their **normalizers** in 4*mm*. Distribute the subgroups into conjugacy classes with the help of their normalizers in 4*mm*.

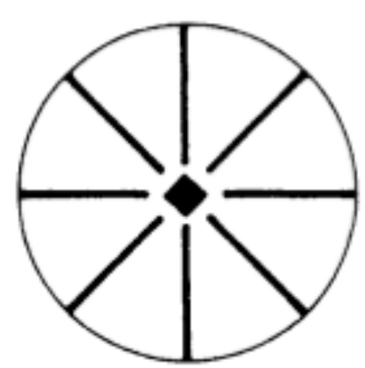


	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
1	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
2	2	1	4^{-1}	4	m_y	m_-	m_x	m_+
4	4	4^{-1}	2	1	m_+	m_y	m_-	m_x
4^{-1}	4^{-1}	4	1	2	m_-	m_x	m_+	m_y
m_x	m_x	m_y	m_-	m_+	1	4^{-1}	2	4
m_+	m_+	m_-	m_x	m_y	4	1	4^{-1}	2
m_y	m_y	m_x	m_+	m_-	2	4	1	4^{-1}
m_-	m_-	m_+	m_y	m_x	4^{-1}	2	4	1

Multiplication table of 4*mm*

Hint: The stereographic projections could be rather helpful





CRYSTALLOGRAPHIC POINT GROUPS IN 2D AND 3D (BRIEF OVERVIEW)

Crystallographic symmetry operations

Problem 1.6.1.11

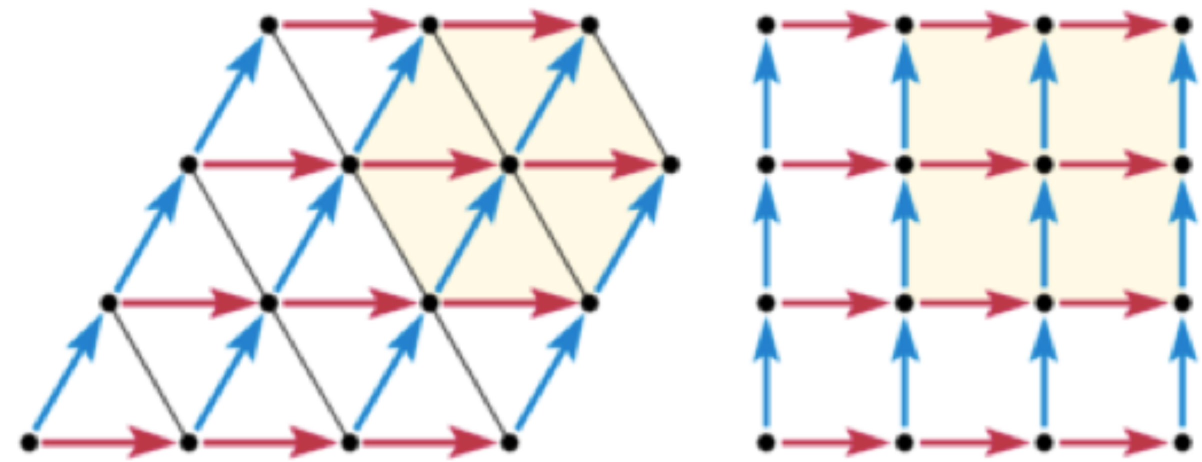
Crystallographic restriction theorem

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.

Tr R = 2cosθ= 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

CRYSTALLOGRAPHIC POINT GROUPS IN THE PLANE

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?

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

-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?

$$2 \times 2 = \begin{array}{|c|c|}\hline -1 & \\ \hline & -1 \\ \hline\end{array} \times \begin{array}{|c|c|}\hline -1 & \\ \hline & -1 \\ \hline\end{array} = \begin{array}{|c|c|}\hline 1 & \\ \hline & 1 \\ \hline\end{array}$$

-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?

$$m \times m = \begin{array}{|c|c|}\hline -1 & \\ \hline & 1 \\ \hline \end{array} \times \begin{array}{|c|c|}\hline -1 & \\ \hline & 1 \\ \hline \end{array} = \begin{array}{|c|c|}\hline 1 & \\ \hline & 1 \\ \hline \end{array}$$

-order of **m**?

-multiplication table

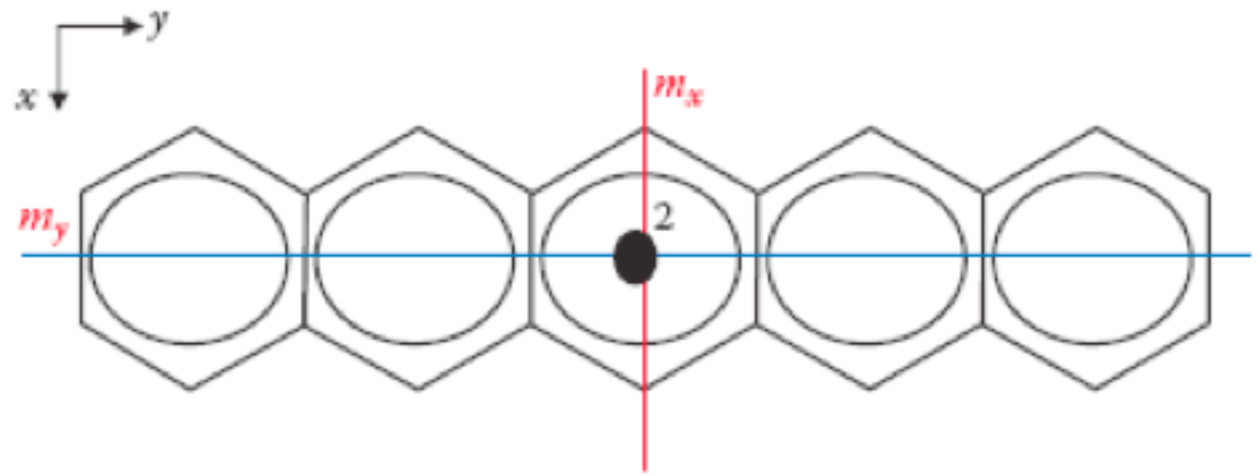
$\times$	1	m_y
1	1	m_y
m_y	m_y	1

-generators of **m**?

Crystallographic Point Groups in 2D

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

Molecule of pentacene



-order of **2mm**?

-group axioms?

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

-multiplication table

$\times$	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

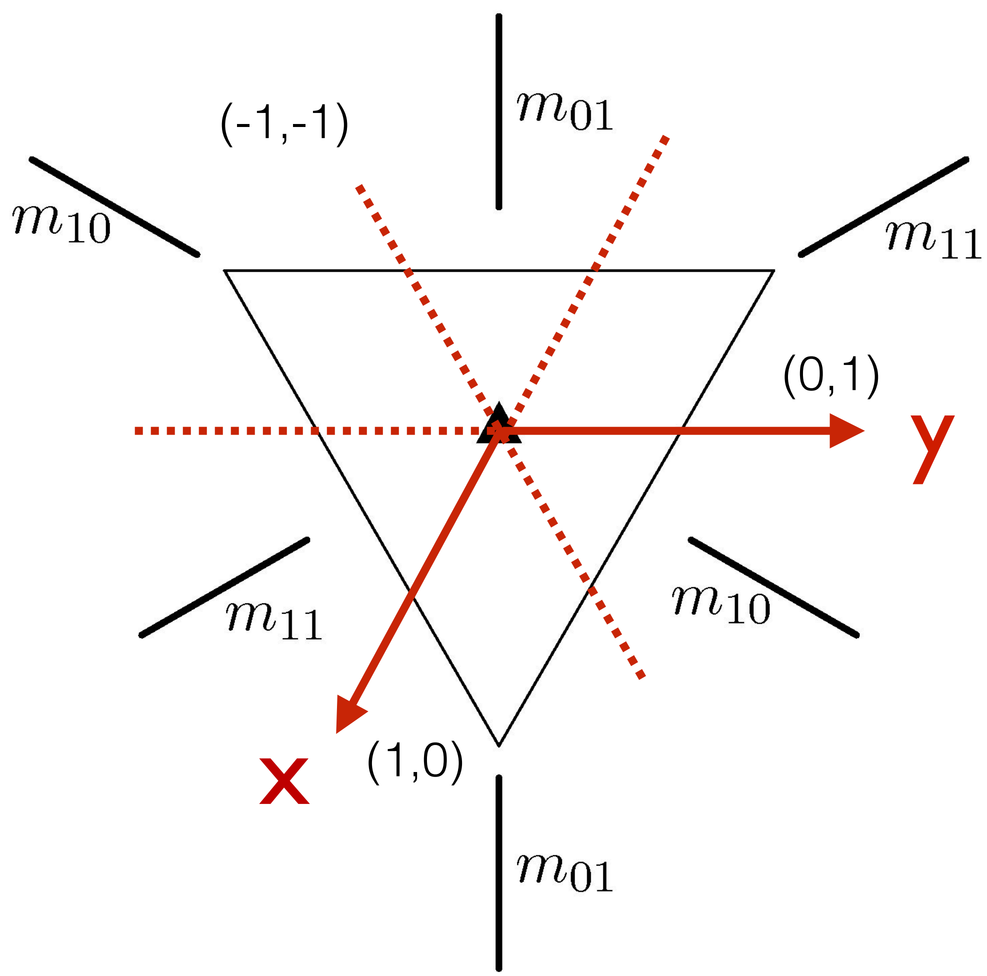
-generators of **mm2**?

Crystallographic Point Groups in 2D

Group of the equilateral triangle

Point group

3m = {1,3+,3-,m_{10}, m_{01}, m_{11}}



	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

Multiplication table of **3m**

Hermann-Mauguin symbolism (International Tables A)

A direction is called a ***symmetry direction*** of a crystal structure if it is parallel to an axis of rotation or to the normal of a reflection.

A symmetry direction is thus the **direction of the geometric element** of a symmetry operation, when the normal of a symmetry plane is used for the description of its orientation.

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

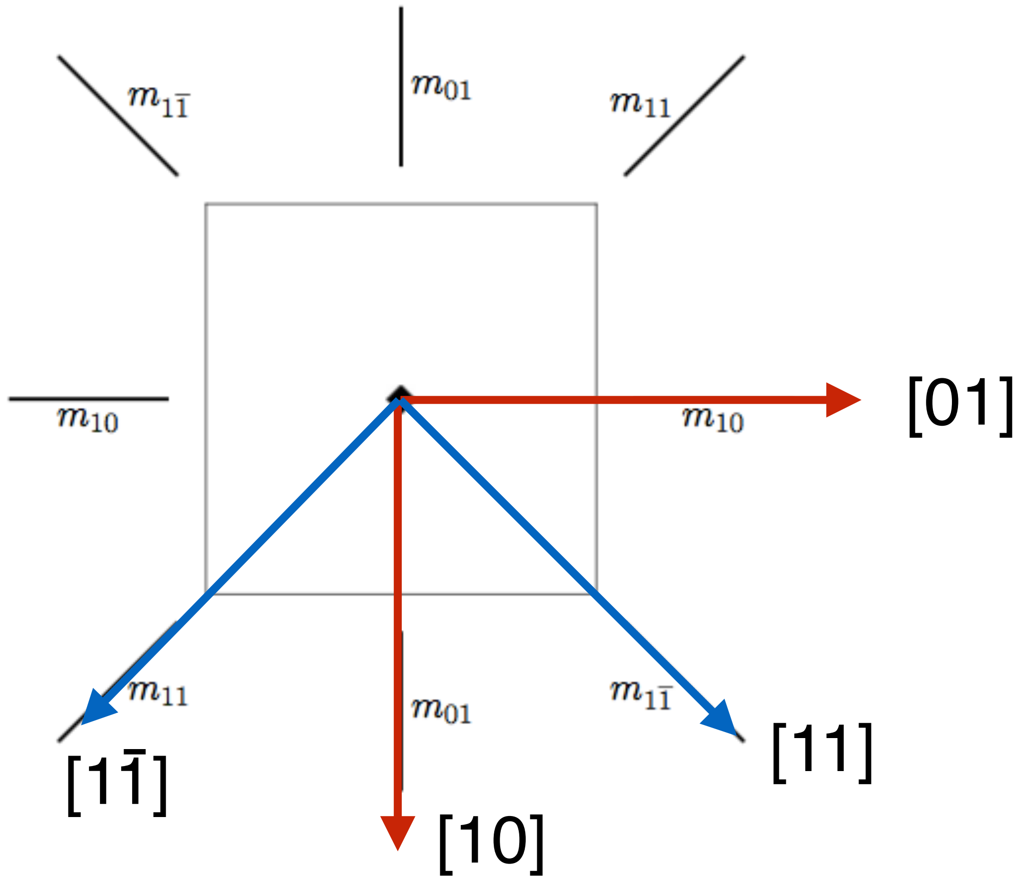
Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Two dimensions			
Oblique *1, 2*	Rotation point in plane		
Rectangular *m, 2mm*		[10]	[01]
Square *4, 4mm*		{[10], [01]}	{$[1\bar{1}]$, [11]}
Hexagonal *3, 3m* *6, 6mm*		{[10], [01], $[\bar{1}\bar{1}]$}	{$[1\bar{1}]$, [12], $[\bar{2}\bar{1}]$}

rotations:
by the axes of rotation

reflections:
by the normals to the planes

Symmetry Directions

tetragonal



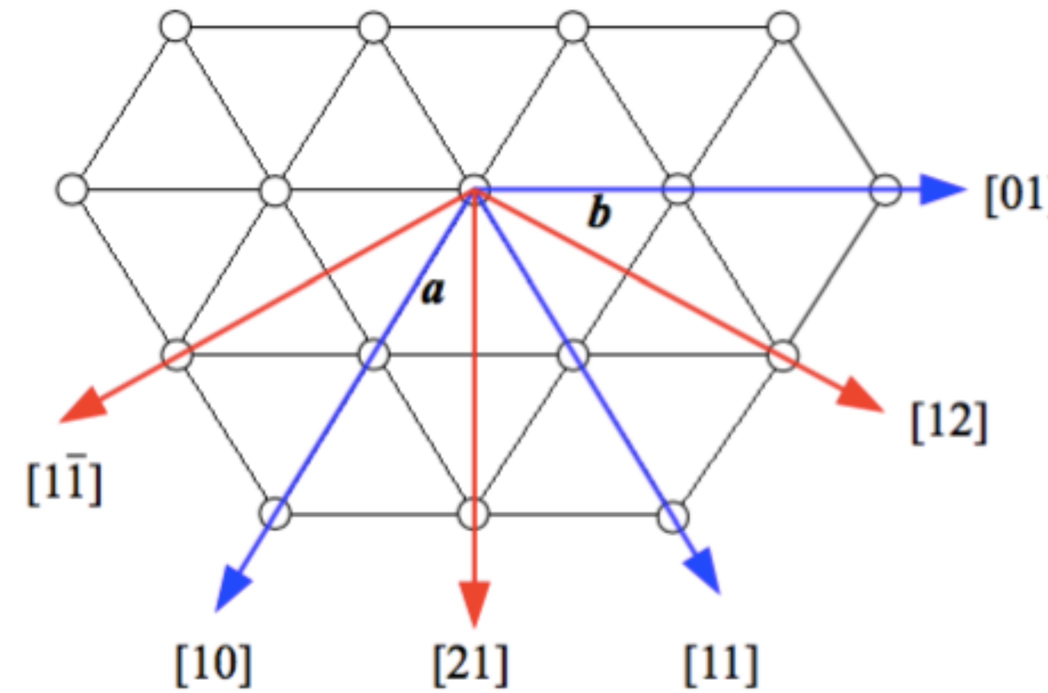
symmetry directions

<10> <1$\bar{1}$>

[10] [1$\bar{1}$]

[01] [11]

hexagonal



symmetry directions

<10> <1$\bar{1}$>

[10] [1$\bar{1}$]

[01] [21]

[11] [12]

Example

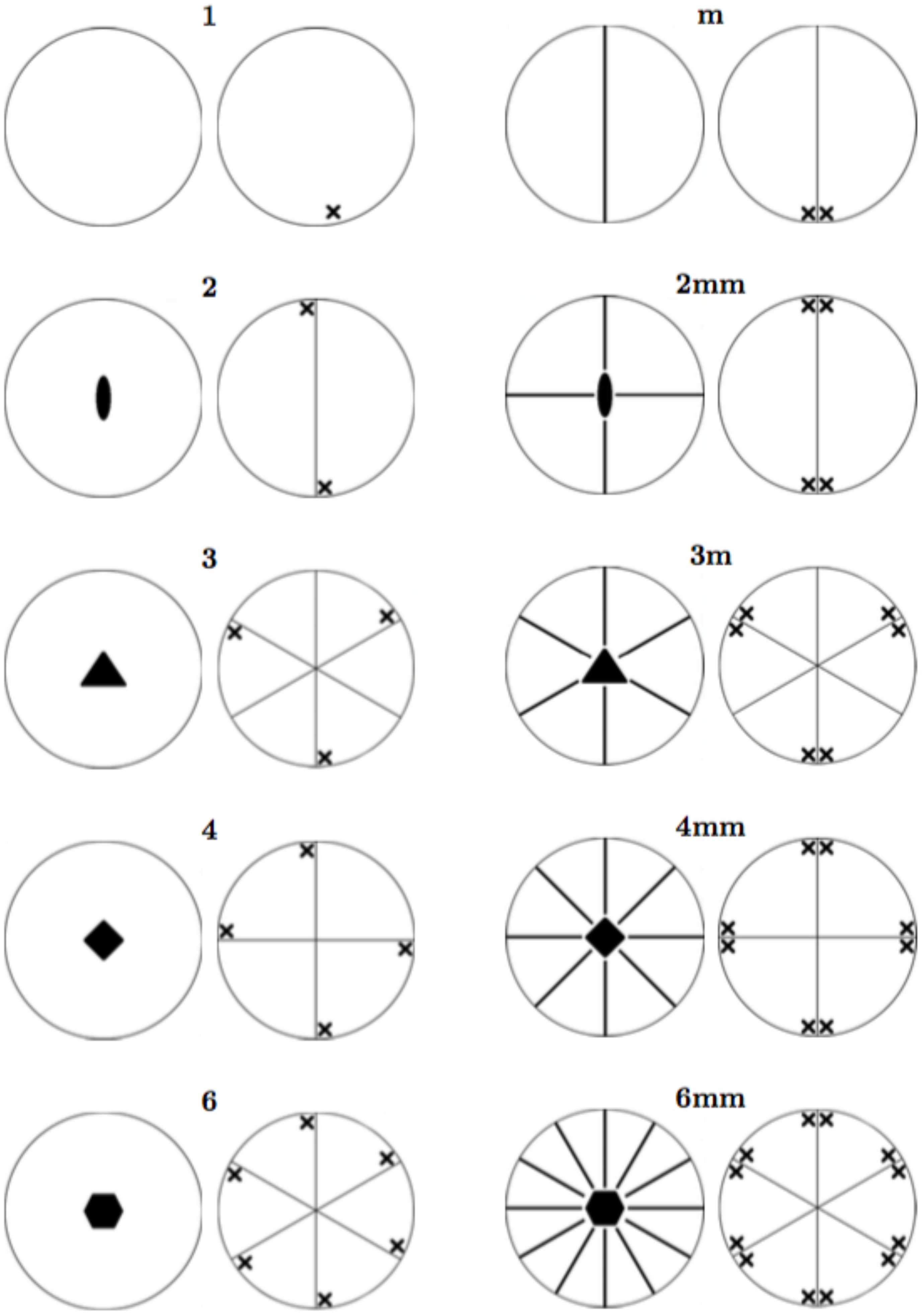
Symmetry-elements diagrams

and

General-positions diagrams

of the

plane point groups.



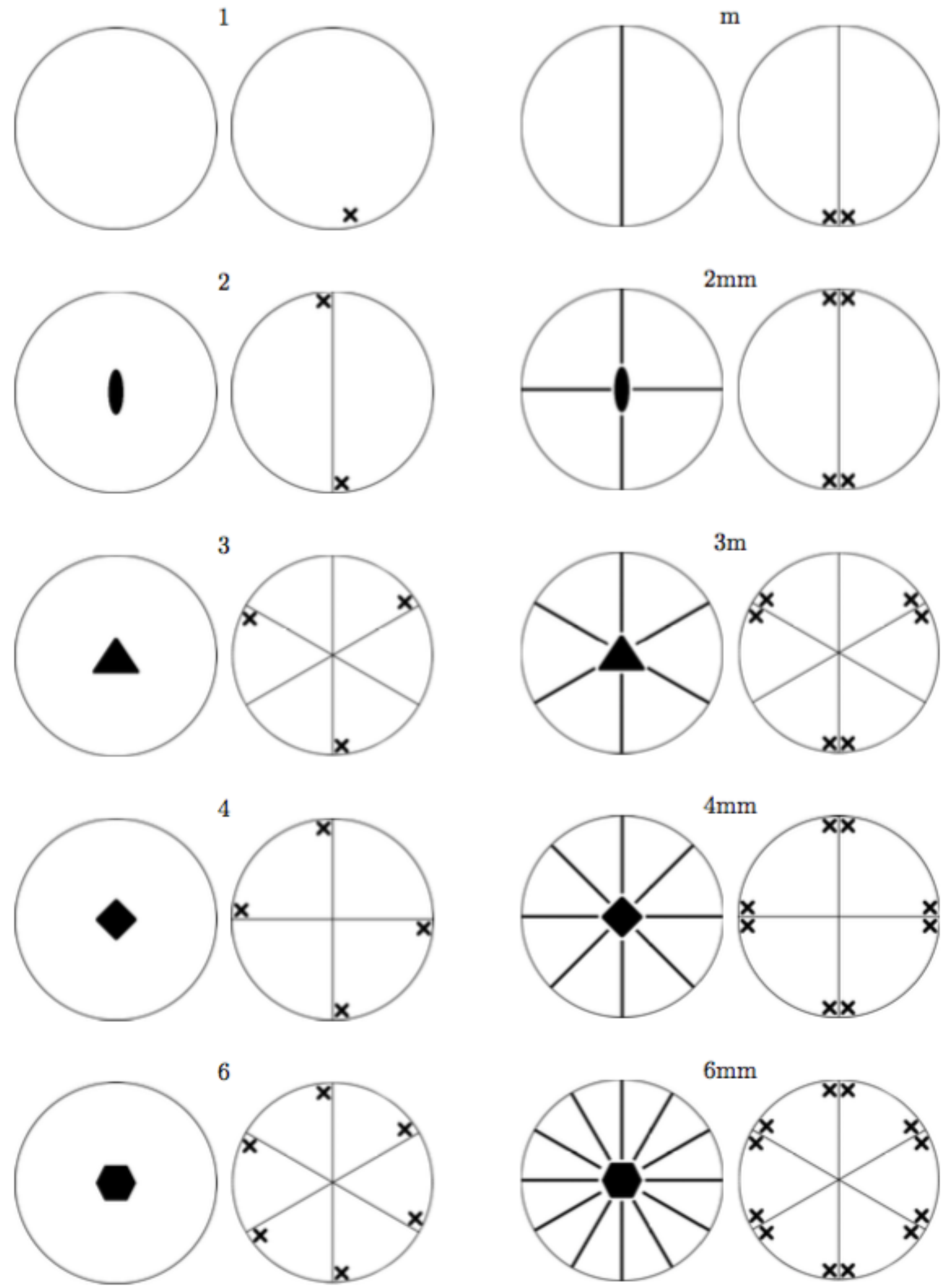
Problem 1.6.1.14

Consider the following 10 figures of the symmetry elements and the general positions of the plane point groups.

1. Determine the order of the point groups and arrange them vertically by descending point-group orders (i.e. the point group of highest order at the top, and that of lowest order at the bottom).

2. Determine the complete group-subgroup graph for all plane point groups.

3. Consider the point group 2mm. Determine its maximal subgroups, its minimal supergroups and the corresponding indices.



CRYSTALLOGRAPHIC POINT GROUPS IN 3D
(brief overview)

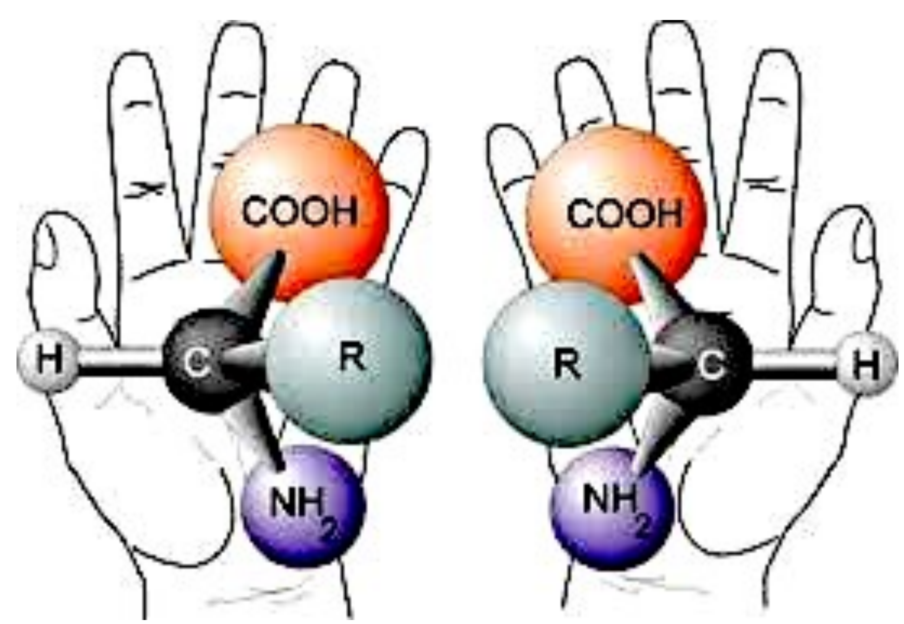
Crystallographic Point Groups in 3D

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

chirality preserving

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

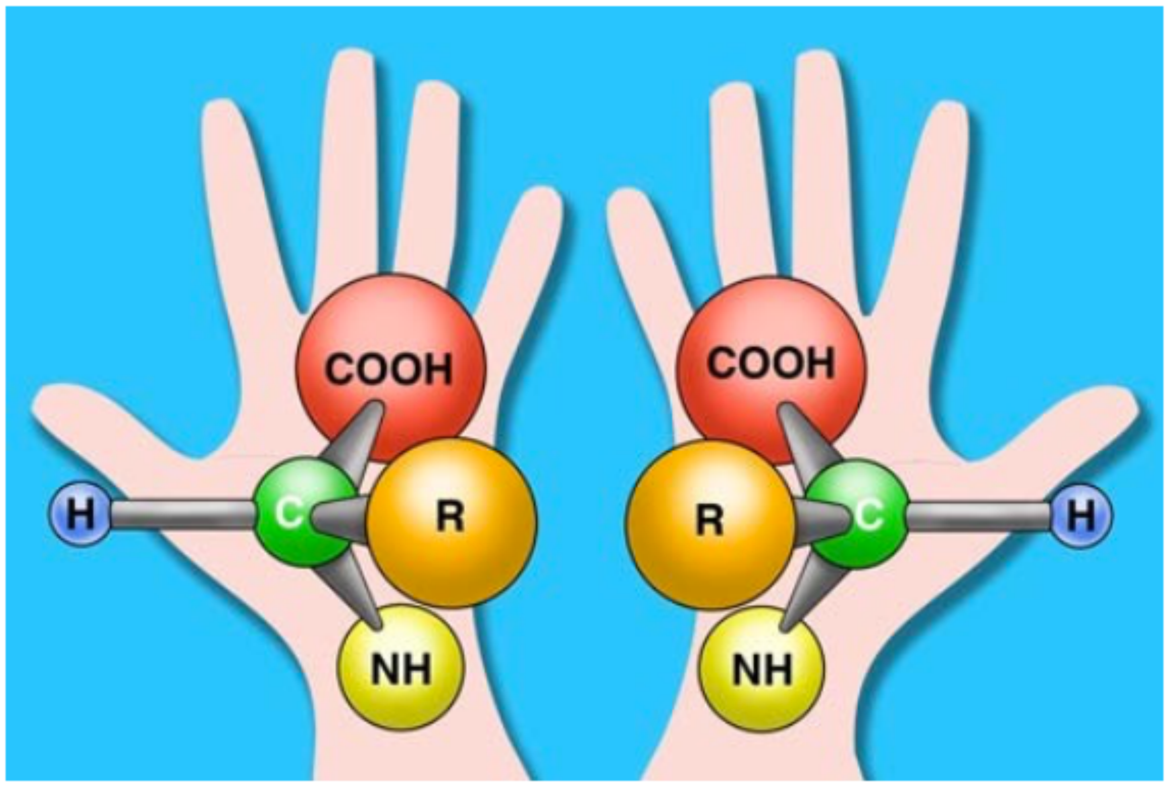
chirality non-preserving

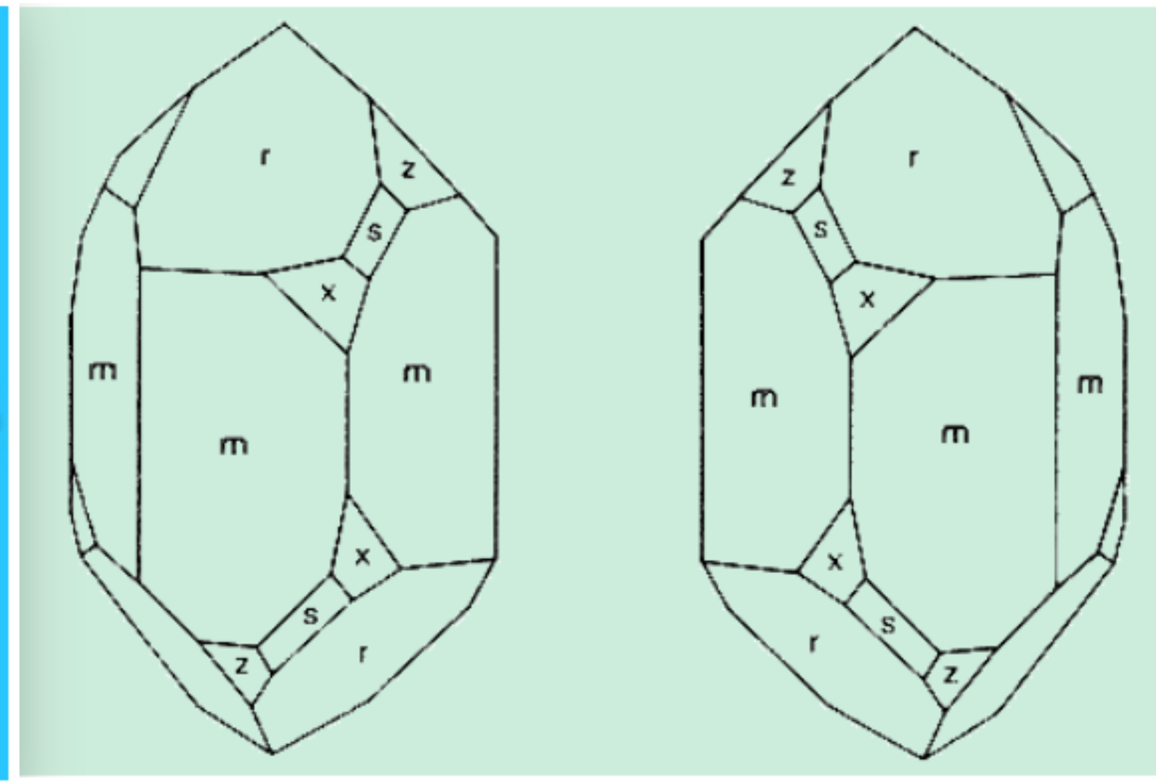


Chirality and chiral objects

Lord Kelvin (1884) "I called any geometrical figure or group of points 'chiral' and say it has chirality if its image in a plane mirror ideally realized, cannot be brought to coincide with itself."

A chiral molecule/object is non-superimposable on its mirror image.
The mirror images of a chiral molecule/object are called enantiomers.





The term *chirality* is derived from the Greek word for hand, χειρ (kheir).

symmetry operations:

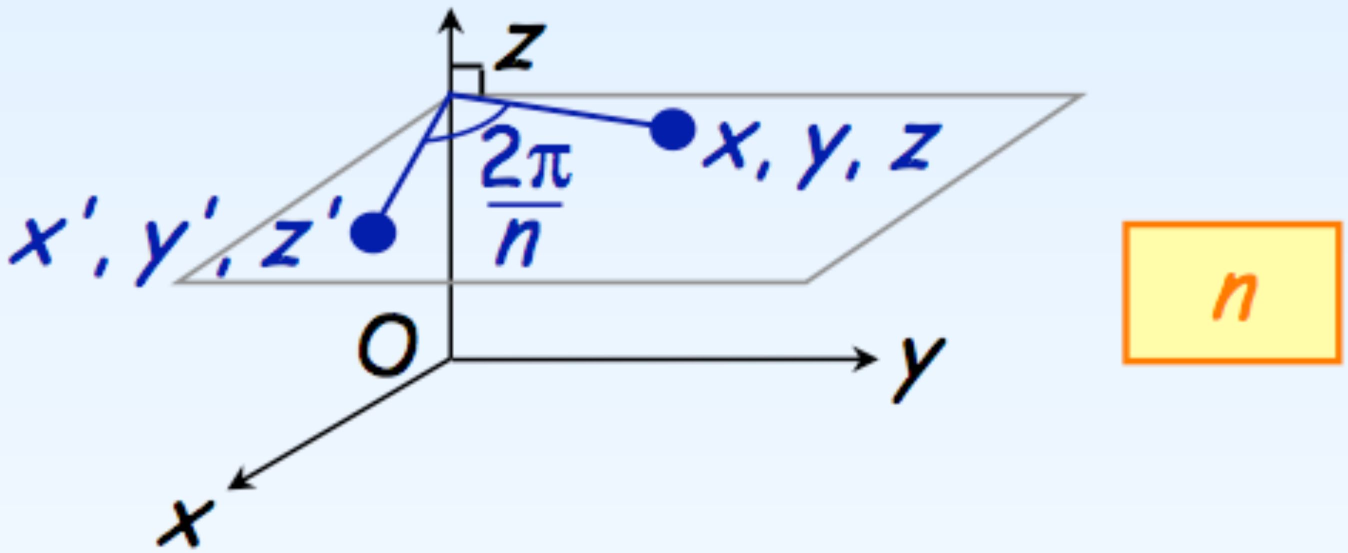
first kind (det=+1): does not change the chirality of a chiral object
second kind (det = -1): change the chirality of a chiral object

Symmetry groups of chiral objects:

Symmetry operations in 3D
Rotations

Rotation (around an axis)

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

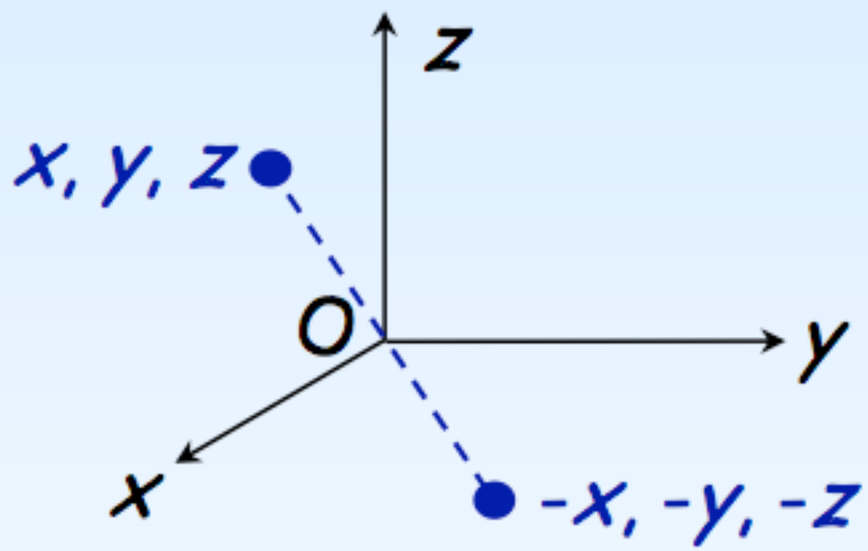


$$\alpha(n) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Det = +1

Symmetry operations in 3D
Inversion

Inversion (through a point)



$\bar{1}$

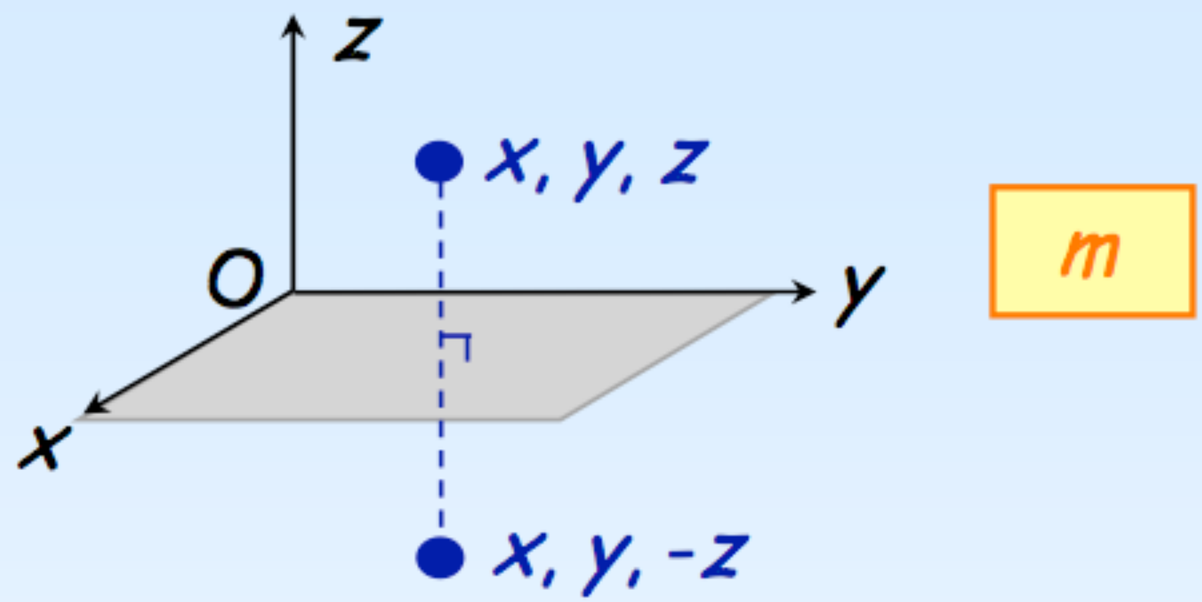
a crystal which has the inversion symmetry is called centrosymmetrical.

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

Det = -1

Symmetry operations in 3D
Reflection

Reflection (through a mirror plane)

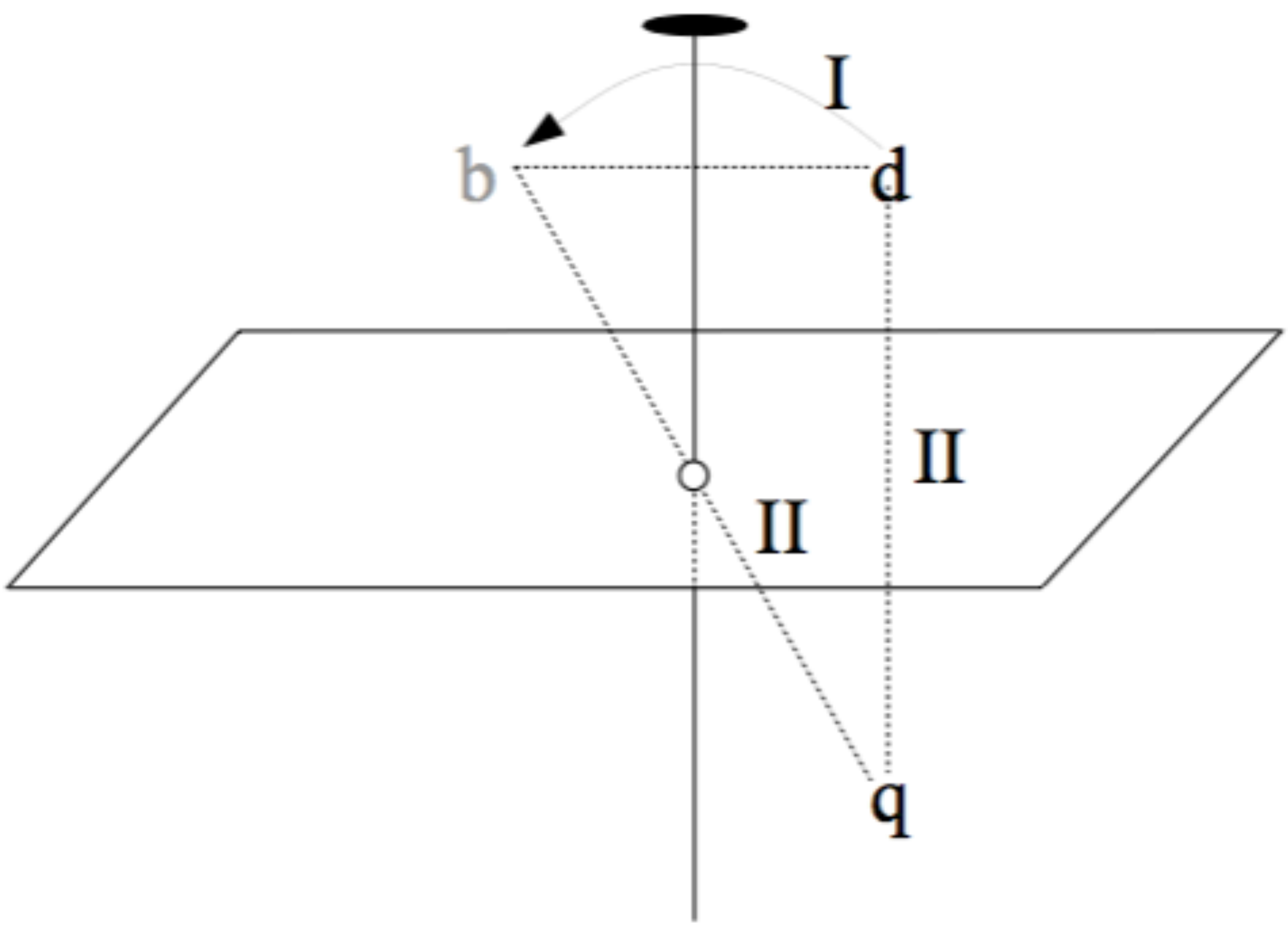


Note that: $m = \bar{2}$!

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

Det = -1

Equivalence of $\bar{2}$ and *m*

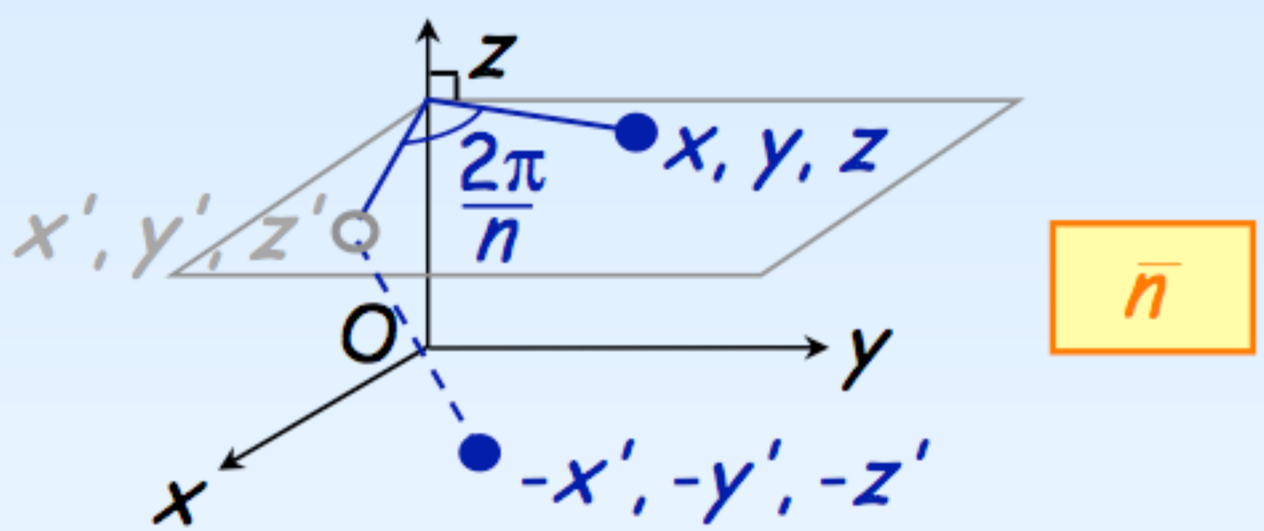


Symmetry operations in 3D
Rotoinversions

Roto-inversion

(around an axis and through a point)

Rotation followed by an inversion



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

Det = -1

Crystallographic Point Groups in 3D

System used in this volume	Point group — International symbol — Short	Point group — International symbol — Full	Schoenflies symbol
Triclinic	1	1	C_1
	$\bar{1}$	$\bar{1}$	$C_i(S_2)$
Monoclinic	2	2	C_2
	m	m	$C_s(C_{1h})$
	$2/m$	$\frac{2}{m}$	C_{2h}
Orthorhombic	222	222	$D_2(V)$
	$mm2$	$mm2$	C_{2v}
	mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}(V_h)$
Tetragonal	4	4	C_4
	$\bar{4}$	$\bar{4}$	S_4
	$4/m$	$\frac{4}{m}$	C_{4h}
	422	422	D_4
	$4mm$	$4mm$	C_{4v}
	$\bar{4}2m$	$\bar{4}2m$	$D_{2d}(V_d)$
	$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	D_{4h}
Trigonal	3	3	C_3
	$\bar{3}$	$\bar{3}$	$C_{3i}(S_6)$
	32	32	D_3
	$3m$	$3m$	C_{3v}
	$\bar{3}m$	$\bar{3}\frac{2}{m}$	D_{3d}
Hexagonal	6	6	C_6
	$\bar{6}$	$\bar{6}$	C_{3h}
	$6/m$	$\frac{6}{m}$	C_{6h}
	622	622	D_6
	$6mm$	$6mm$	C_{6v}
	$\bar{6}2m$	$\bar{6}2m$	D_{3h}
	$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}
Cubic	23	23	T
	$m\bar{3}$	$\frac{2}{m}\bar{3}$	T_h
	432	432	O
	$\bar{4}3m$	$\bar{4}3m$	T_d
	$m\bar{3}m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	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 $\alpha = \gamma = 90°$ c-unique setting $\alpha = \beta = 90°$	[010] ('unique axis b') [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

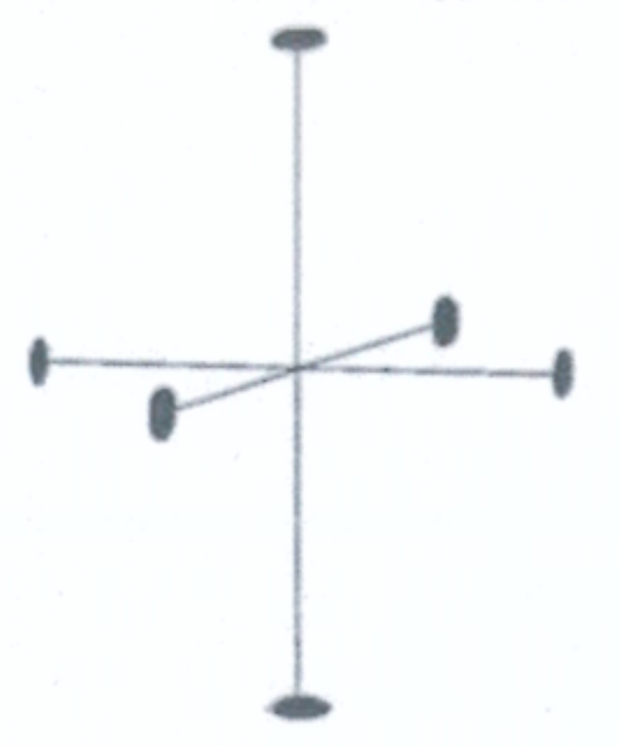
Crystal system	Crystallographic point groups†	Restrictions on cell parameters	primary	secondary	ternary
Trigonal	3, $\bar{3}$ 32, $3m$, $\bar{3}m$	$a = b$ $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$			
		$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell)	[111]	$\{[1\bar{1}0],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

Rotation Crystallographic Point Groups in 3D

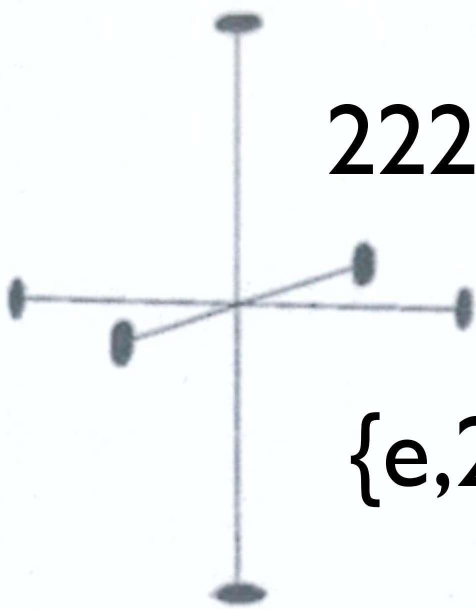
Cyclic: 1(C_1), 2(C_2), 3(C_3), 4(C_4), 6(C_6)

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

Cubic: 23 (T), 432 (O)

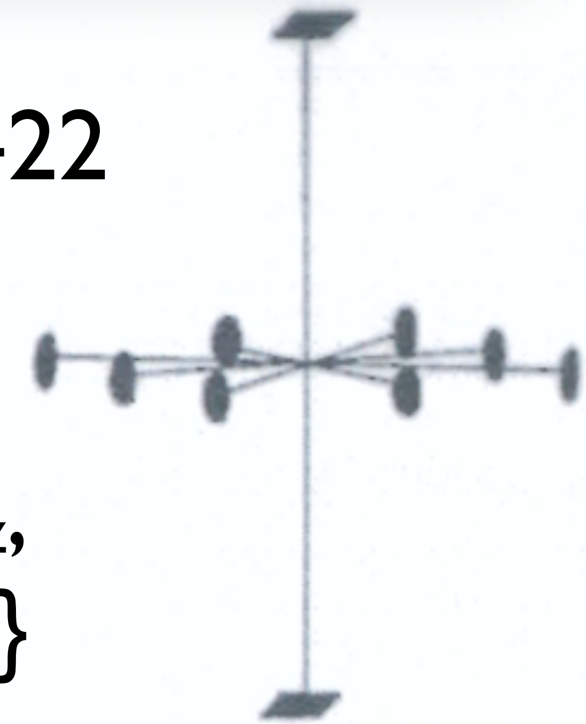


Dihedral Point Groups



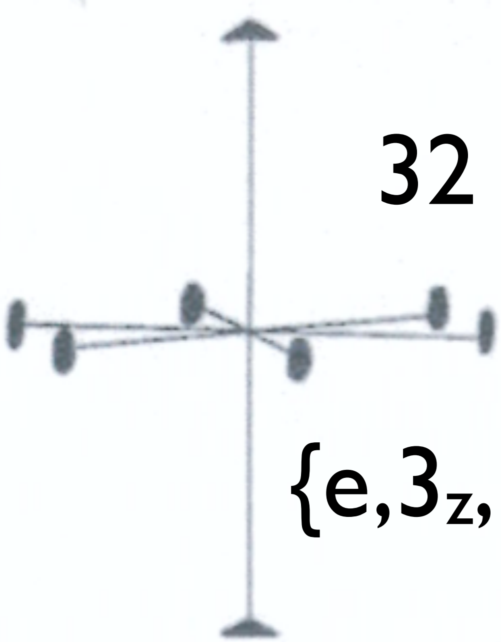
222

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



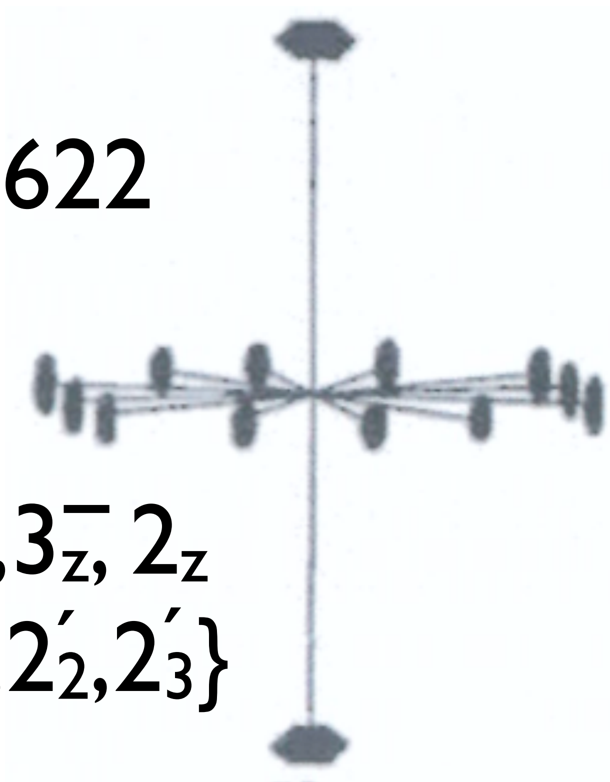
422

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



32

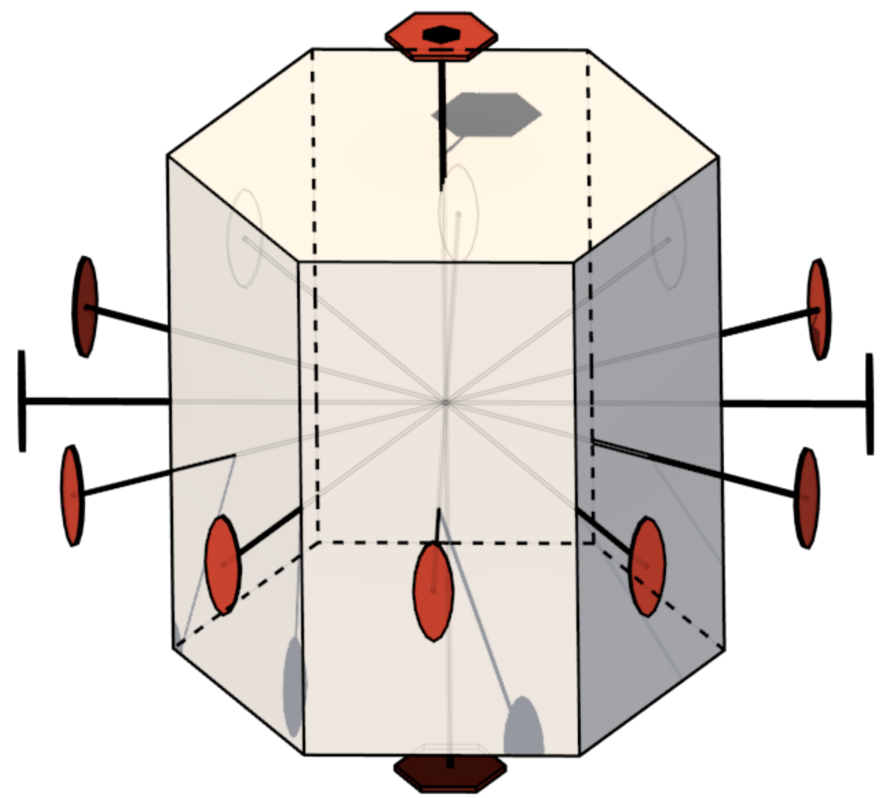
$\{e, 3_z, 3_{\bar{z}}, 2_1, 2_2, 2_3\}$



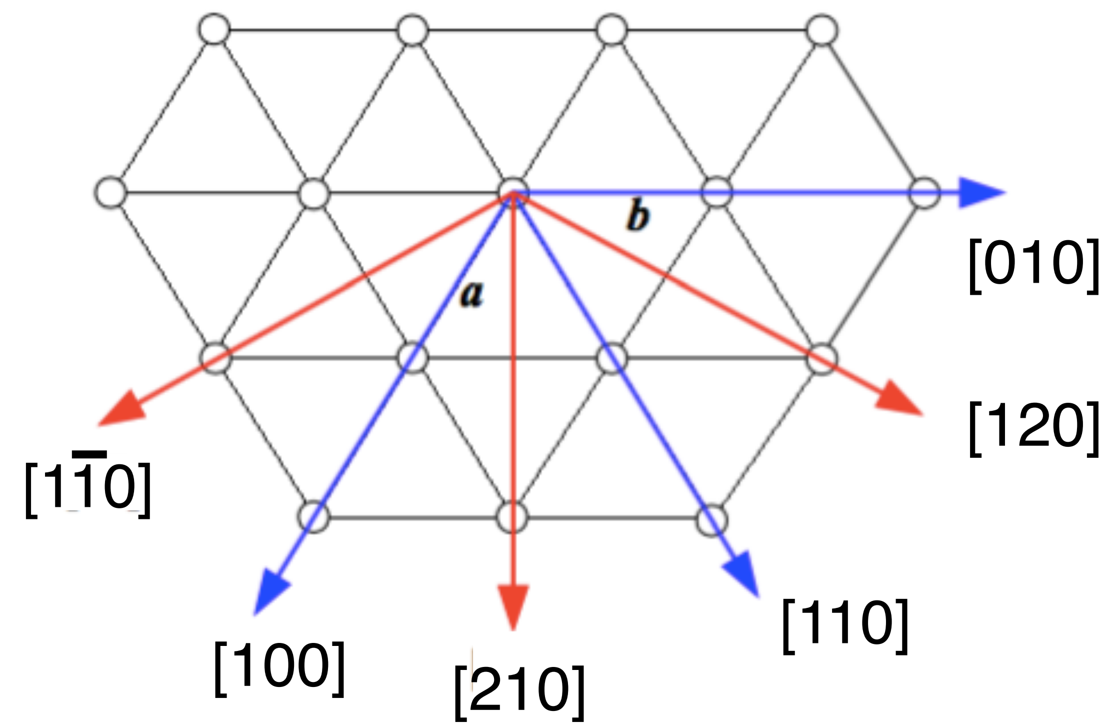
622

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

622 (D_6)



regular
hexagonal prism



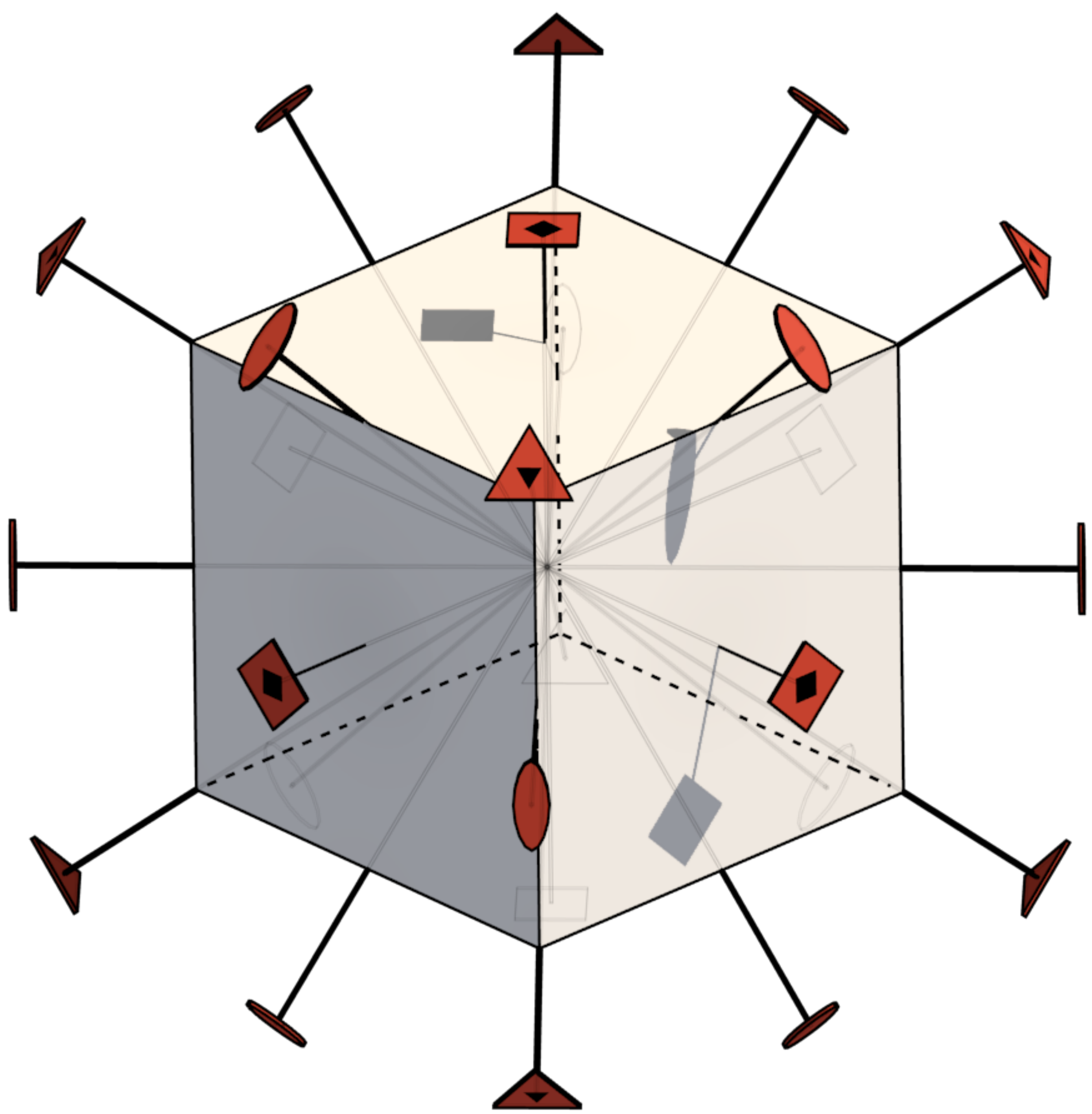
1

$6_{001}, 6_{\overline{001}}, 3_{001}, 3_{\overline{001}}, 2_{001}$

$2_{100}, 2_{010}, 2_{110},$
$2_{1\bar{1}0}, 2_{210}, 2_{120}$

Cubic Rotational Point Groups

432(O)



Cube

1

$4_{100}, \bar{4}_{100}, 4_{010}, \bar{4}_{010}, 4_{001}, \bar{4}_{001}$

$2_{100}, 2_{010}, 2_{001}$

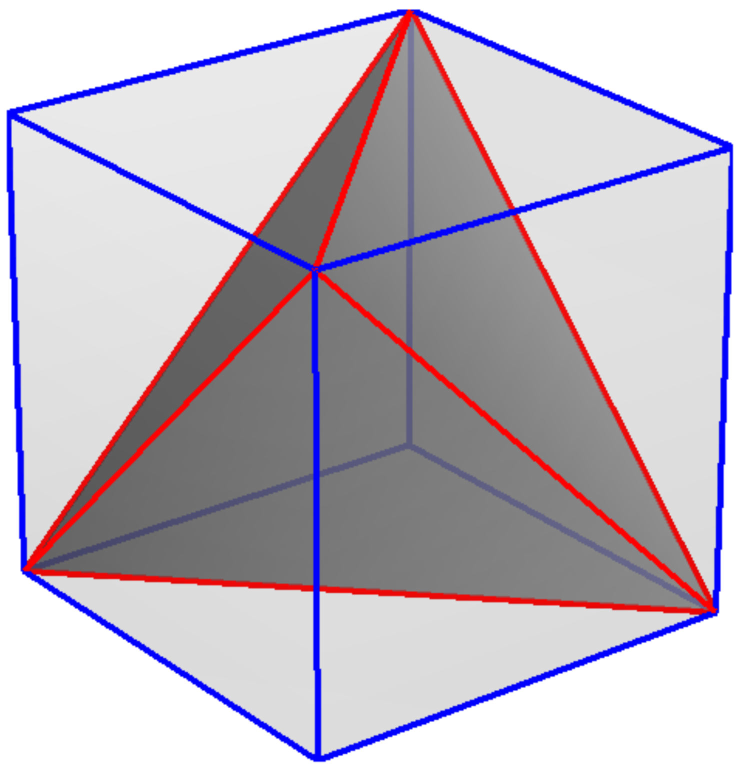
$3_{111}, \bar{3}_{111}, 3_{1\bar{1}\bar{1}}, \bar{3}_{1\bar{1}\bar{1}}$

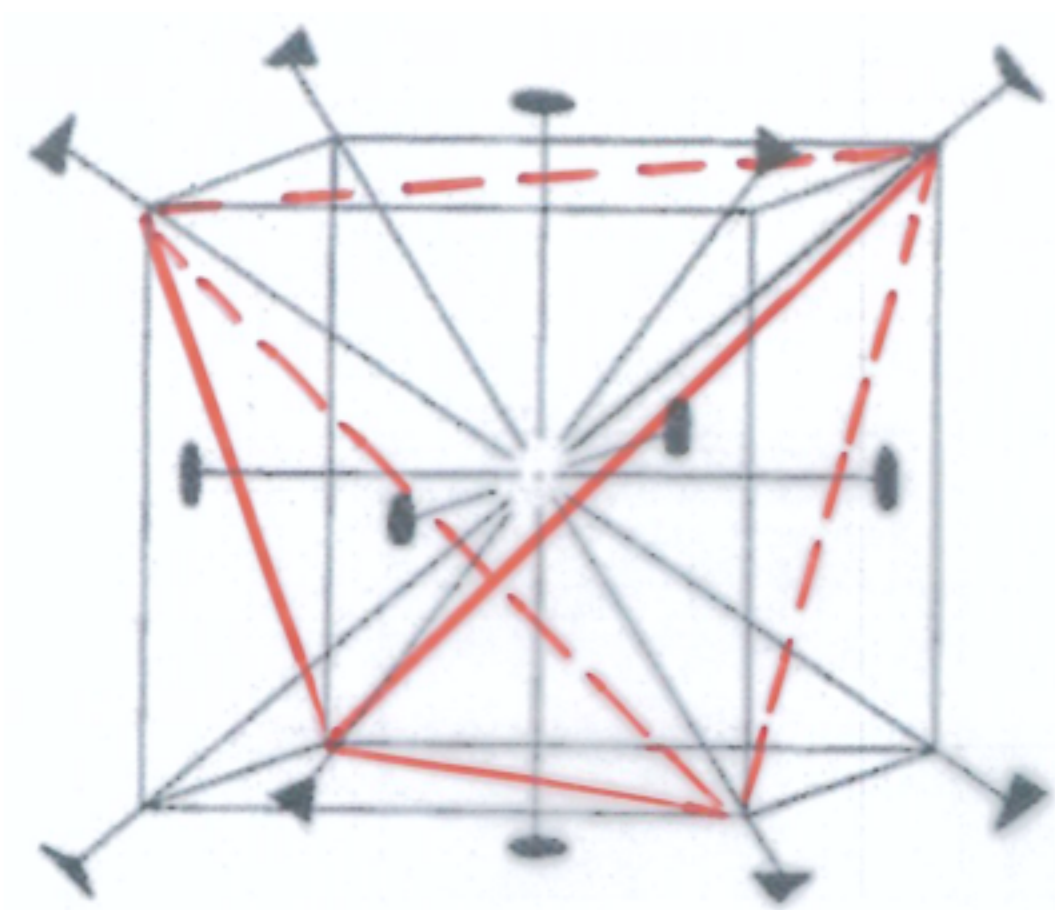
$3_{\bar{1}1\bar{1}}, \bar{3}_{\bar{1}1\bar{1}}, 3_{1\bar{1}\bar{1}}, \bar{3}_{1\bar{1}\bar{1}}$

$2_{1\bar{1}0}, 2_{110}, 2_{01\bar{1}}, 2_{011}, 2_{\bar{1}01}, 2_{101}$

23 (T)

Cubic Rotational Point Groups





regular tetrahedron

1

$2_{100}, 2_{010}, 2_{001}$

$3_{111}, \bar{3}_{111}, 3_{1\bar{1}\bar{1}}, \bar{3}_{1\bar{1}\bar{1}}$

$3_{\bar{1}1\bar{1}}, \bar{3}_{\bar{1}1\bar{1}}, 3_{1\bar{1}\bar{1}}, \bar{3}_{1\bar{1}\bar{1}}$

Centro-symmetrical groups

G_I: rotational groups $G_2=\{I,\bar{I}\}$ group of inversion

$G_I \otimes \{I,\bar{I}\}=G_I+\bar{I}.G_I$

2/m

$\{1,2_{001}\} \otimes \{I,\bar{I}\}=$

$\{1.1,\ 2_{001}.1,\ 1.\bar{1},\ 2_{001}.\bar{1}\}$

$\{1,2_{001},\bar{1},m_{001}=2/m\}$

mmm

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

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

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

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

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

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

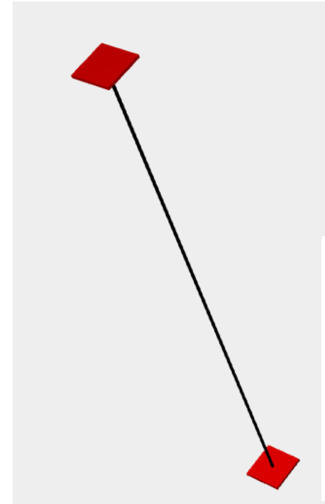
$G_1 \otimes G_2 = \{1.1,\ 2_{001}.1,\ 1.m_{100},\ 2_{001} m_{100} = m_{010}\}$

Crystallographic Point Groups

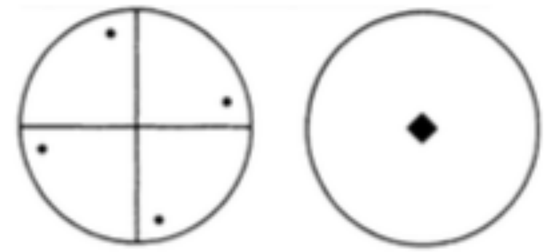
G	$G+\bar{1}G$	G(G')	$G'+\bar{1}(G-G')$
1 (C_1)	$1+\bar{1}.1=\bar{1}$ (C_i)	----	-----
2 (C_2)	$2+\bar{1}.2=2/m$ (C_{2h})	2(1)	m (C_s)
3 (C_3)	$3+\bar{1}.3=\bar{3}$ (C_{3i} or S_6)	----	----
4 (C_4)	$4+\bar{1}.4=4/m$ (C_{4h})	4(2)	$\bar{4}$ (S_4)
6 (C_6)	$6+\bar{1}.6=6/m$ (C_{6h})	6(3)	$\bar{6}$ (C_{3h})

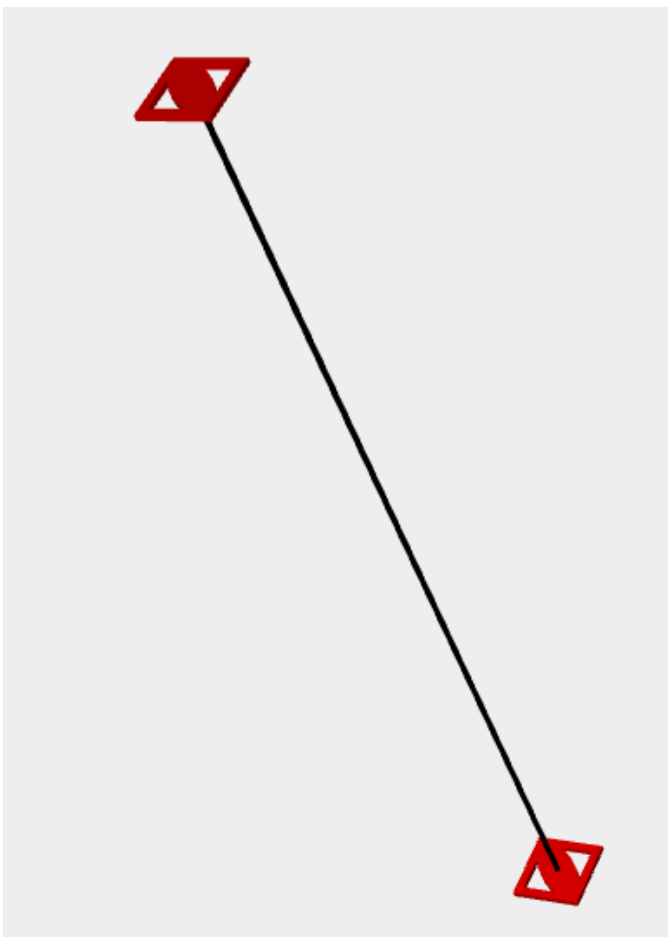
Problem 1.6.1.12

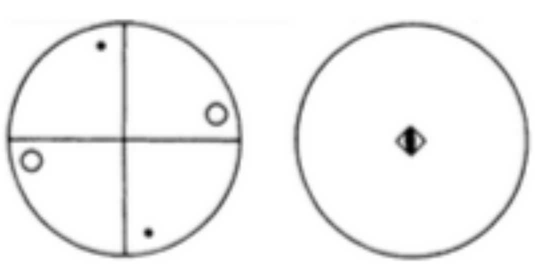
Shaw that the symmetry operations of the point groups $\bar{6}$ and 3/m are identical



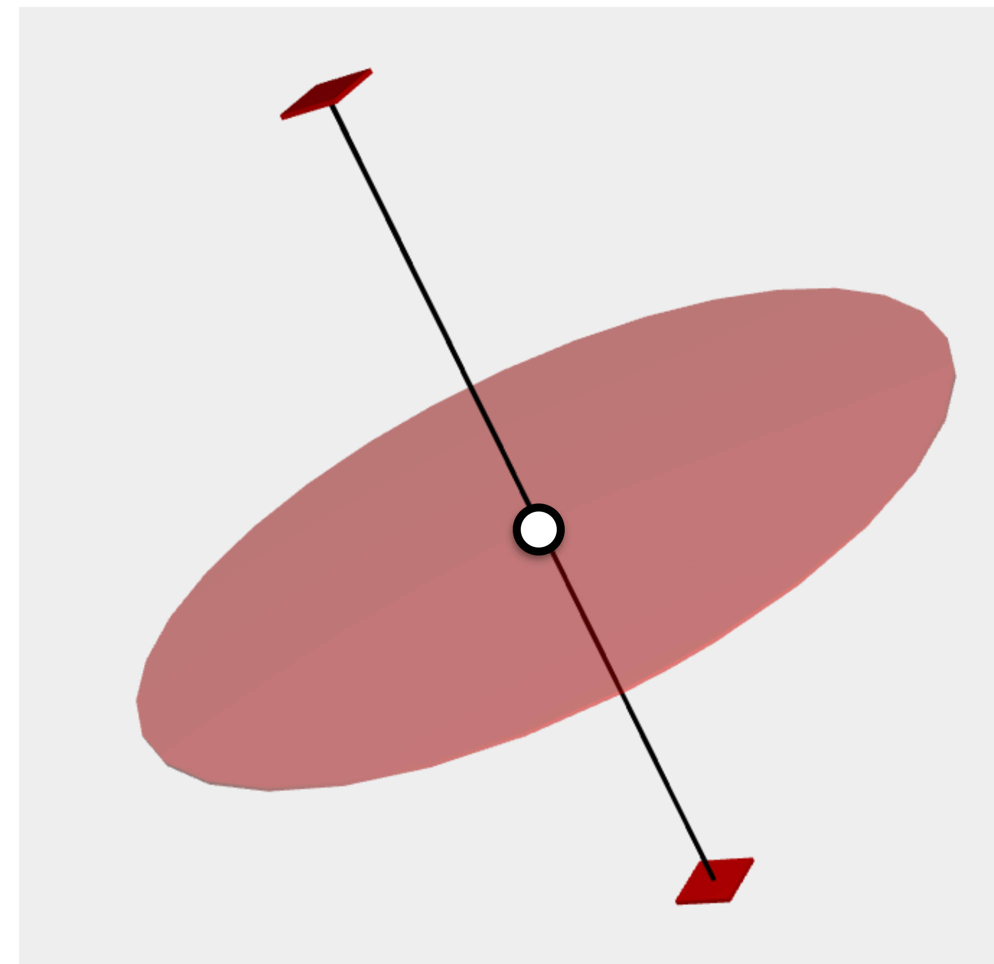
4 (C_4)

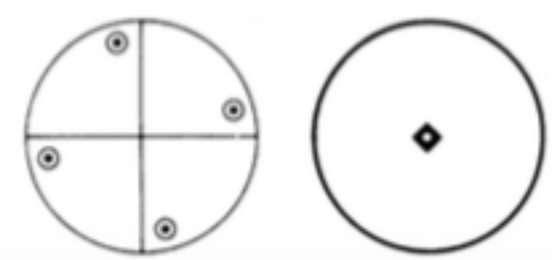






4(2) $\bar{4}$ (S_4)



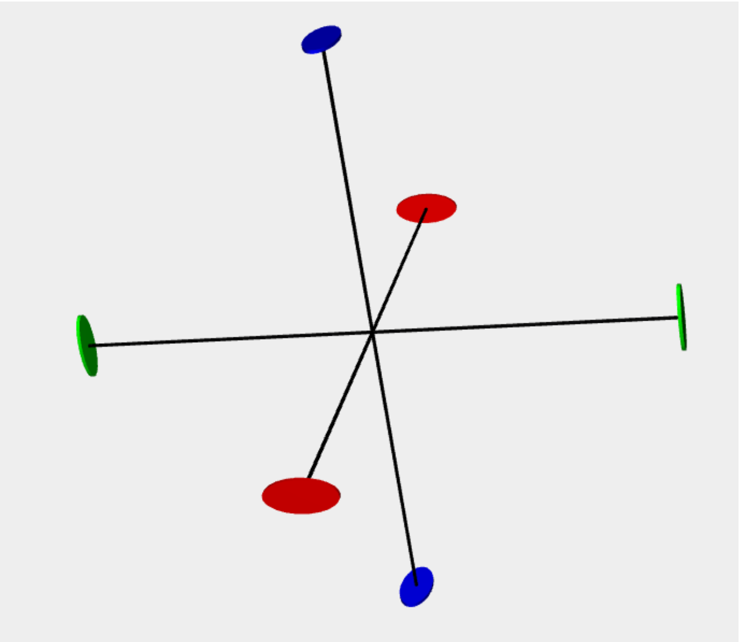


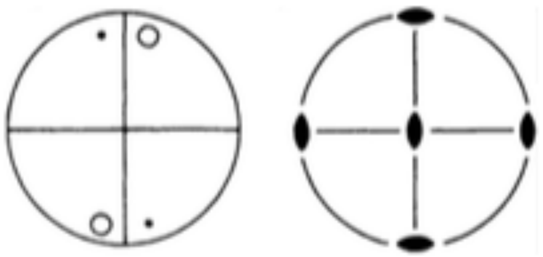
$4+\bar{1}.4=4/m$ (C_{4h})

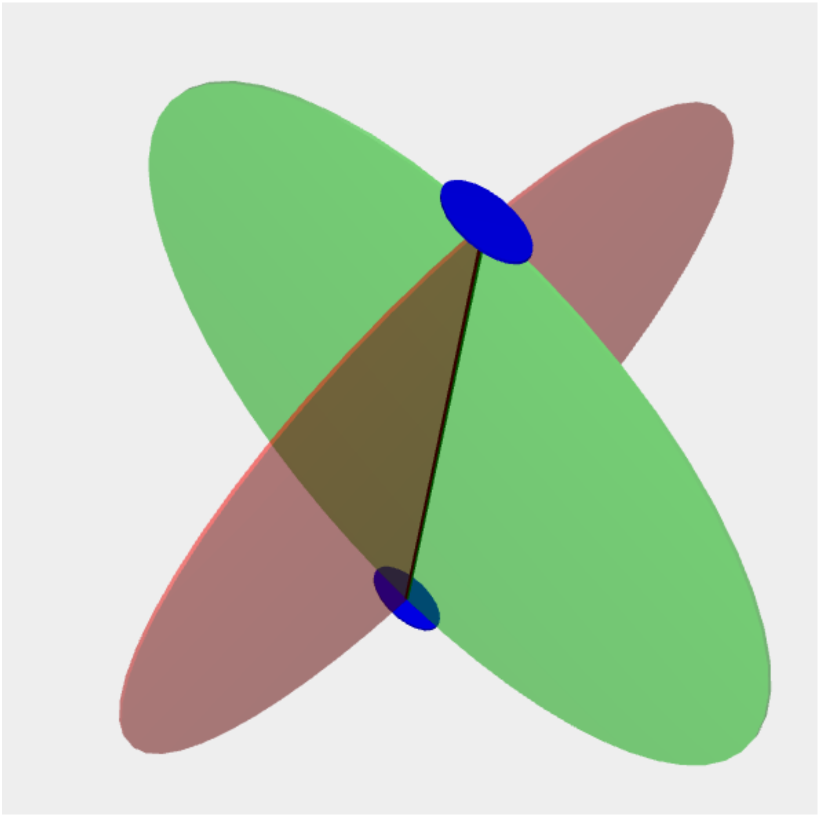
Crystallographic Point Groups

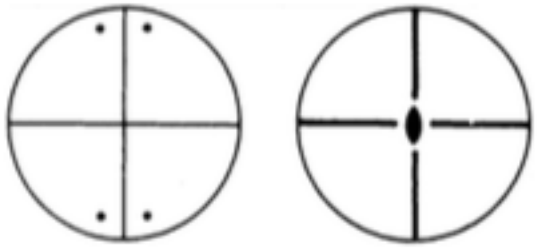
G	$G+\bar{1}G$	G(G')	$G'+\bar{1}(G-G')$
222 (D_2)	$222+\bar{1}.222=2/m2/m2/m$ mmm (D_{2h})	222(2)	2mm (C_{2v})
32 (D_3)	$32+\bar{1}.32=\bar{3}2/m$ $\bar{3}m$(D_{3d})	32(3)	3m (C_{3v})
422 (D_4)	$422+\bar{1}.422=4/m2/m2/m$ 4/mmm(D_{4h})	422(4) 422(222)	4mm (C_{4v}) $\bar{4}2m$ (D_{2d})
622 (D_6)	$622+\bar{1}.622=6/m2/m2/m$ 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)

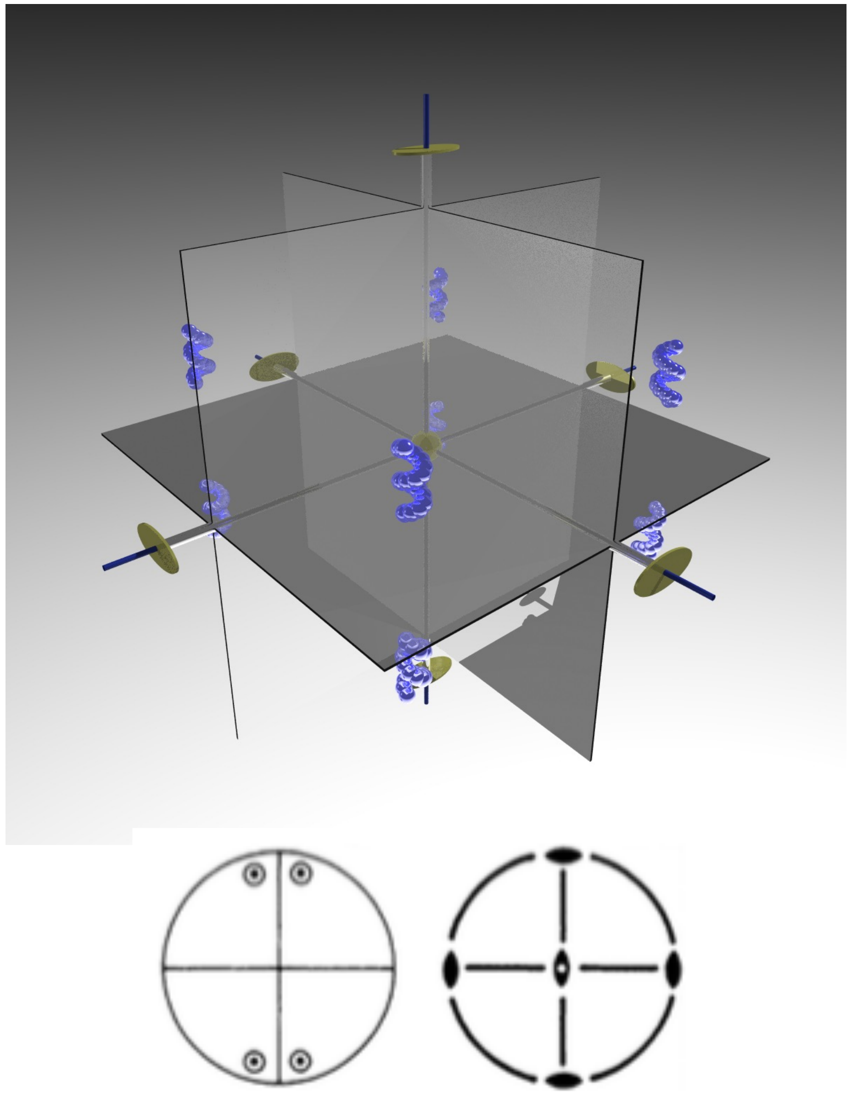
222 (D_2)











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

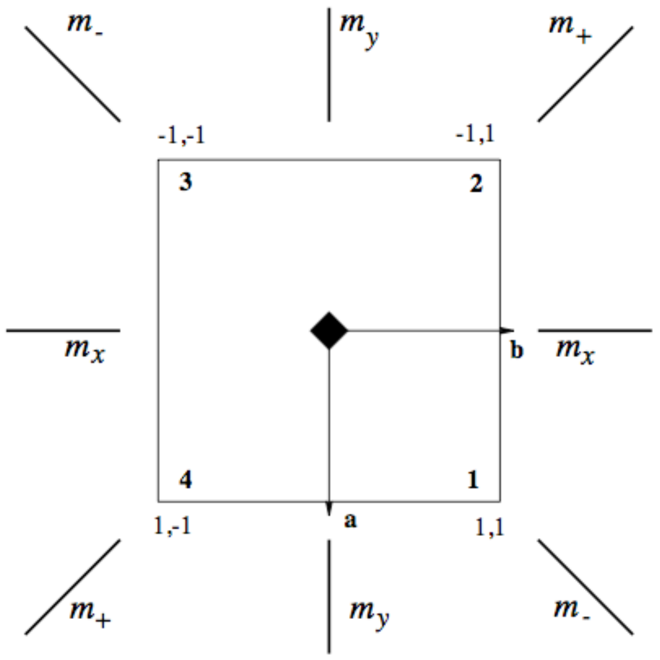
$222+\bar{1}.222=2/m2/m2/m$

mmm (D_{2h})

Crystallographic Point Groups

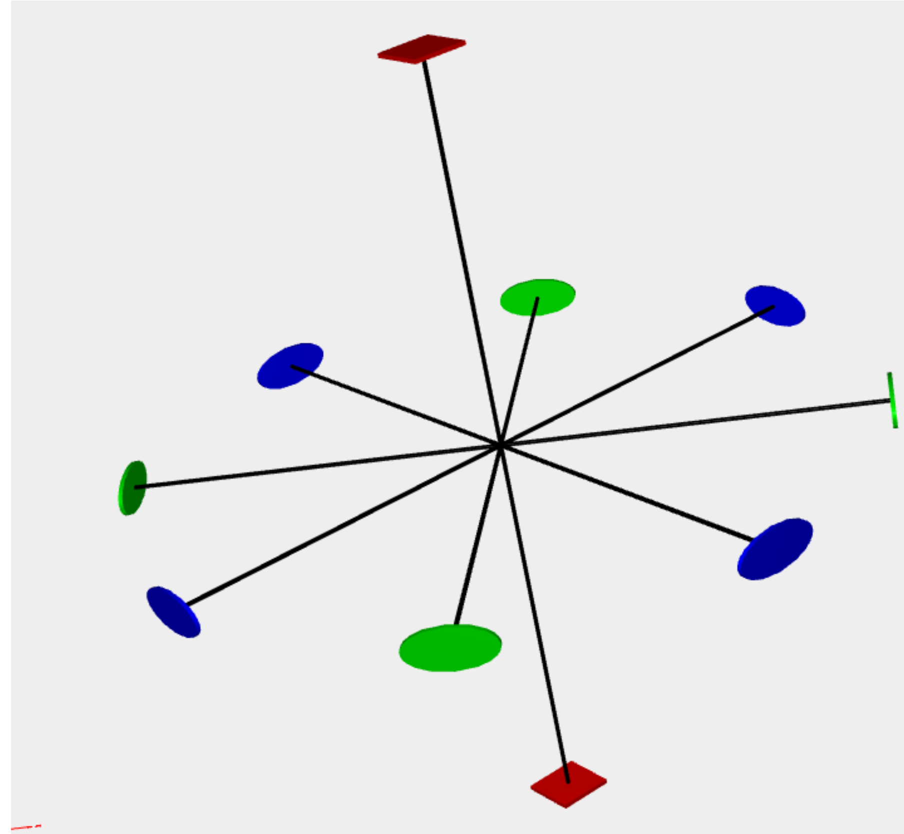
Groups isomorphic to 422

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	$2_+ 2_-$

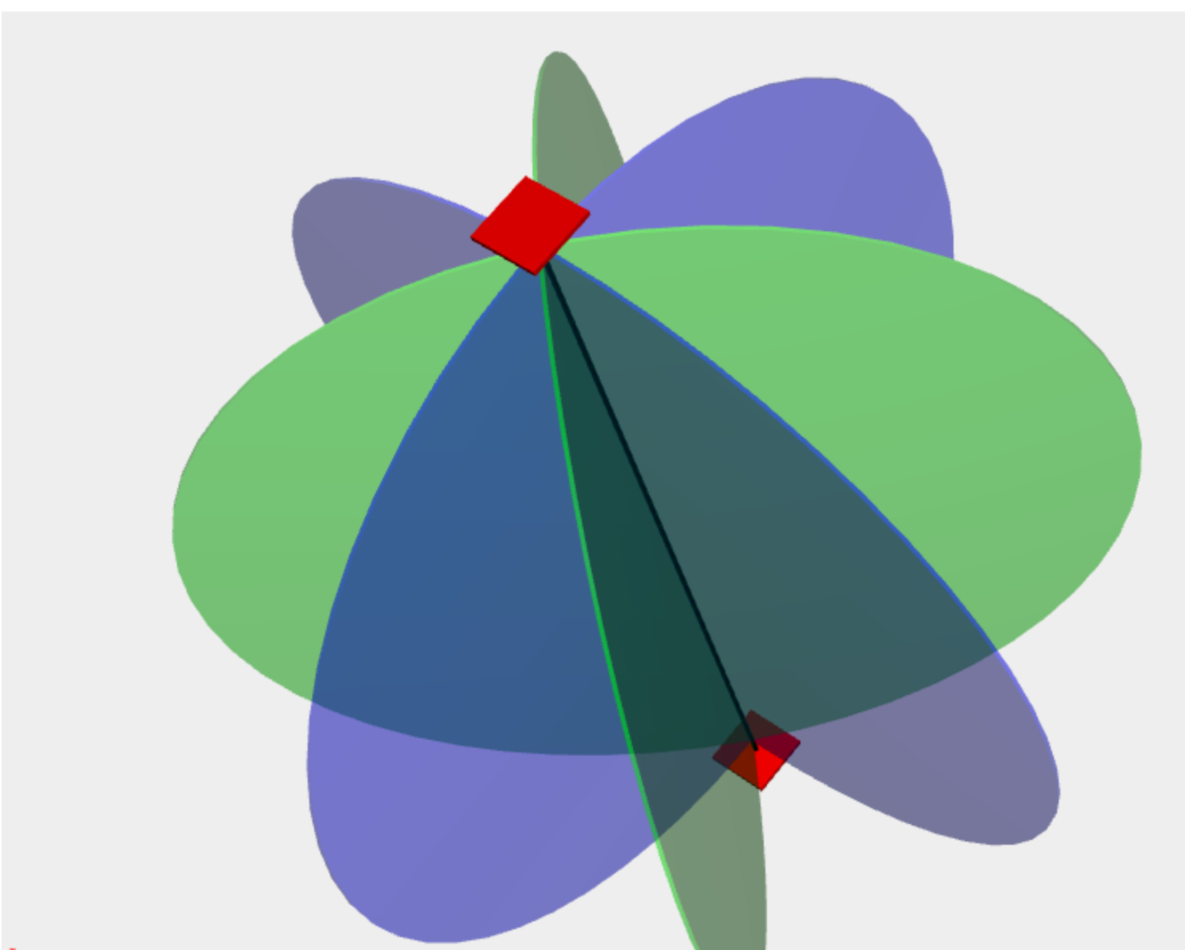


Groups isomorphic to 622

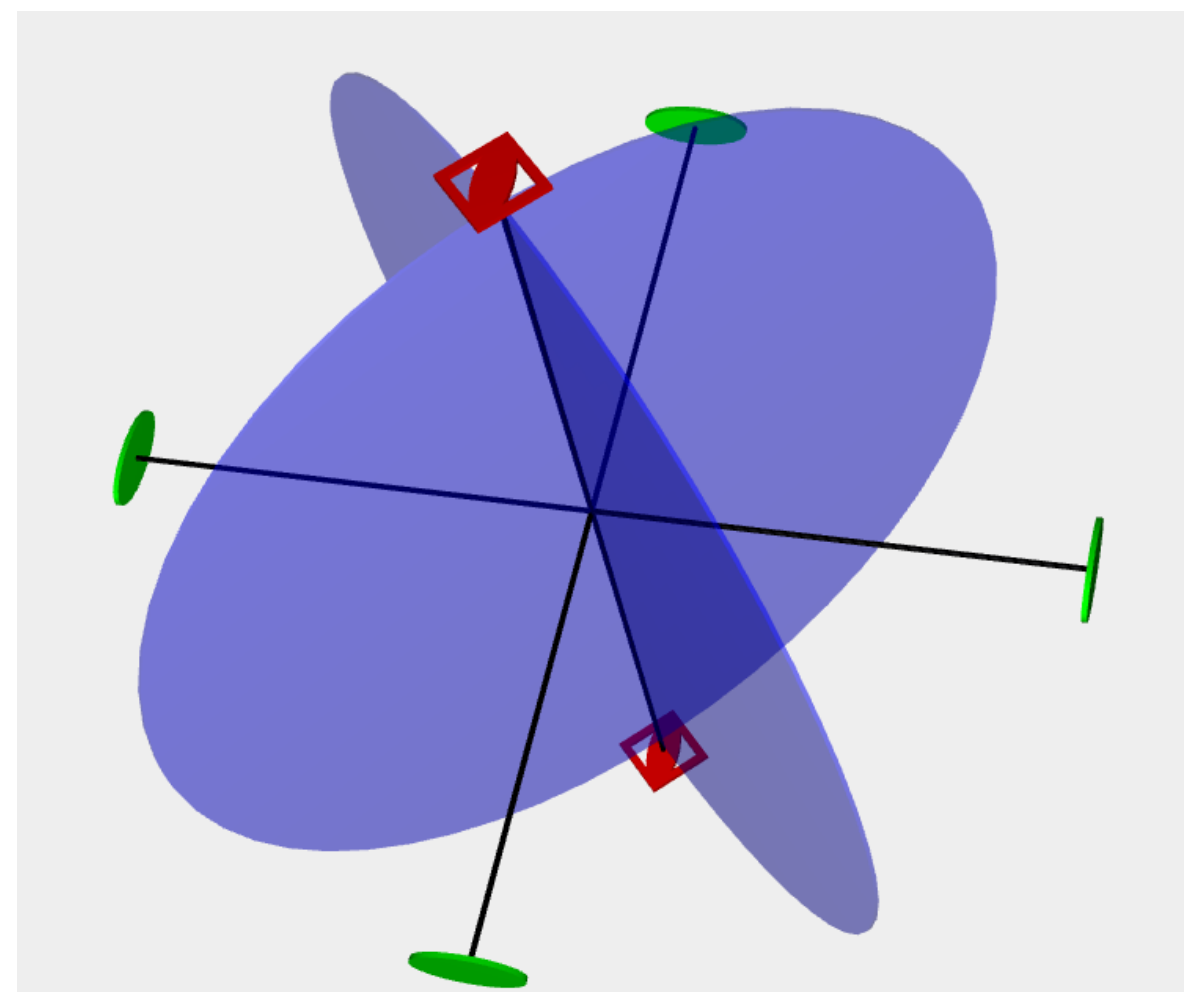
622	e	$6_z 6_z^{-}$	$3_z 3_z^{-}$	2_z	$2_1 2_2 2_3$	$2'_1 2'_2 2'_3$
6mm	e	$6_z 6_z^{-}$	$3_z 3_z^{-}$	2_z	$m_1 m_2 m_3$	$m'_1 m'_2 m'_3$
$\bar{6}$2m	e	$\bar{6}_z \bar{6}_z^{-}$	$3_z 3_z^{-}$	m_z	$2_1 2_2 2_3$	$m'_1 m'_2 m'_3$
$\bar{6}$m2	e	$\bar{6}_z \bar{6}_z^{-}$	$3_z 3_z^{-}$	m_z	$m_1 m_2 m_3$	$2'_1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



422 (D_4)



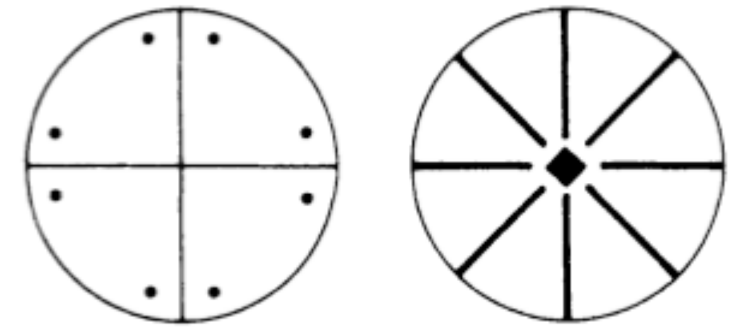
422(4) 4mm (C_{4v})



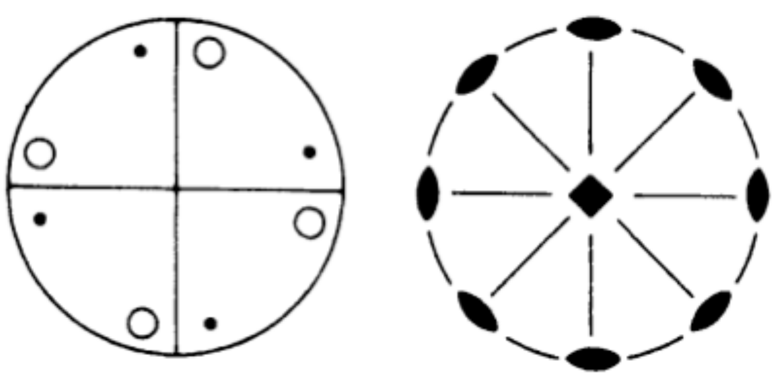
422(222) $\bar{4}2m$ (D_{2d})

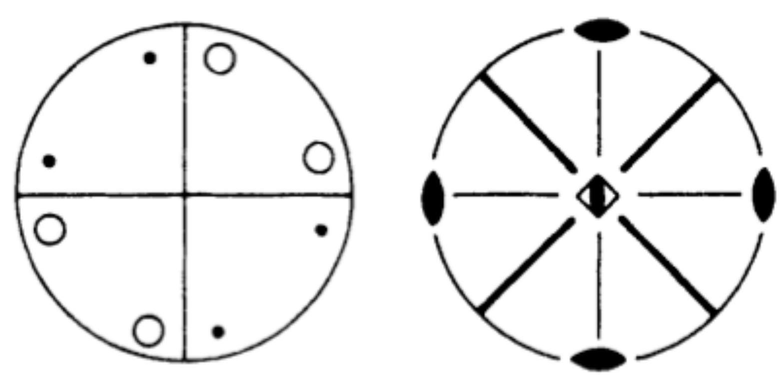
Problem 1.6.1.13

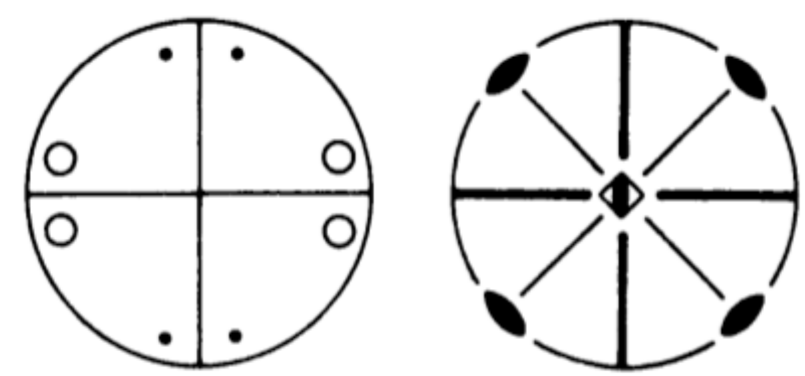
4mm



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***.

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

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

Step 1:

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

Step 2:

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

Step 3:

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

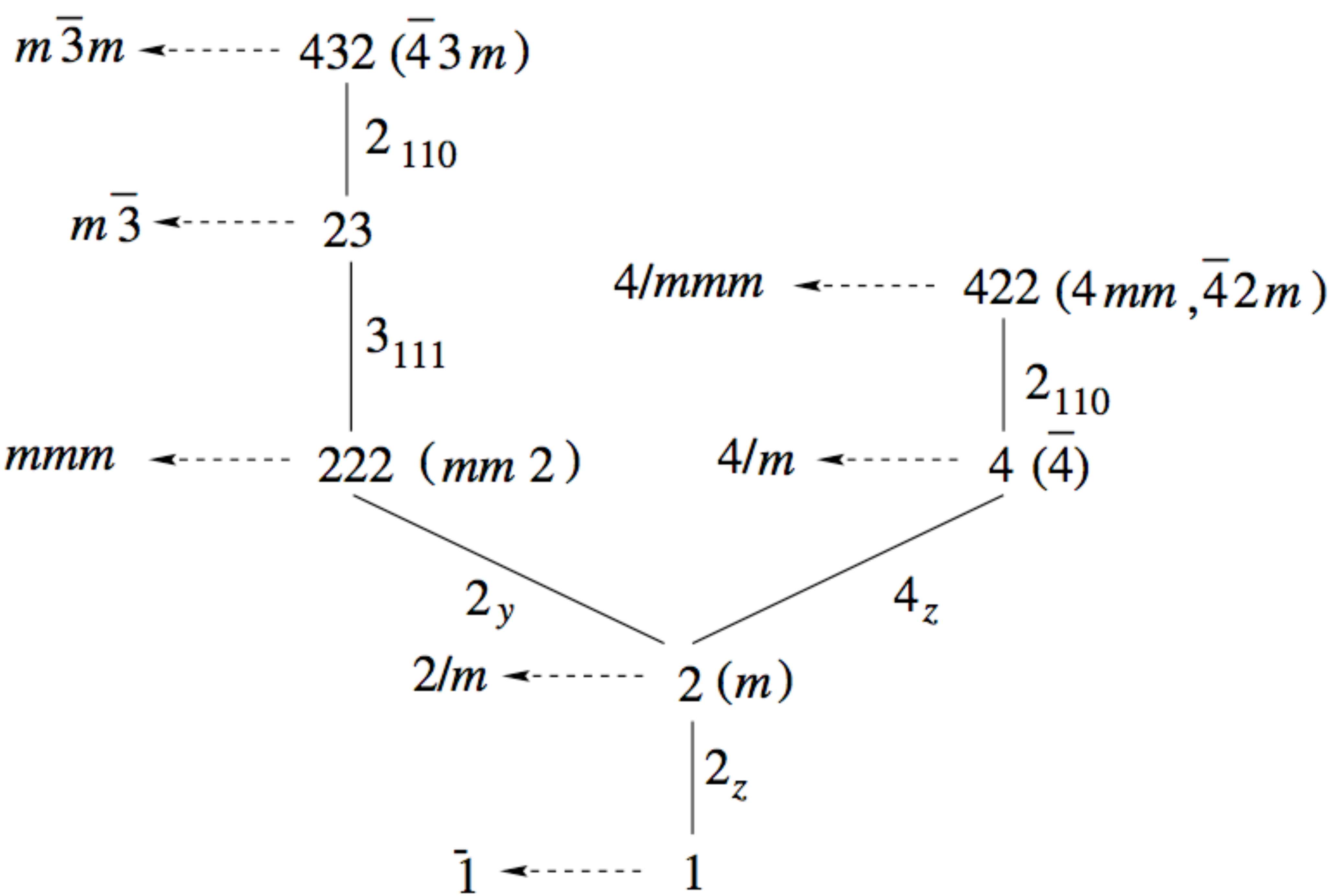
Step 4:

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

	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 $4mm$

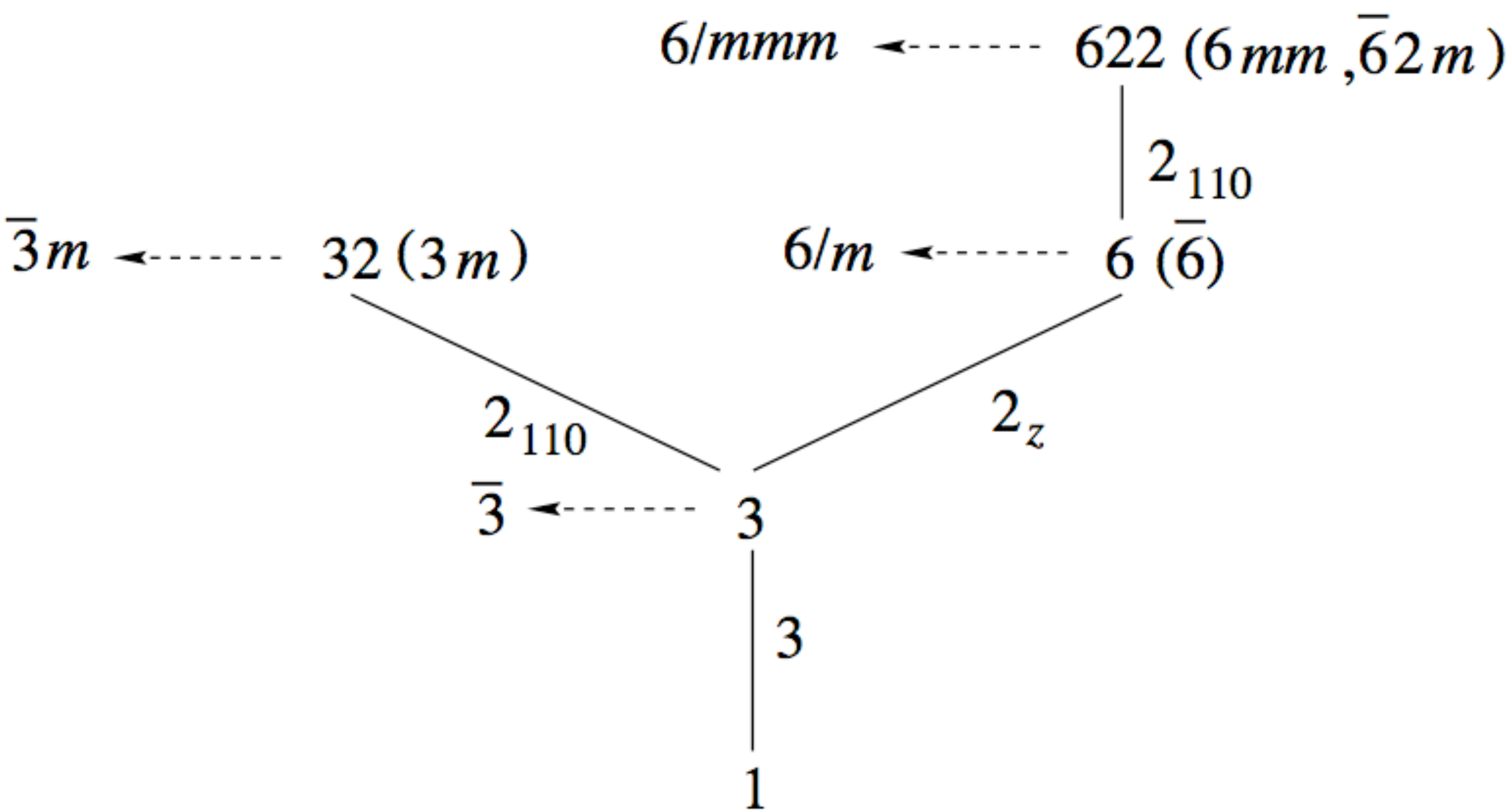
Generation of sub-cubic point groups



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 1.6.1.16

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.