



Българско Кристалографско Дружество
Bulgarian Crystallographic Society

Основано 2009

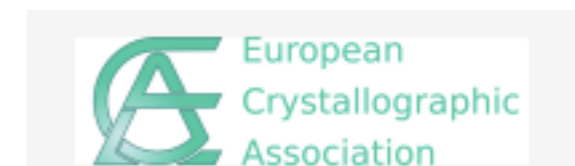


***IUCr Commission on Mathematical and
Theoretical Crystallography***



INTERNATIONAL AUTUMN SCHOOL ON FUNDAMENTAL AND ELECTRON CRYSTALLOGRAPHY

8-13 October 2017, Sofia, Bulgaria



I. CRYSTALLOGRAPHIC POINT GROUPS (brief revision)

GROUP THEORY (few basic facts)

I. Crystallographic symmetry operations

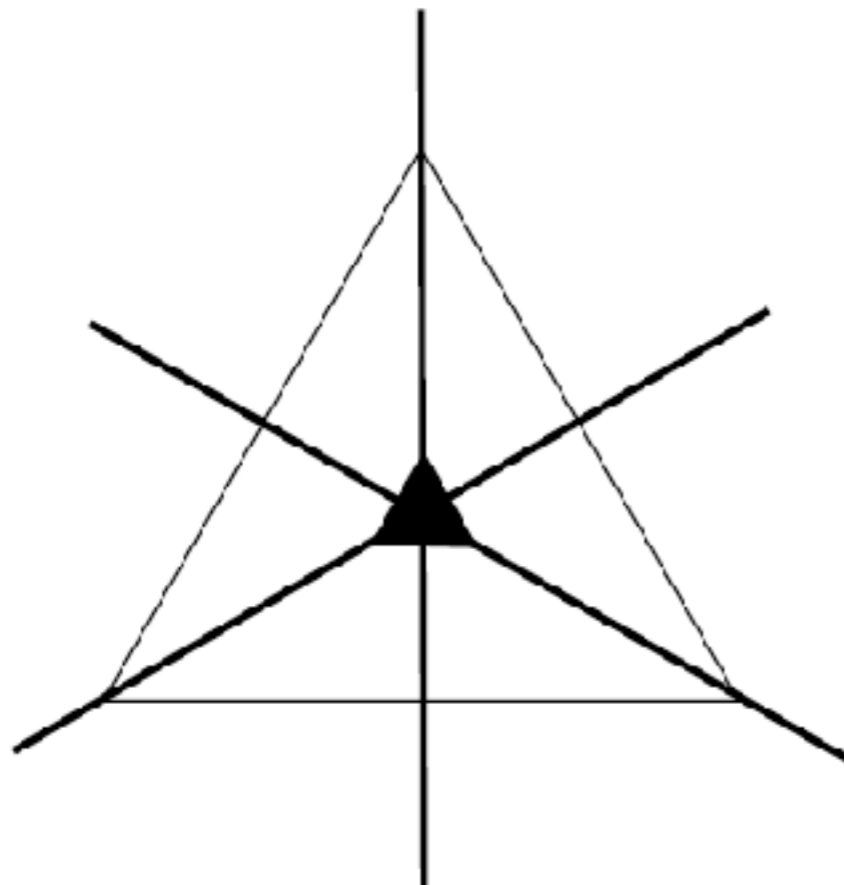
Symmetry operations of an object

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*.

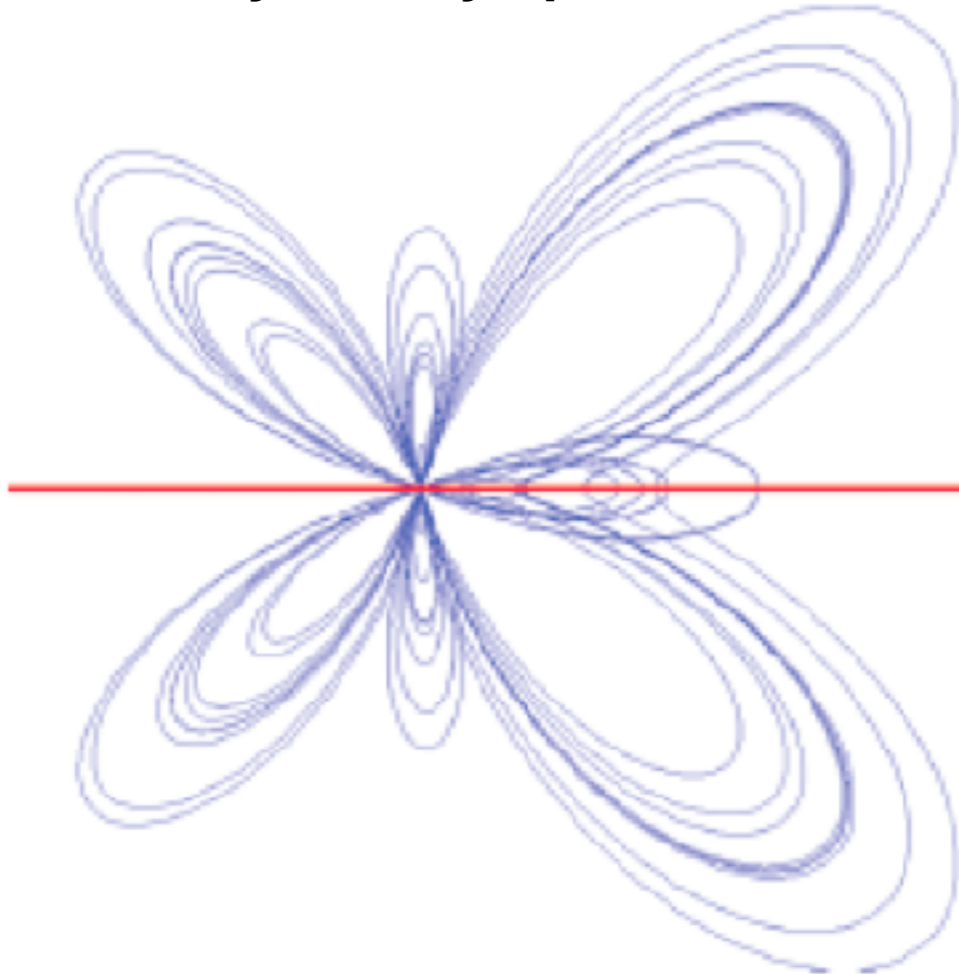


The equilateral triangle allows six symmetry operations: rotations by 120 and 240 around its centre, reflections through the three thick lines intersecting the centre, and the identity operation.

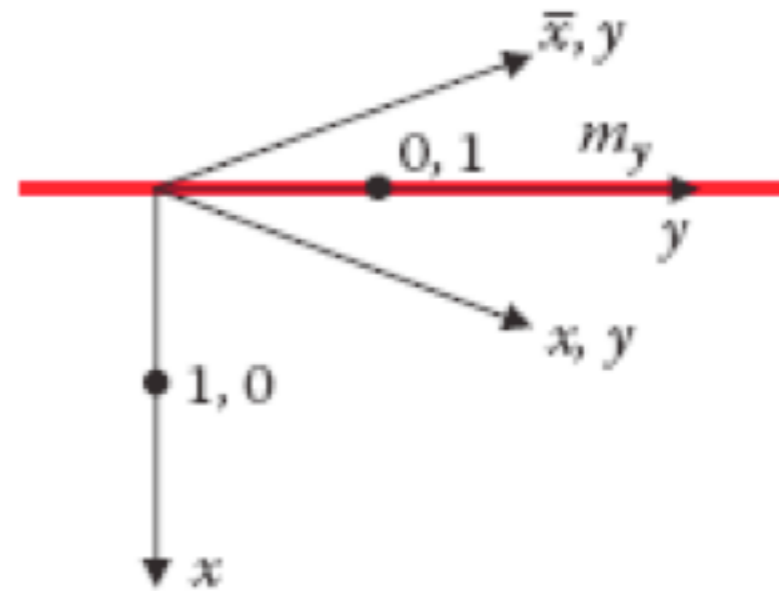
Symmetry operations in the plane

Matrix representations

Mirror symmetry operation



Mirror line m_y at $0, y$



Matrix representation

$$m_y \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -x \\ y \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\det \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = ? \quad \text{tr} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = ?$$

Fixed points

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

drawing: M.M. Julian
Foundations of Crystallography
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2. Group axioms

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

DEFINITION. A **group** is a set $G = \{e, g_1, g_2, g_3 \dots\}$ 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:**

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

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

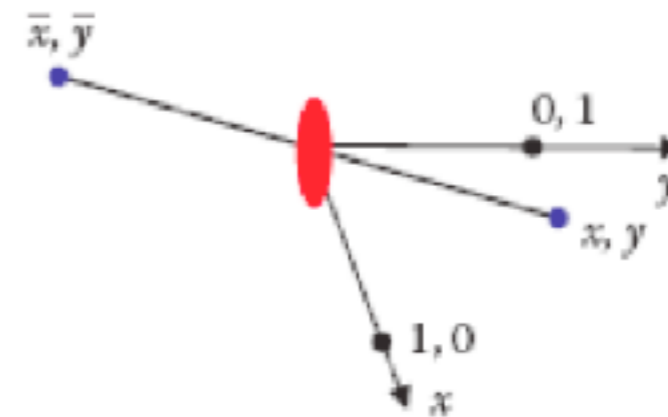
a set of elements such that each element of the group can be obtained as a product of the generators

Crystallographic Point Groups in 2D

Motif with
symmetry of **2**



Where is the two-fold
point?



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

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

$$\text{tr} \begin{bmatrix} -1 & \\ & -1 \end{bmatrix} = ?$$

Crystallographic Point Groups in 2D

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

Motif with
symmetry of **2**



-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**?

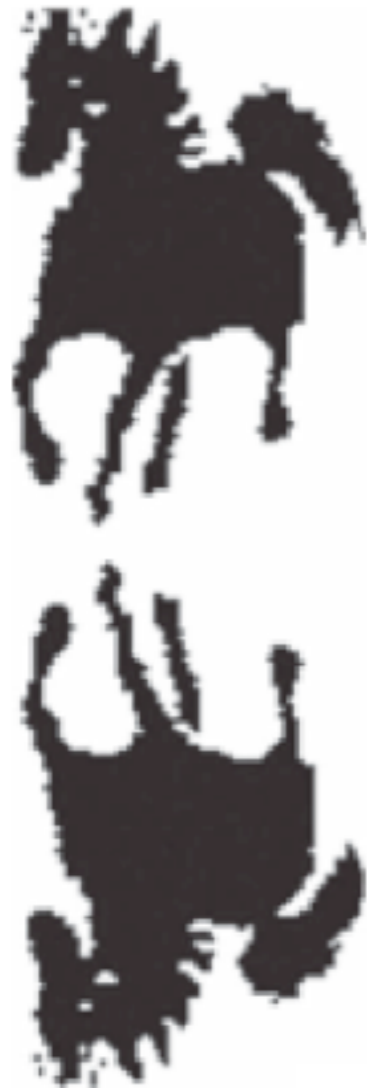
-multiplication table

	×	1	2
1		1	2
2		2	1

-generators of **2**?

Crystallographic symmetry operations in the plane

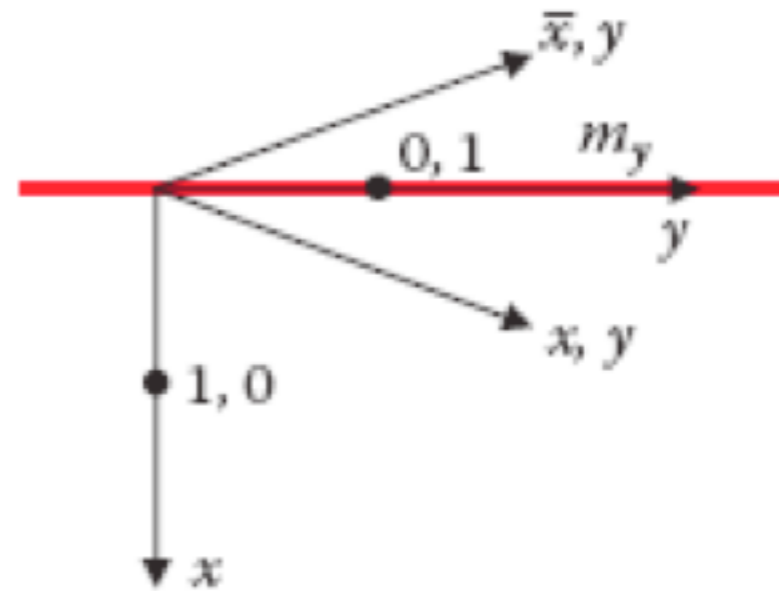
Mirror symmetry operation



Where is the mirror line?

drawing: M.M. Julian
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Mirror line m_y at $0, y$



Matrix representation

$$m_y \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -x \\ y \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\det \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = ? \quad \text{tr} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = ?$$

Crystallographic Point Groups in 2D

Point group $m = \{1, m\}$

Motif with symmetry of m



-group axioms?

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

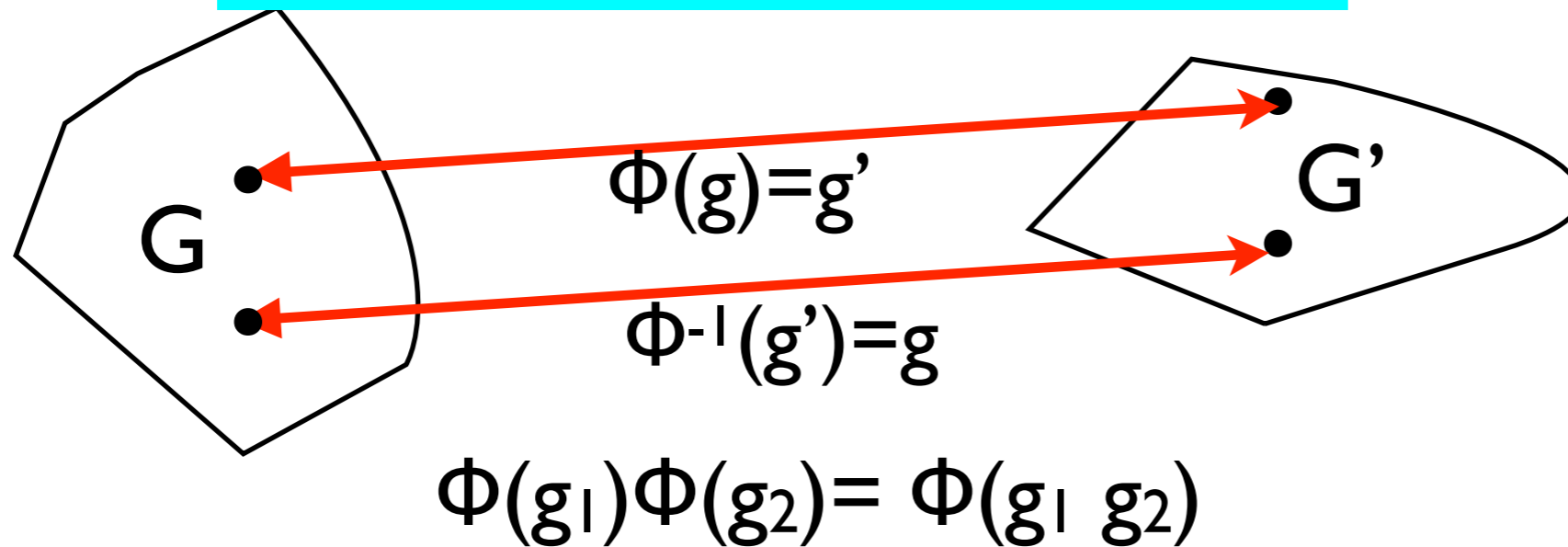
-order of m ?

-multiplication table

\times	1	m_y
1	1	m_y
m_y	m_y	1

-generators of m ?

Isomorphic groups



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

\times	1	2
1	1	2
2	2	1

Point group $\mathbf{m} = \{1, m\}$

\times	1	m_y
1	1	m_y
m_y	m_y	1

-groups with the same multiplication table

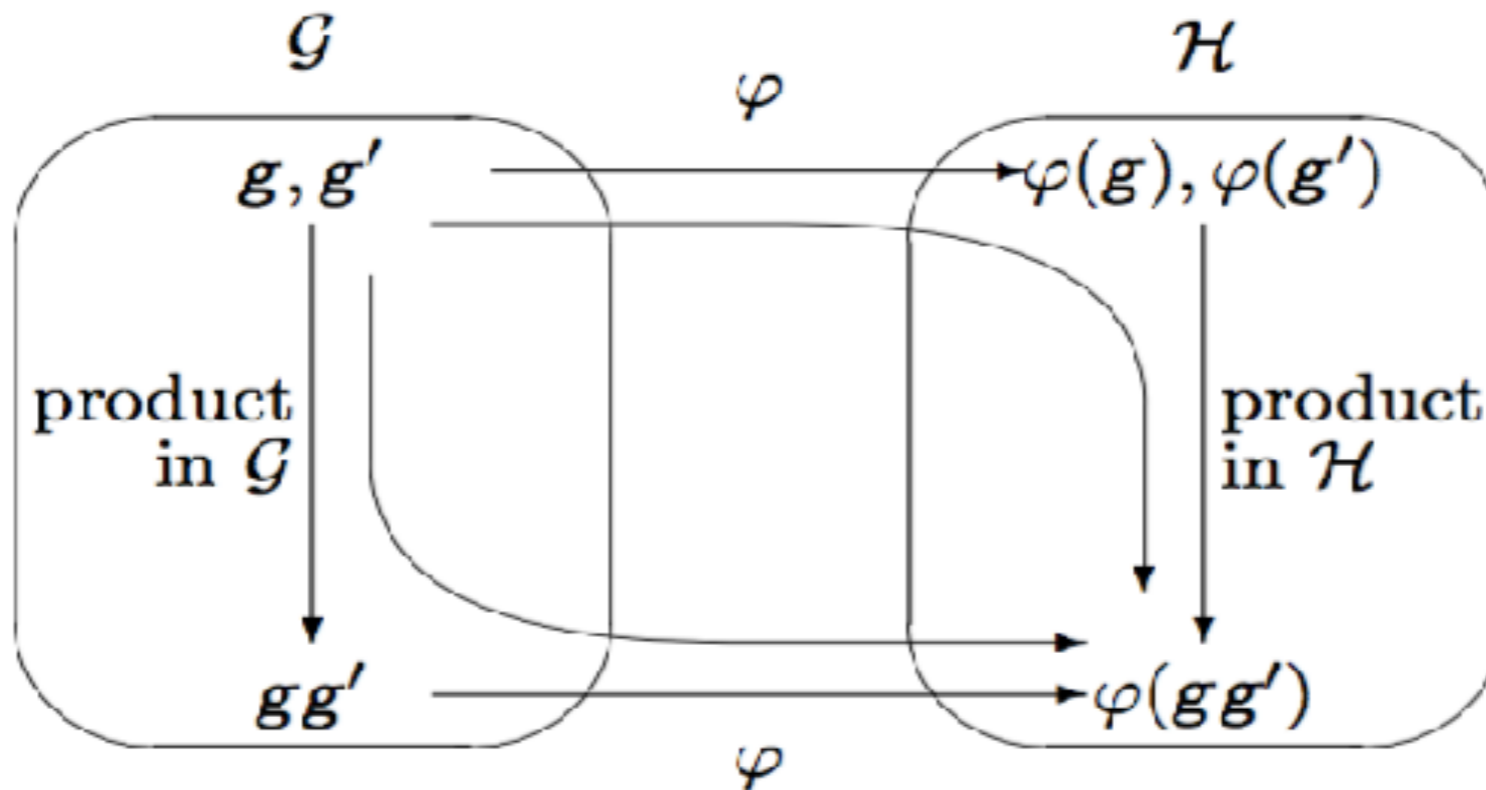
Homomorphism

mapping

$$G = \{g\} \xrightarrow{\varphi(g)=h} H = \{h\}$$

homomorphic
condition

$$\varphi(gg') = \varphi(g)\varphi(g') \text{ for all } g, g' \in G.$$



Crystallographic Point Groups in 2D

Point group **1** = {1}

Motif with
symmetry of **1**



drawing: M.M. Julian
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-group axioms?

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

-order of **1**?

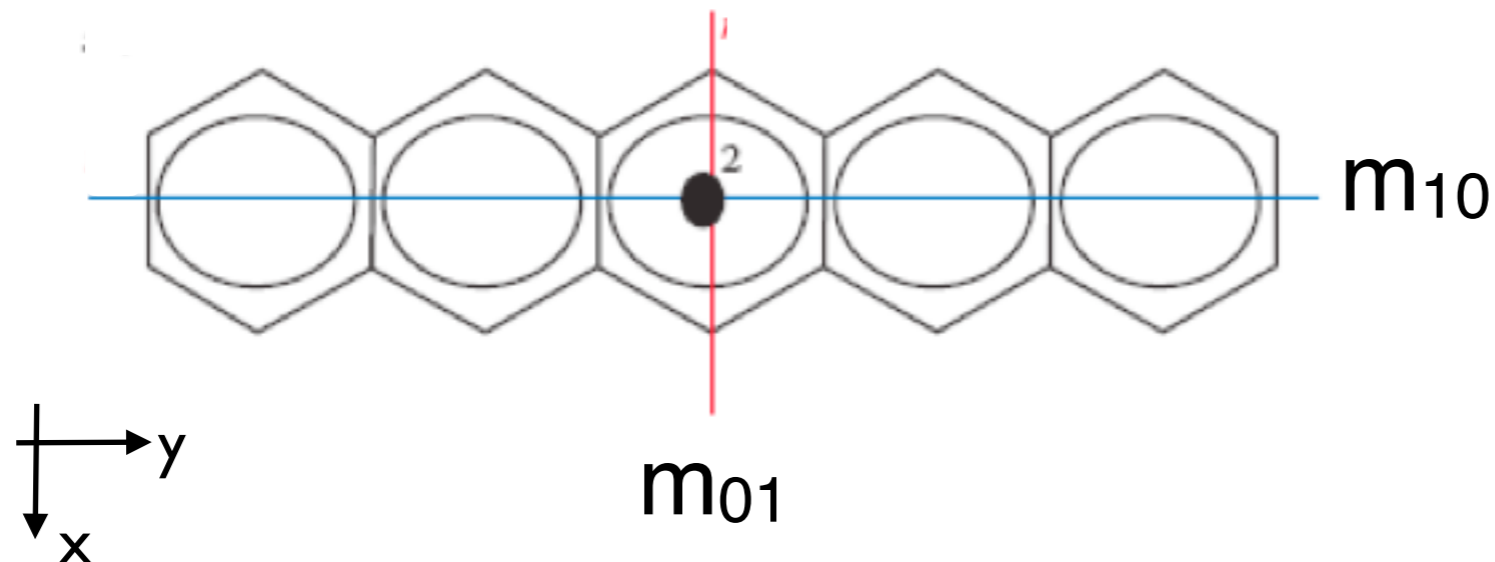
-multiplication table

	x		1
1			1

-generators of **1**?

Problem 2.2.1

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

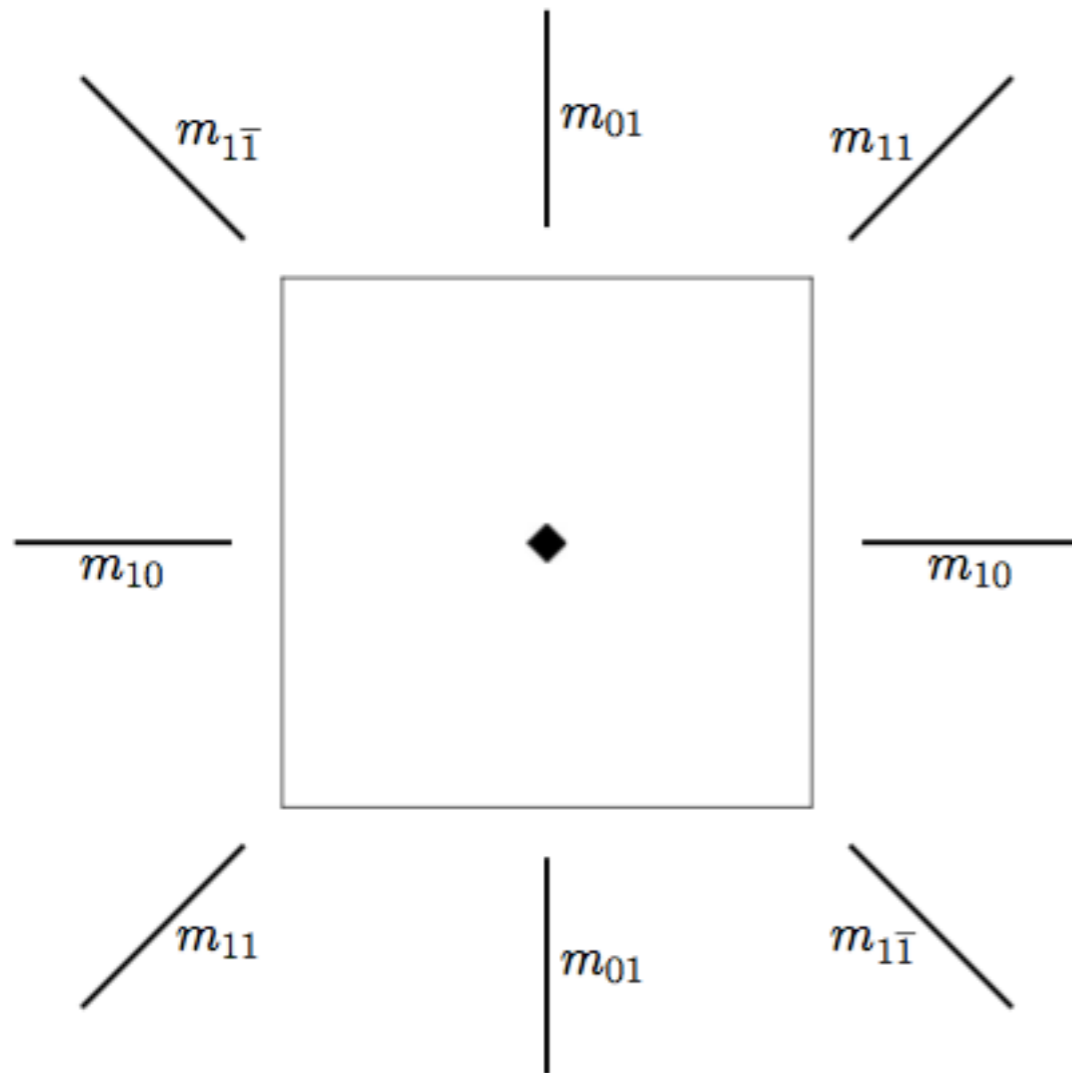


Determine:

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

Problem 2.2.2

Consider the symmetry group of the square. Determine:



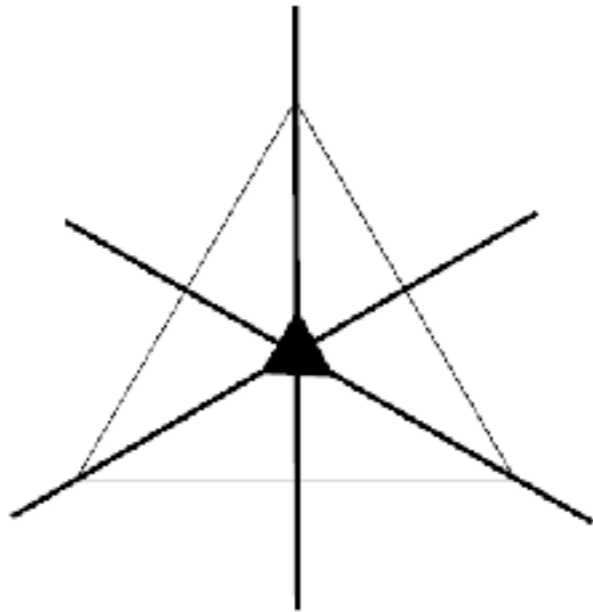
symmetry operations:
matrix and (x,y)
presentation

generators

multiplication table

Problem 2.2.3 (additional)

Consider the symmetry group of the equilateral triangle. Determine:



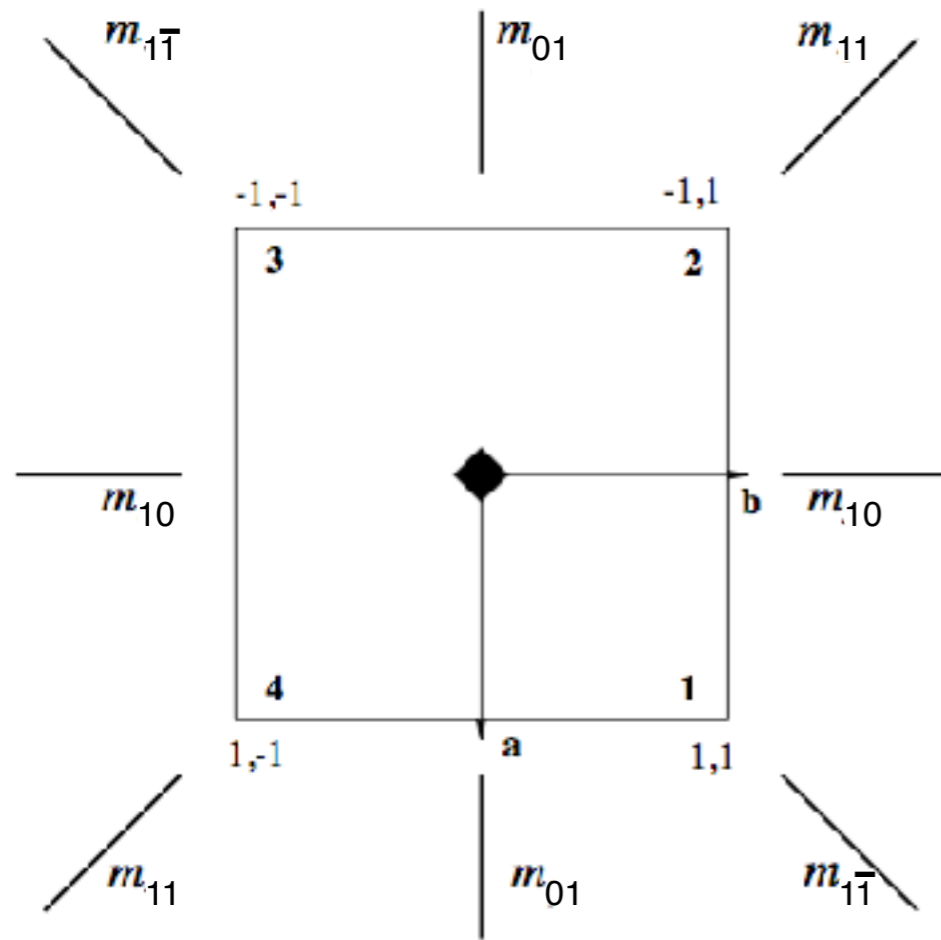
-symmetry operations:
matrix and (x,y)
presentation

-general-position and symmetry-
elements stereographic
projection diagrams;

-generators

-multiplication table

Conjugate elements



4mm

4^+
 $m_{10} \sim m_{01}$
 $m_{11} \sim ?$

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

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

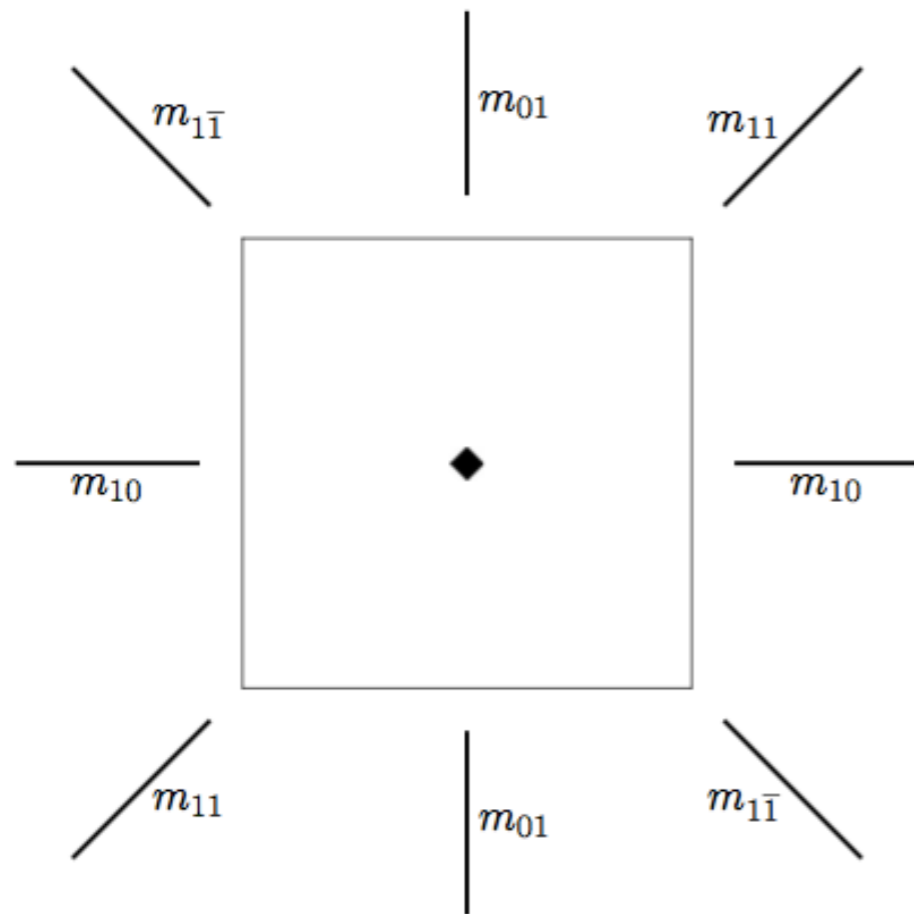
Conjugation-properties

- (i) $L(g_i) \cap L(g_j) = \{\emptyset\}$, 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 $(g_i)^k = (g_j)^k = e$

Example (Problem 2.2.2):

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 ₁₁ ⁻
1	1	2	4 ⁺	4 ⁻	m ₁₀	m ₀₁	m ₁₁	m ₁₁ ⁻
2	2	1	4 ⁻	4 ⁺	m ₀₁	m ₁₀	m ₁₁ ⁻	m ₁₁
4 ⁺	4 ⁺	4 ⁻	2	1	m ₁₁	m ₁₁ ⁻	m ₀₁	m ₁₀
4 ⁻	4 ⁻	4 ⁺	1	2	m ₁₁ ⁻	m ₁₁	m ₁₀	m ₀₁
m ₁₀	m ₁₀	m ₀₁	m ₁₁ ⁻	m ₁₁	1	2	4 ⁻	4 ⁺
m ₀₁	m ₀₁	m ₁₀	m ₁₁	m ₁₁ ⁻	2	1	4 ⁺	4 ⁻
m ₁₁	m ₁₁	m ₁₁ ⁻	m ₁₀	m ₀₁	4 ⁺	4 ⁻	1	2
m ₁₁ ⁻	m ₁₁ ⁻	m ₁₁	m ₀₁	m ₁₀	4 ⁻	4 ⁺	2	1

EXERCISES

Problem 2.2.1 (cont)

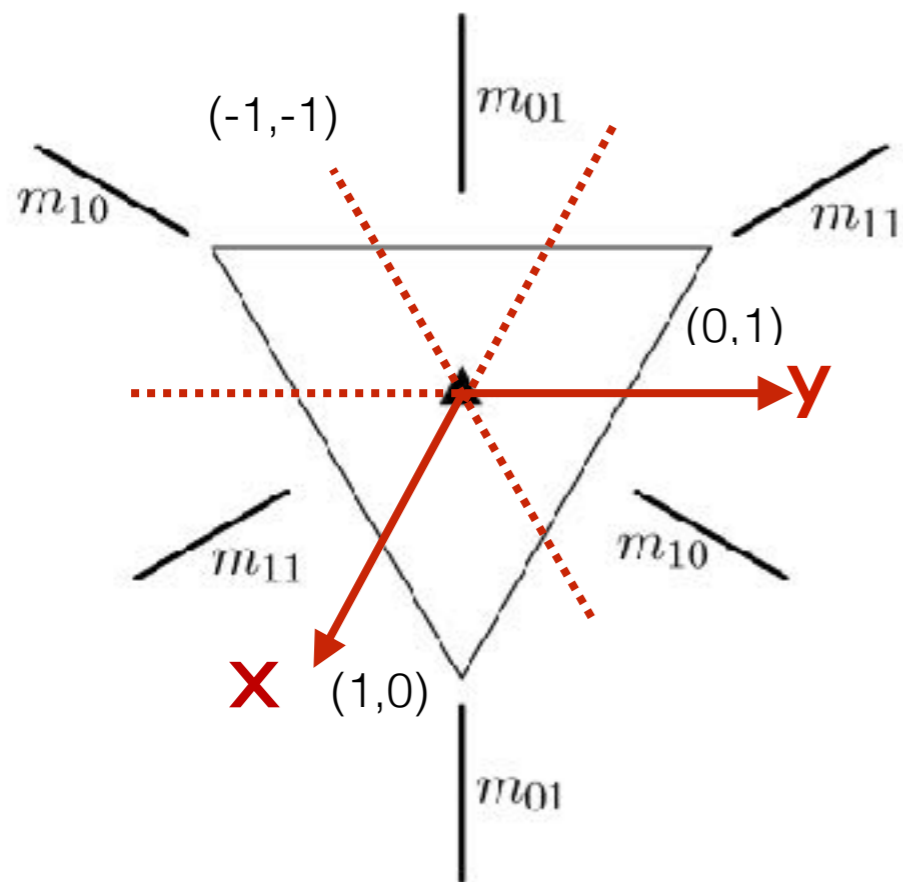
Distribute the symmetry elements of the group $mm2 = \{1, 2_z, m_x, m_y\}$ in classes of conjugate elements.

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

Problem 2.2.5 (additional)

Consider the group of the equilateral triangle and distribute its symmetry operations into conjugacy classes



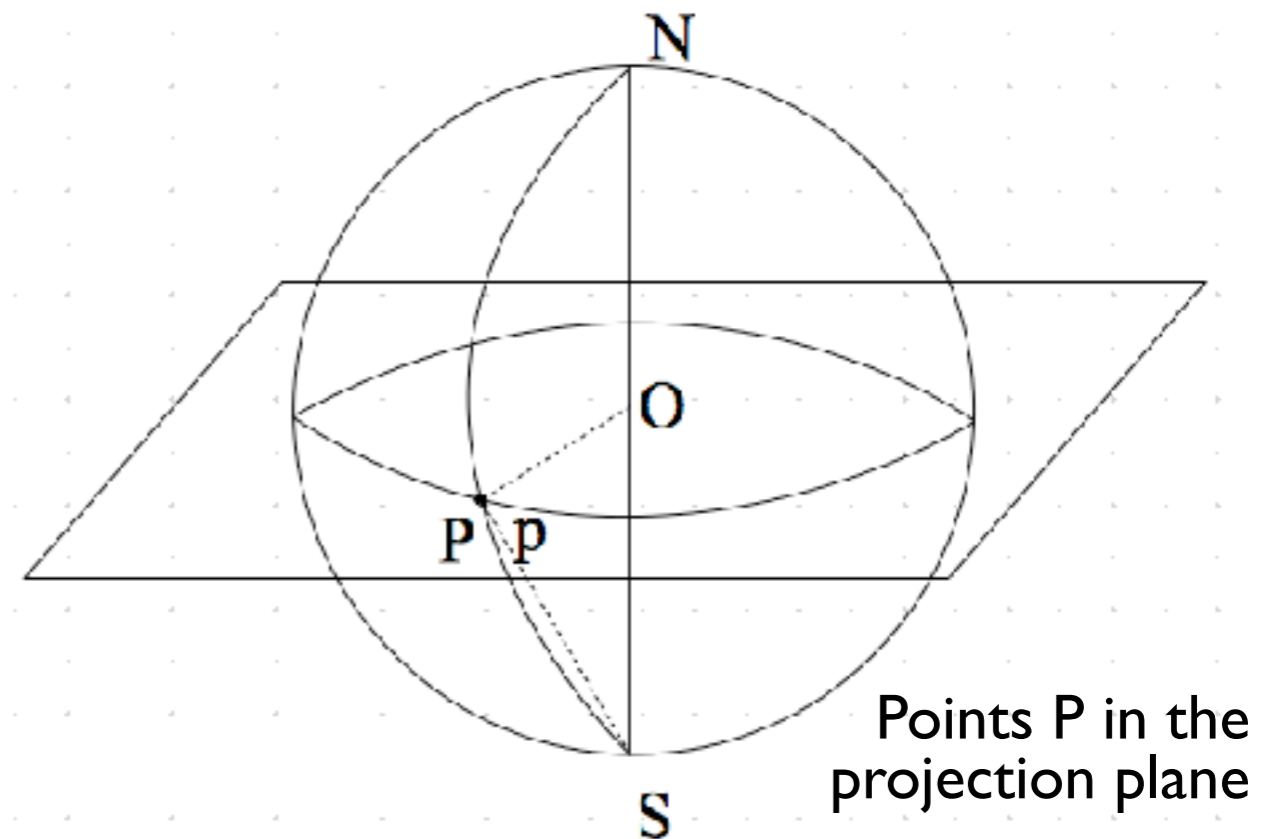
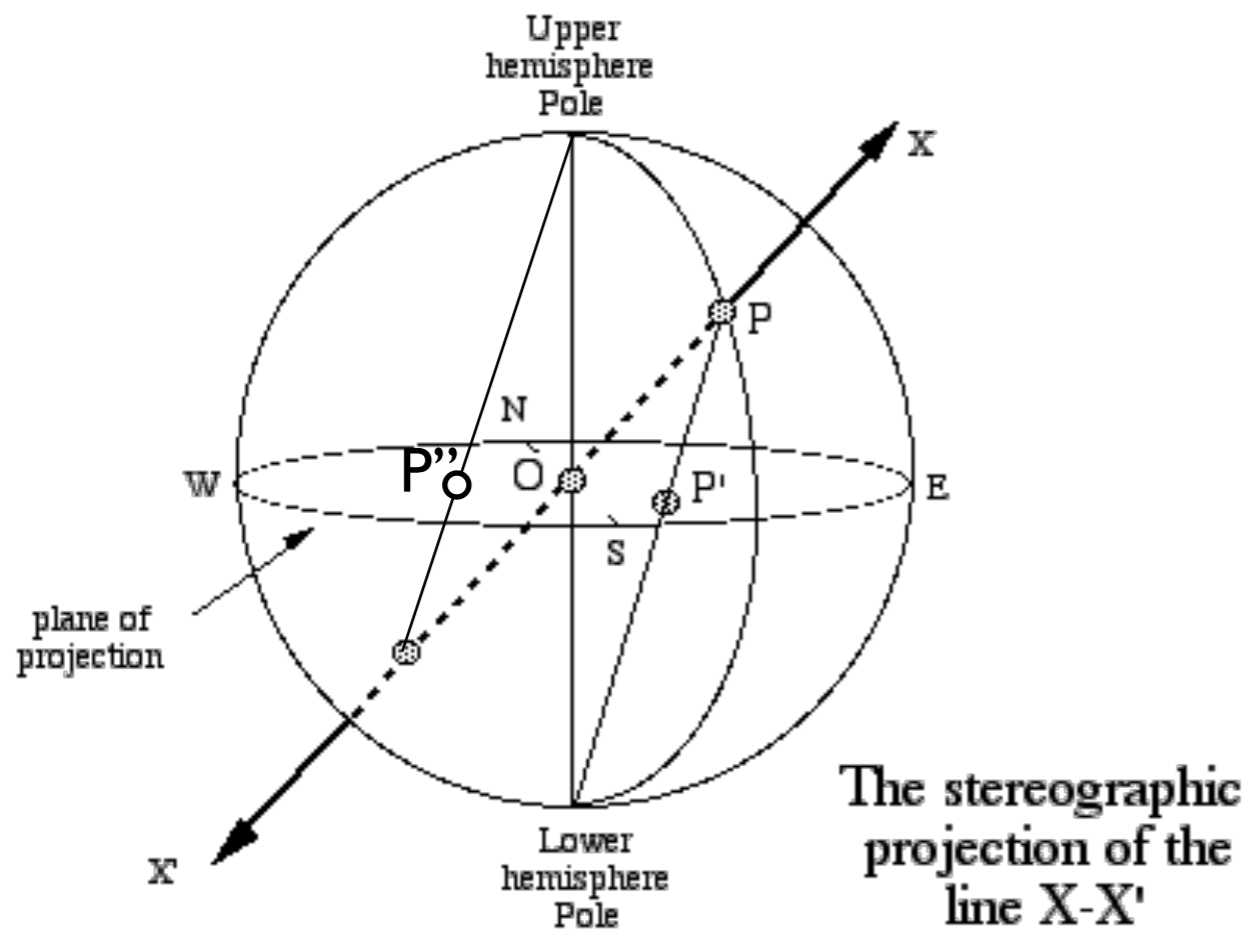
	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

Multiplication table of $3m$

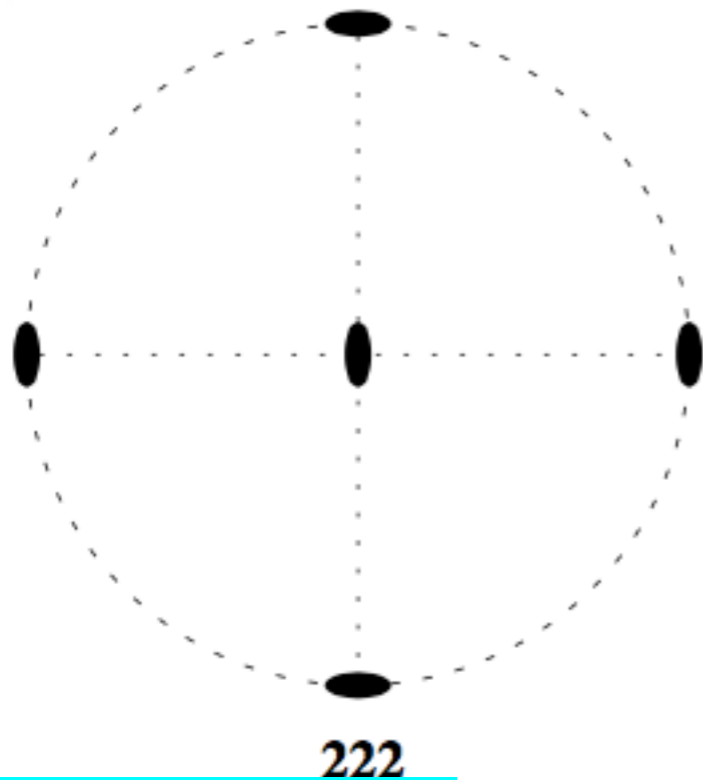
Visualization of Crystallographic Point Groups

- general position diagram
- symmetry elements diagram

Stereographic Projections

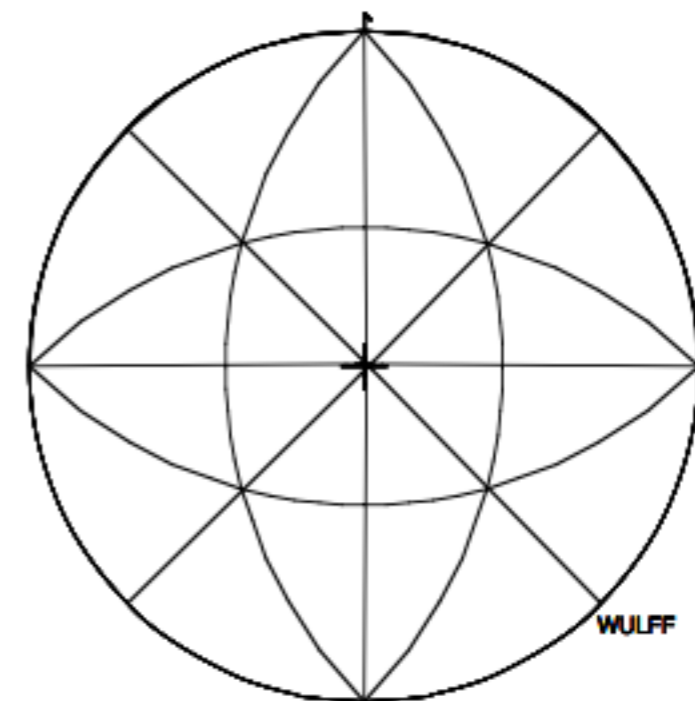
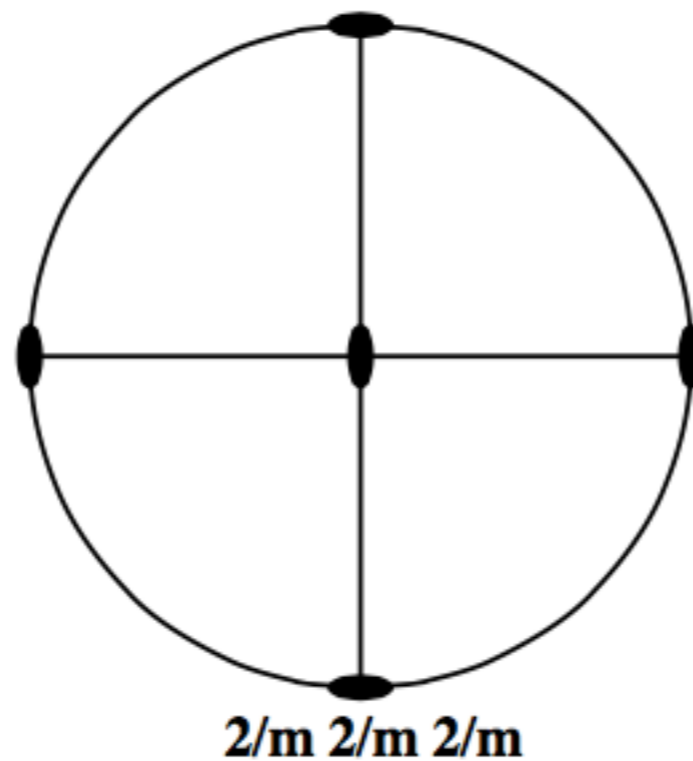
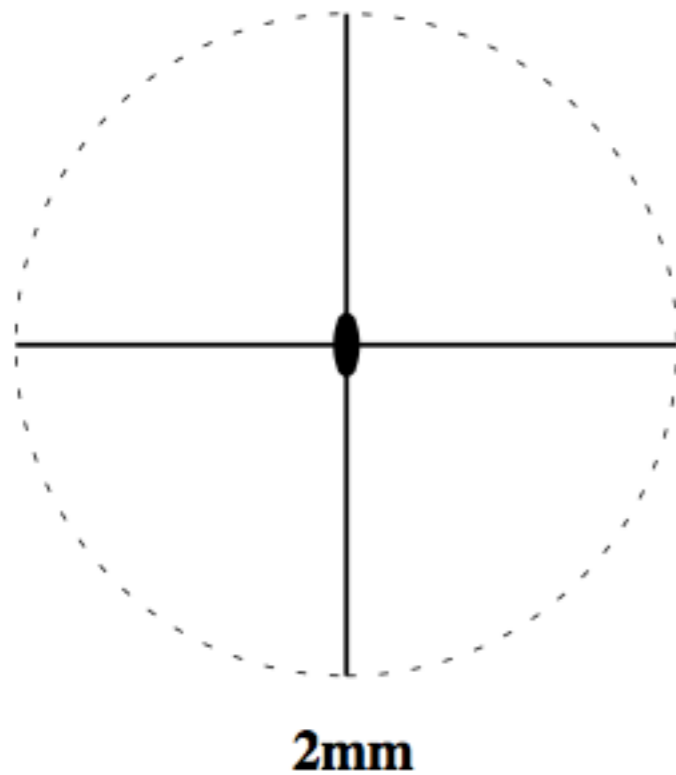


Rotation axes



- 6-fold
- 4-fold
- ▲ 3-fold
- 2-fold

Mirror planes

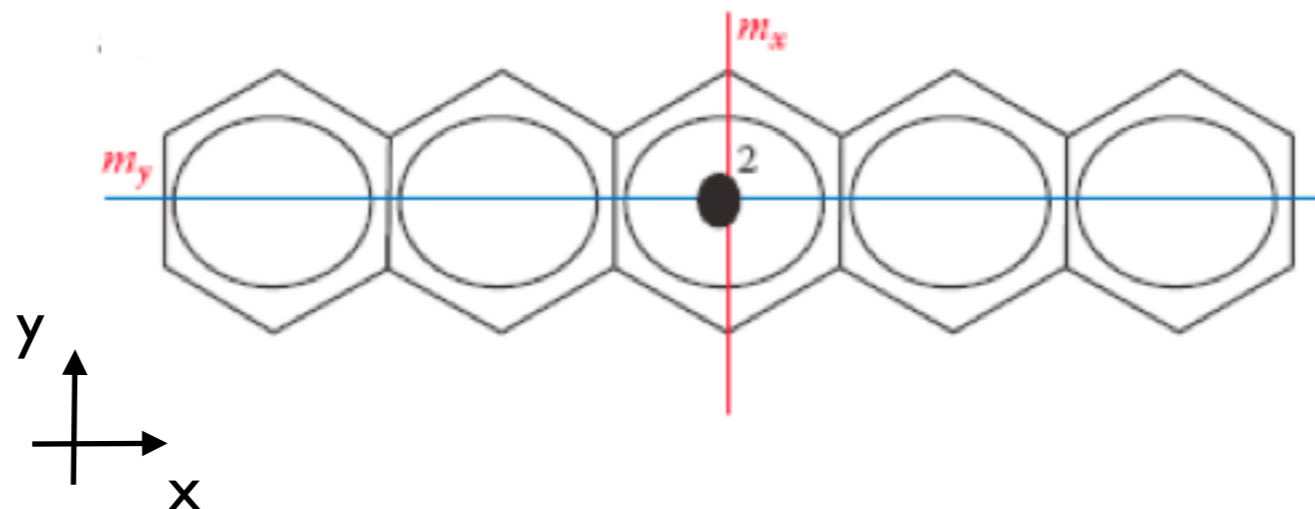


EXAMPLE

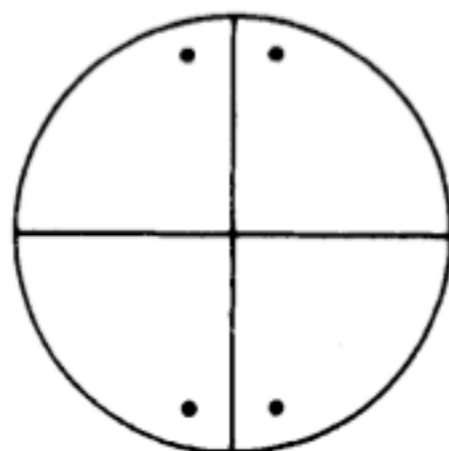
Stereographic Projections of $mm2$

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

Molecule of pentacene



Stereographic projections diagrams



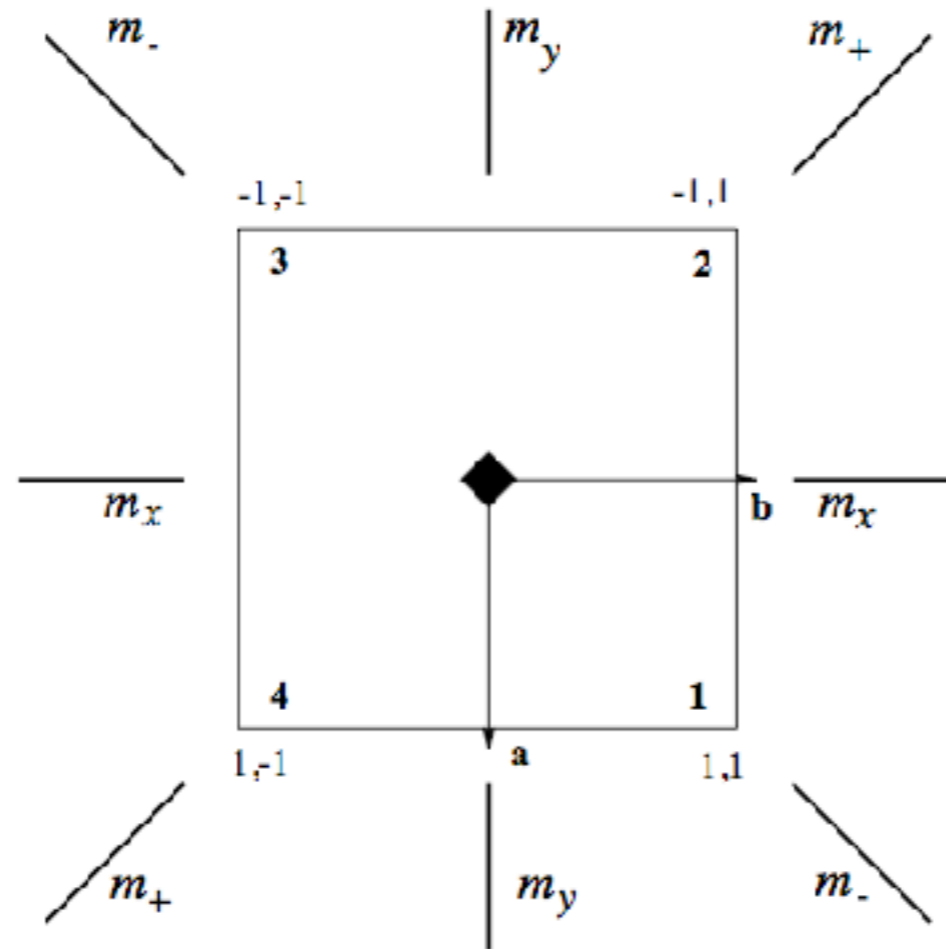
general position



symmetry elements

Problem 2.2.2 (cont.)

Stereographic Projections of $4mm$



general position
diagram

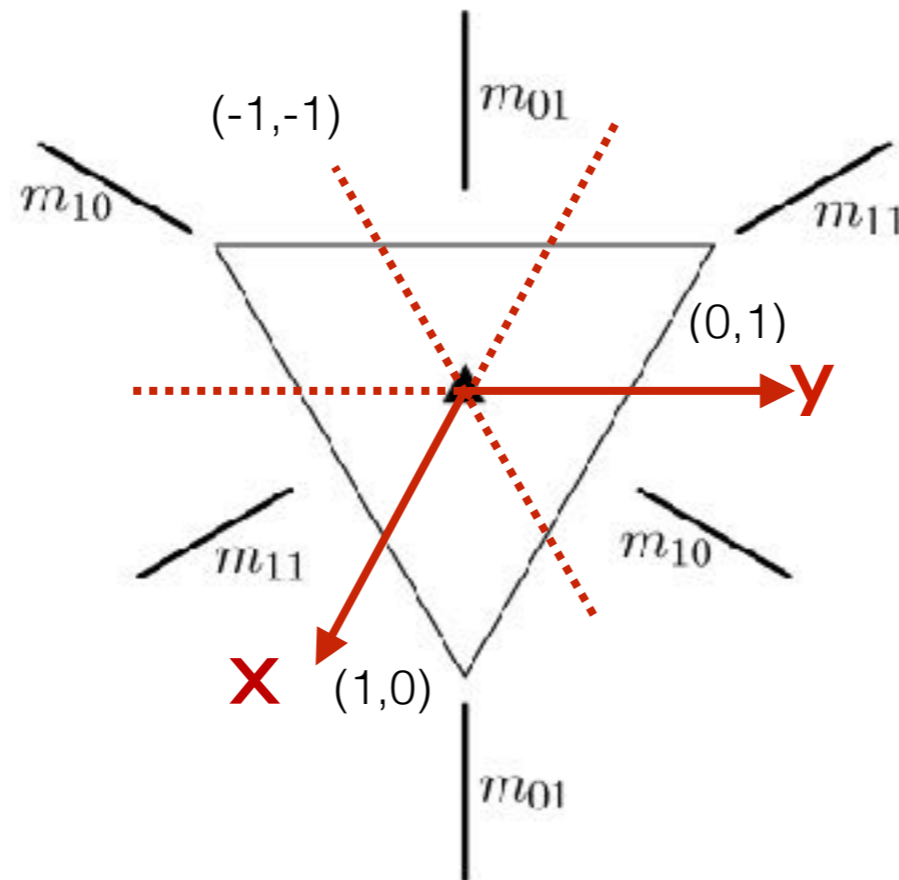
?

symmetry elements
diagram

?

Problem 2.2.2 (cont.)

Stereographic Projections of $3m$



general position
diagram



symmetry elements
diagram



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. $H = \{e, h_1, h_2, \dots, h_k\} \subset G$
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)

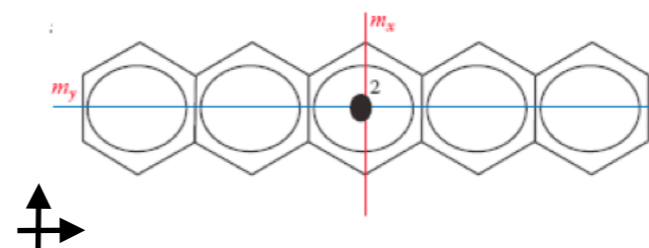
Maximal subgroup H of G

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

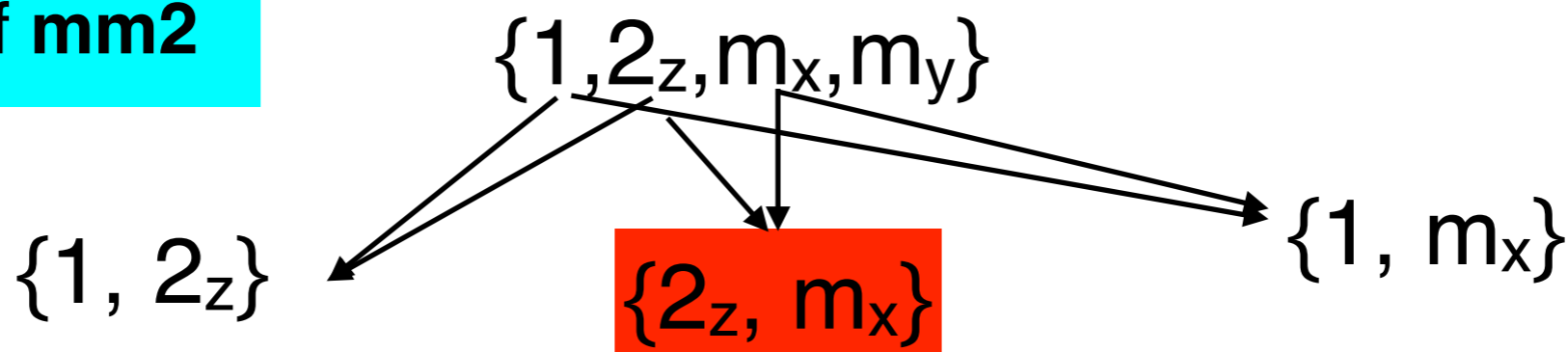
Example

Subgroups of point groups

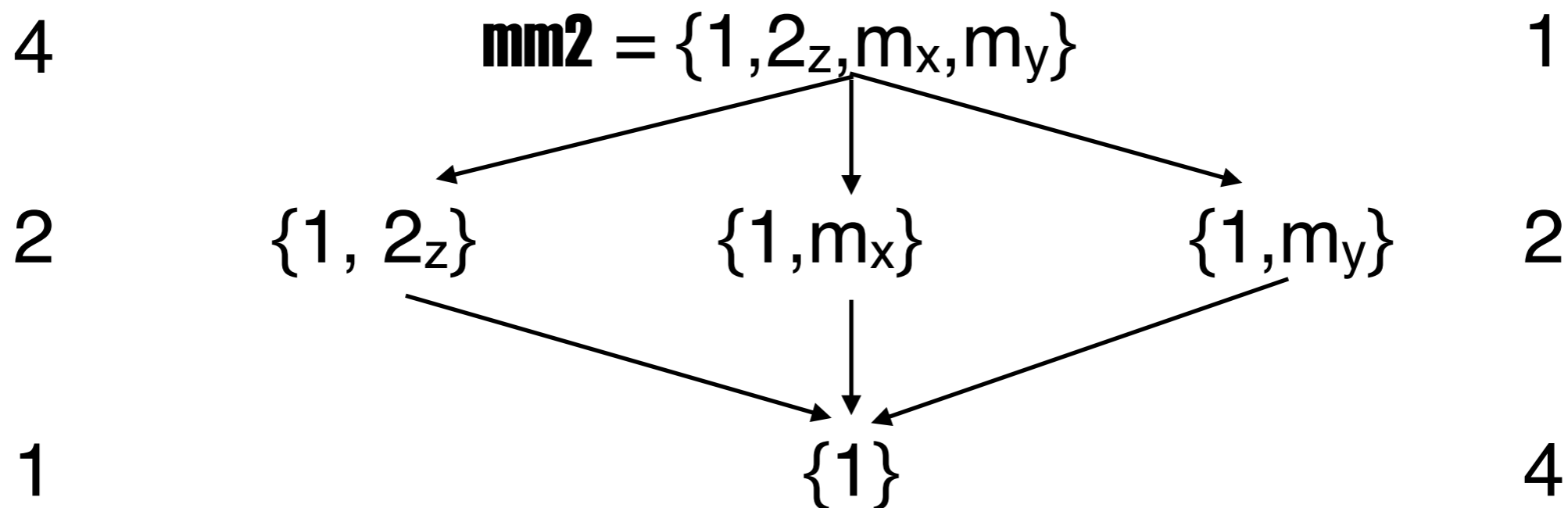
Molecule of pentacene



Subgroups of mm2

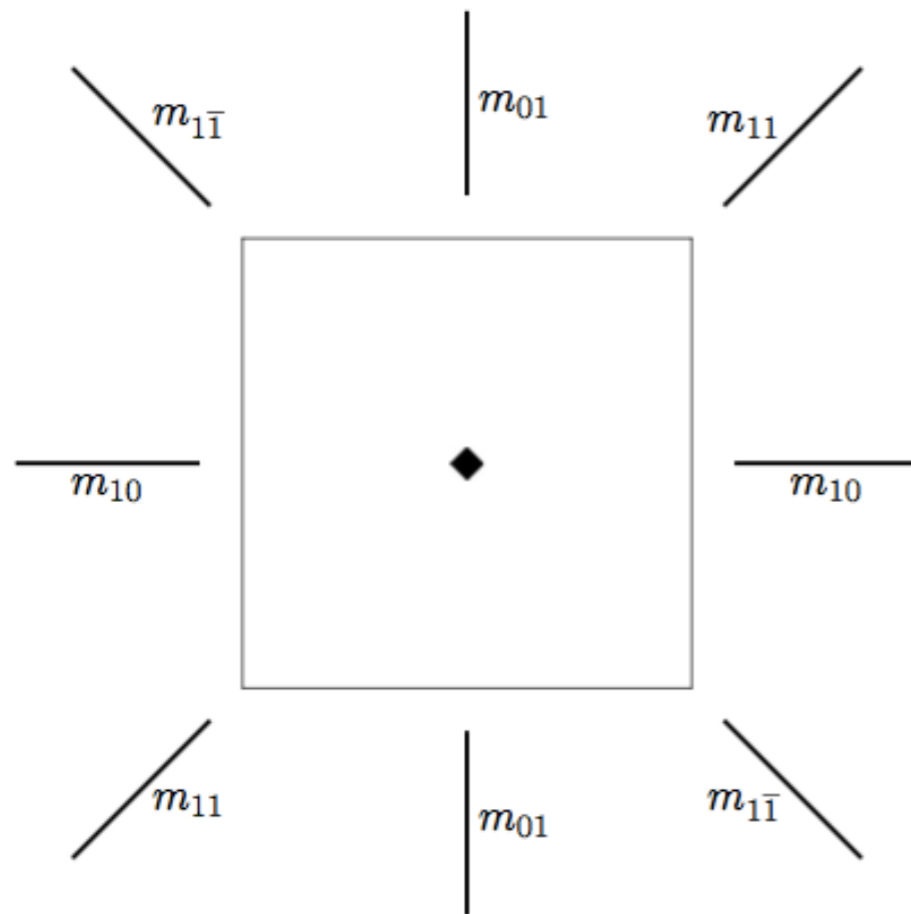


Subgroup graph



Problem 2.2.4

Consider the group of the square and determine its subgroups. Construct the corresponding graph of maximal subgroups.

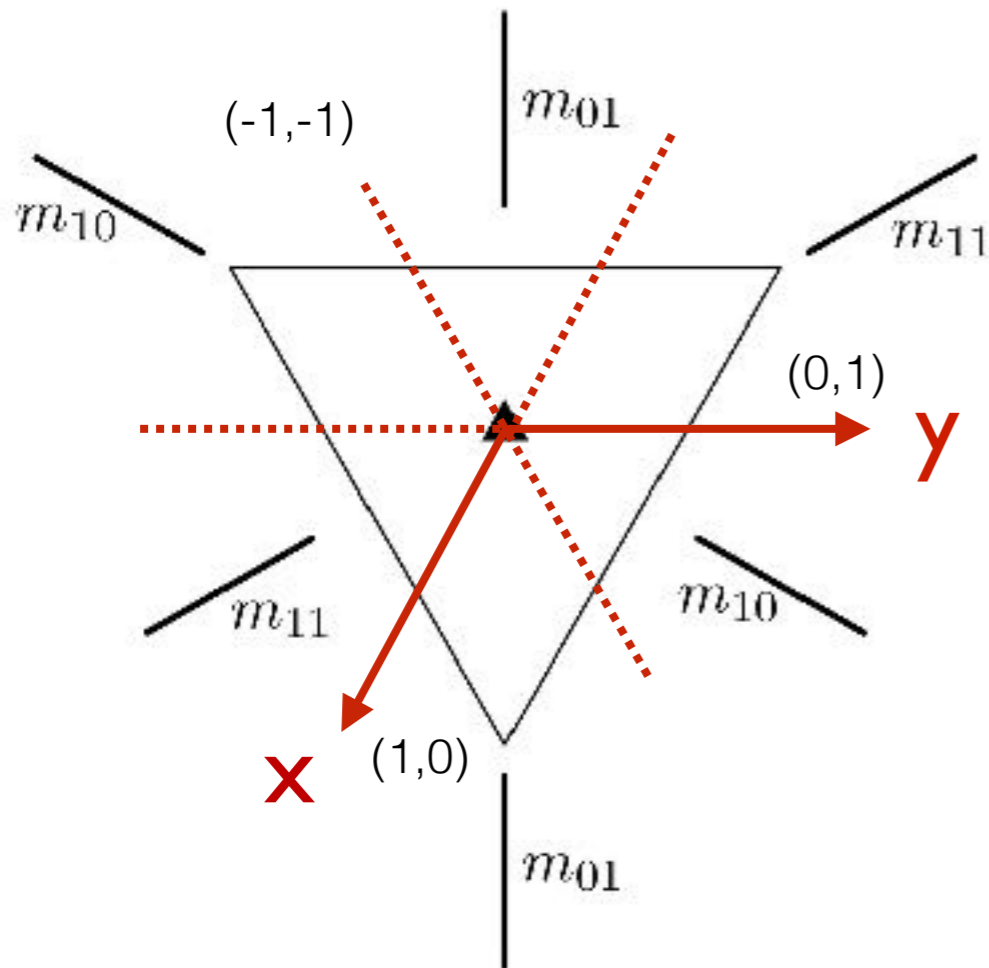


	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
1	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
2	2	1	4^-	4^+	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
4^+	4^+	4^-	2	1	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
4^-	4^-	4^+	1	2	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	1	2	4^-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

Problem 2.2.5

- (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

$$G = H + g_2H + \dots + g_mH, \quad g_i \notin H, \\ m = \text{index of } H \text{ in } G$$

right coset
decomposition

$$G = H + Hg_2 + \dots + Hg_m, \quad g_i \notin H \\ m = \text{index of } H \text{ in } G$$

Coset decomposition-properties

- (i) $g_iH \cap g_jH = \{\emptyset\}$, if $g_i \notin g_jH$
- (ii) $|g_iH| = |H|$
- (iii) $g_iH = g_jH$, $g_i \in g_jH$

Coset decomposition $G:H$

Normal
subgroups

$$Hg_j = g_jH, \text{ for all } g_j = 1, \dots, [i]$$

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 $|G|$

EXERCISES

Problem 2.2.6

Consider the subgroup $\{e, 2\}$ of $4mm$, of index 4:

-Write down and compare the right and left coset decompositions of $4mm$ with respect to $\{e, 2\}$;

-Are the right and left coset decompositions of $4mm$ with respect to $\{e, 2\}$ equal or different? Can you comment why?

Problem 2.2.7

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 $\exists g \in G: g^{-1}H_1g = H_2$

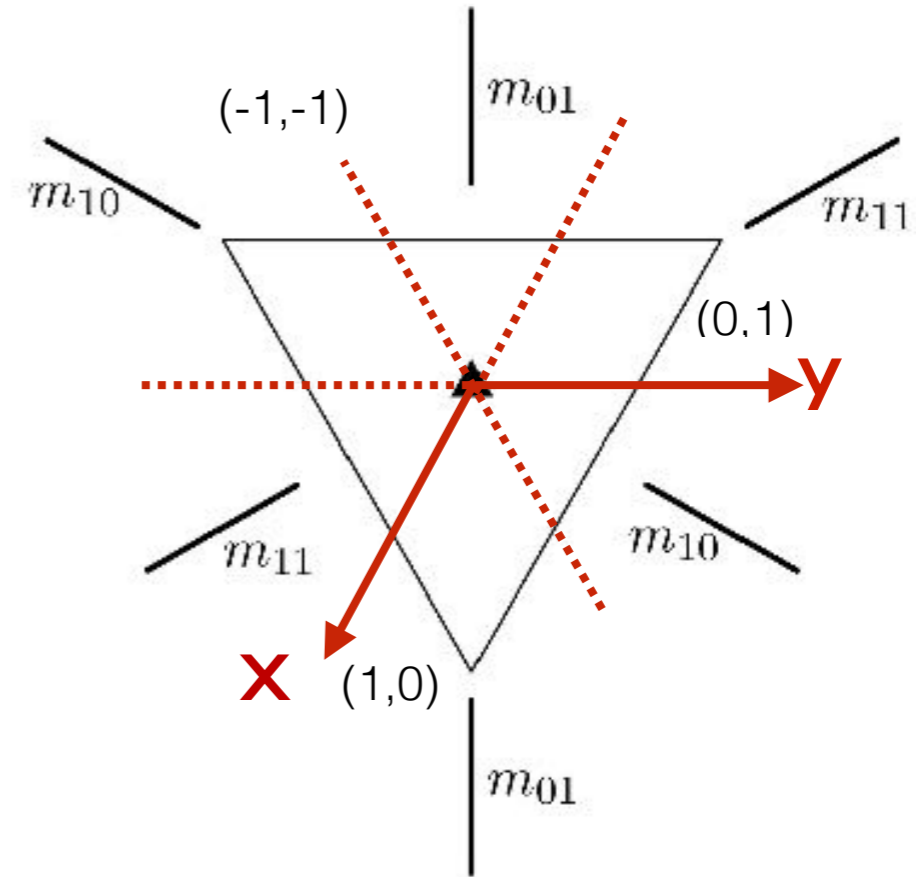
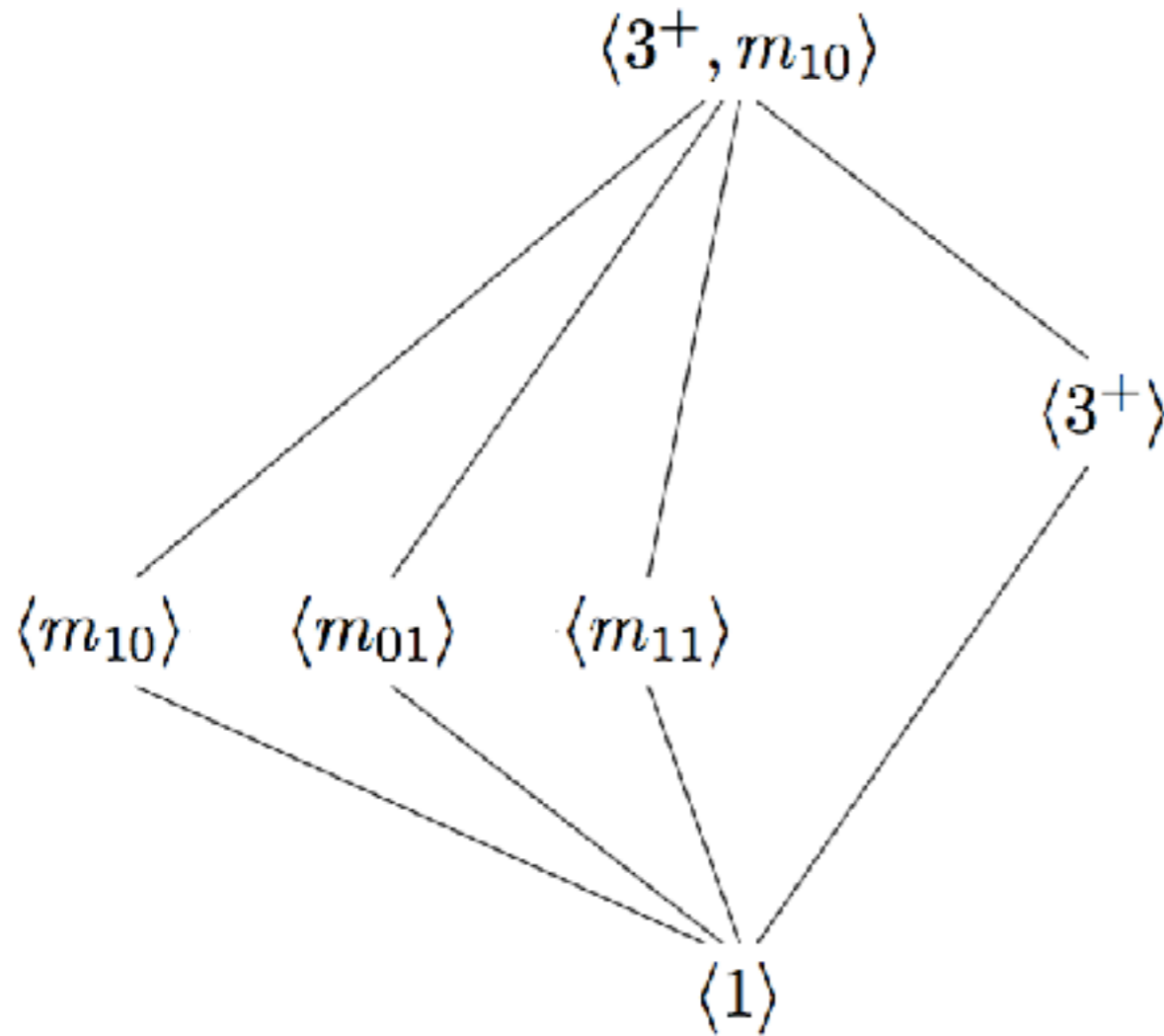
- (i) Classes of conjugate subgroups: $L(H)$
- (ii) If $H_1 \sim H_2$, then $H_1 \cong H_2$
- (iii) $|L(H)|$ is a divisor of $|G|/|H|$

Normal subgroup

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

Problem 2.2.5

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



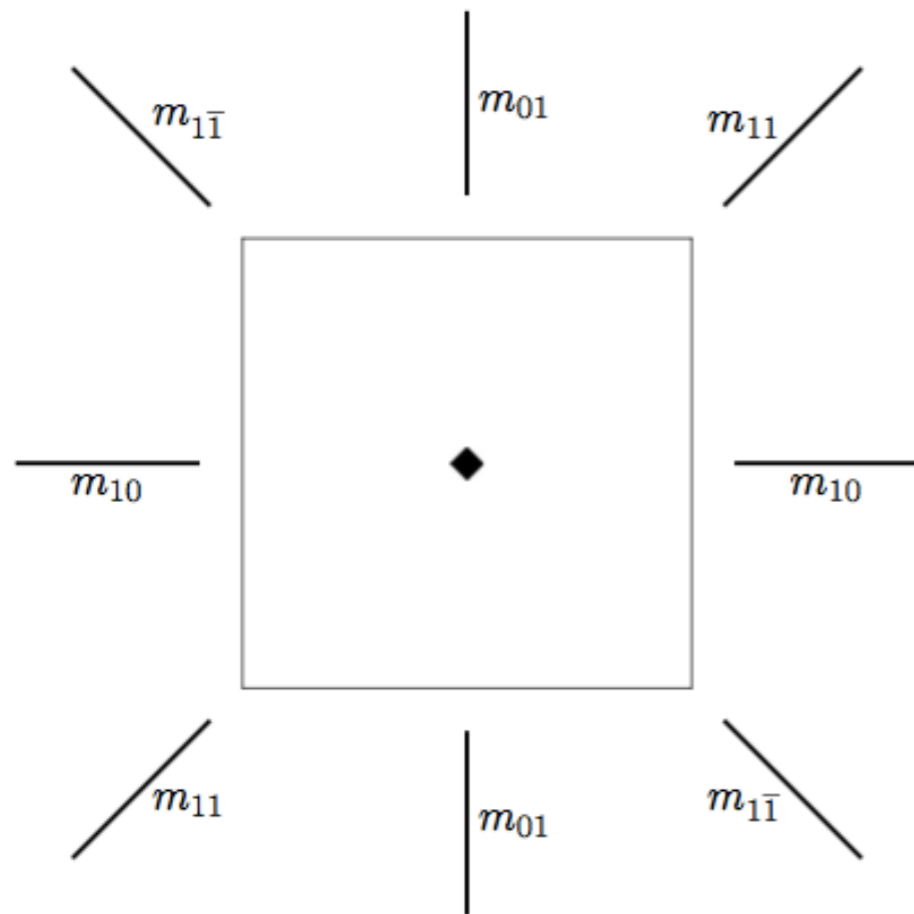
Multiplication table of $3m$

	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

EXERCISES

Problem 2.4 (cont)

Distribute the subgroups of the group of the square into classes of conjugate subgroups

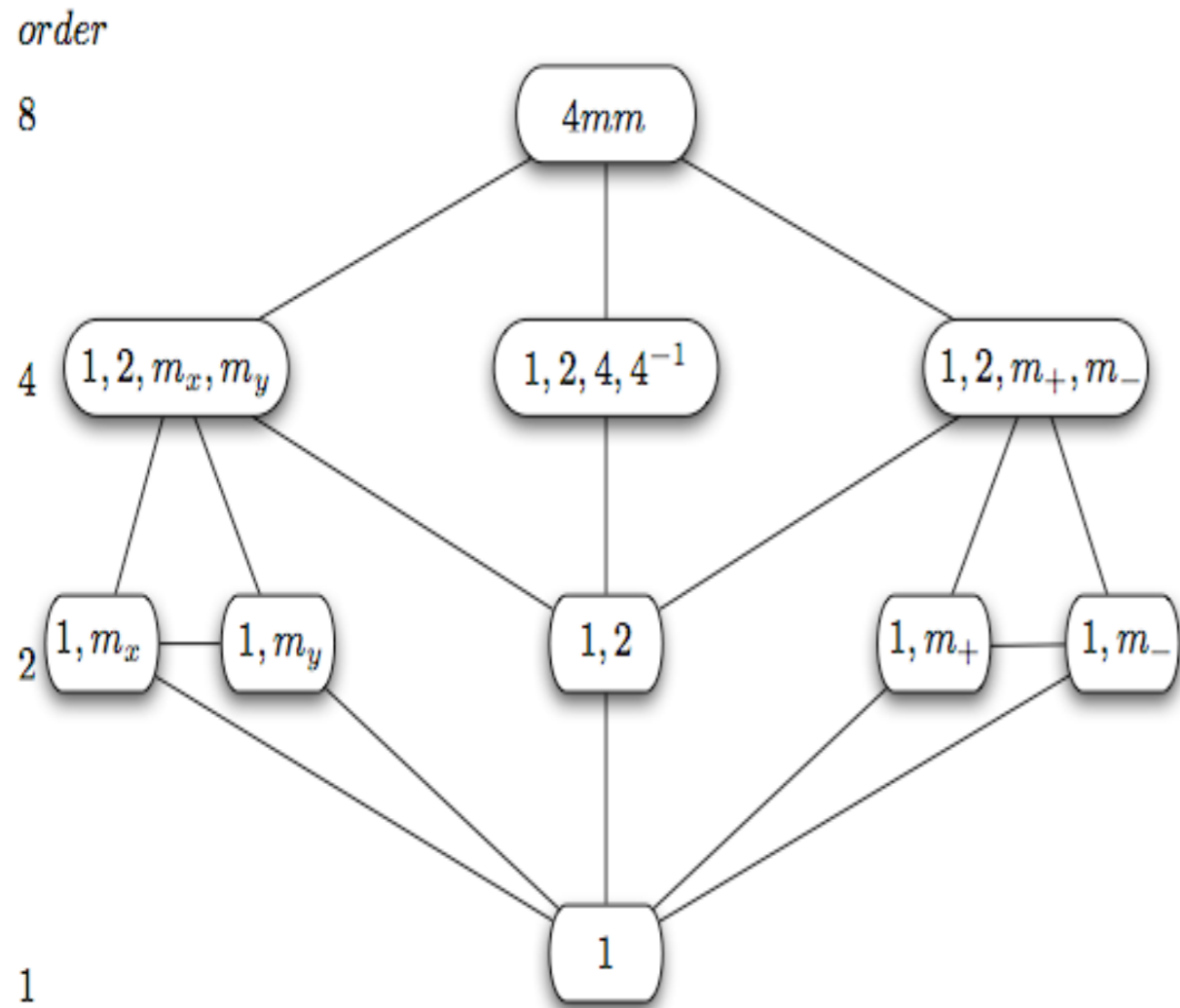


	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
1	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
2	2	1	4^-	4^+	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
4^+	4^+	4^-	2	1	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
4^-	4^-	4^+	1	2	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	1	2	4^-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

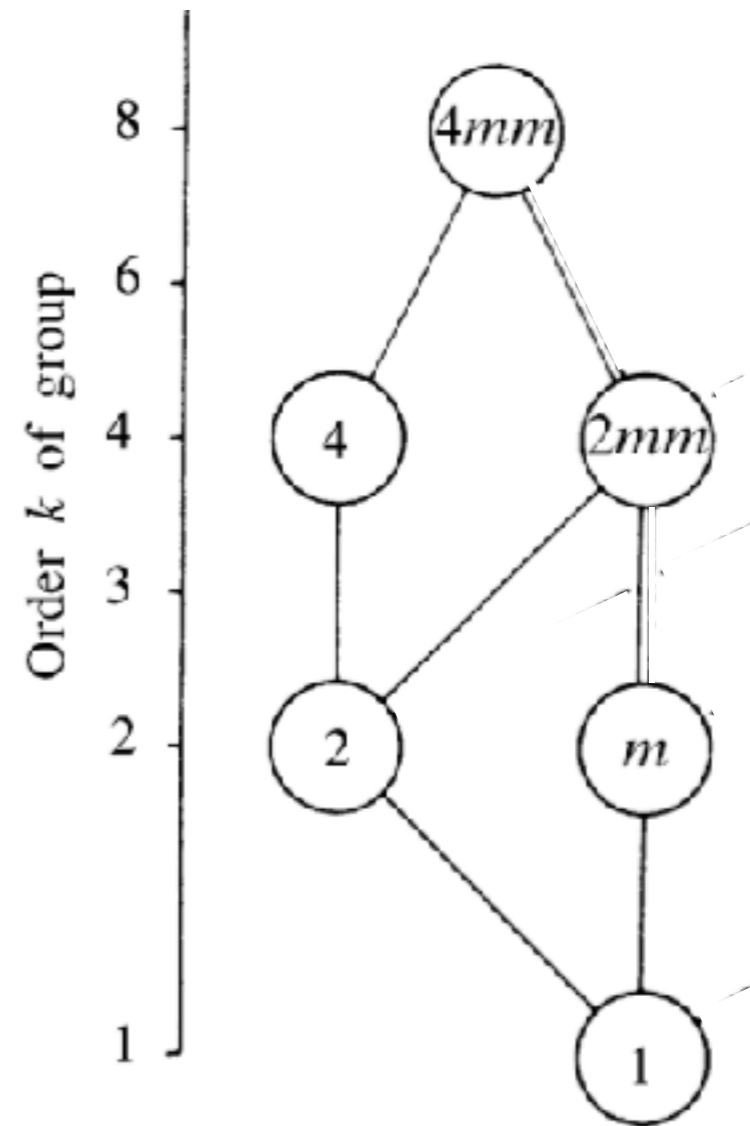
Multiplication table of $4mm$

Hint: The stereographic projections could be rather helpful

Complete and contracted group-subgroup graphs



Complete graph of maximal subgroups



Contracted graph of maximal subgroups

Group-subgroup relations of point groups

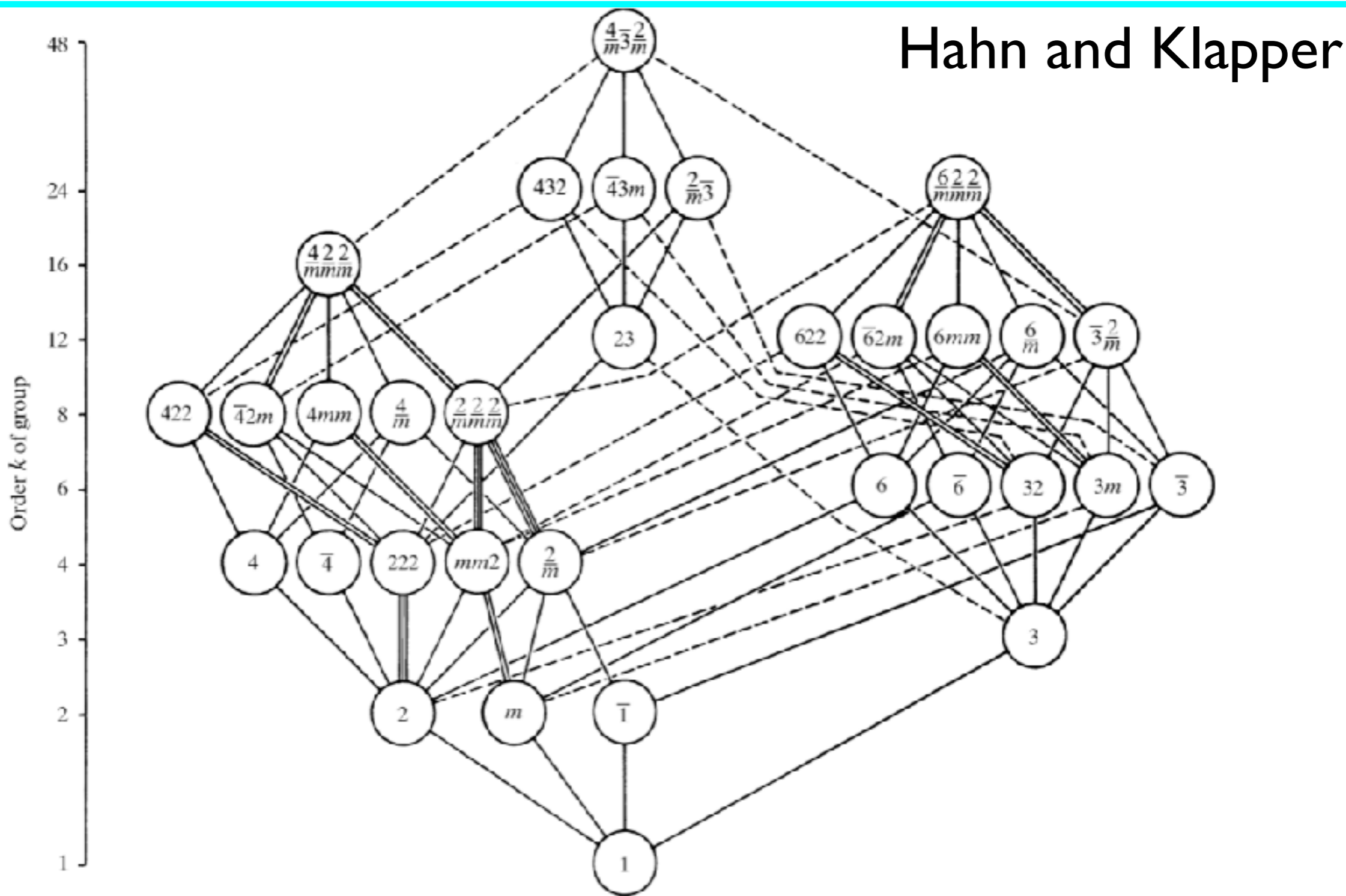


Fig. 10.1.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal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

**GENERAL
AND SPECIAL
WYCKOFF POSITIONS**

Group Actions

Group Actions

A *group action* of a group \mathcal{G} on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair (g, ω) an object $\omega' = g(\omega)$ of Ω such that the following hold:

- (i) applying two group elements g and g' consecutively has the same effect as applying the product $g'g$, i.e. $g'(g(\omega)) = (g'g)(\omega)$
- (ii) applying the identity element e of \mathcal{G} has no effect on ω , i.e. $e(\omega) = \omega$ for all ω in Ω .

Orbit and Stabilizer

The set $\omega^{\mathcal{G}} := \{g(\omega) \mid g \in \mathcal{G}\}$ of all objects in the orbit of ω is called the *orbit of ω under \mathcal{G}* .

The set $S_{\mathcal{G}}(\omega) := \{g \in \mathcal{G} \mid g(\omega) = \omega\}$ of group elements that do not move the object ω is a subgroup of \mathcal{G} called the *stabilizer of ω in \mathcal{G}* .

Equivalence classes

Often, two objects ω and ω' are regarded as *equivalent* if there is a group element moving ω to ω' .

Via this equivalence relation, the action of \mathcal{G} partitions the objects in Ω into *equivalence classes*.

General and special Wyckoff positions

Orbit of a point X_0 under P : $P(X_0) = \{W X_0, W \in P\}$
Multiplicity

Site-symmetry group $S_0 = \{W\}$ of a point X_0

$$W X_0 = X_0$$

a	b	c	x_0
d	e	f	y_0
g	h	i	z_0

 =

x_0
y_0
z_0

Multiplicity: $|P|/|S_0|$

General position X_0

$$S_0 = 1 = \{1\}$$

Multiplicity: $|P|$

Special position X_0

$$S_0 > 1 = \{1, \dots, \}$$

Multiplicity: $|P|/|S_0|$

Site-symmetry groups: oriented symbols

Example

General and special Wyckoff positions

Point group $\mathbf{2} = \{1, 2_z\}$

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

$$S_o = \mathbf{2}$$

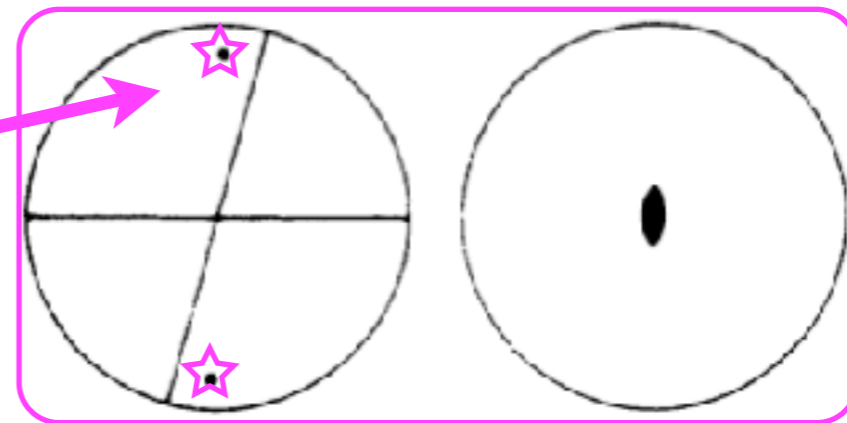
$$WX_o = X_o$$

$$2_z: \begin{array}{|c|c|c|c|} \hline -1 & & & 0 \\ \hline & -1 & & 0 \\ \hline & & 1 & z \\ \hline \end{array} = \begin{array}{|c|} \hline 0 \\ \hline 0 \\ \hline z \\ \hline \end{array}$$

Multiplicity: $|P|/|S_o|$

$$2 \text{ b } 1 \quad (x, y, z) \quad (-x, -y, z)$$

$$1 \text{ a } 2 \quad (0, 0, z)$$



Example

General and special Wyckoff positions

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

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

$$S_o = \mathbf{mm2}$$

$$WX_o = X_o$$

$$2_z: \begin{array}{|c|c|c|c|} \hline -1 & & & 0 \\ \hline & -1 & & 0 \\ \hline & & 1 & z \\ \hline \end{array} = \begin{array}{|c|} \hline 0 \\ \hline 0 \\ \hline z \\ \hline \end{array}$$

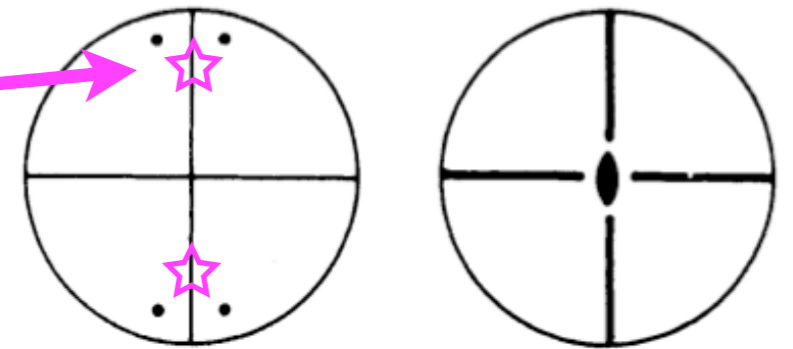
$$m_y: \begin{array}{|c|c|c|c|} \hline 1 & & & 0 \\ \hline & -1 & & 0 \\ \hline & & 1 & z \\ \hline \end{array} = \begin{array}{|c|} \hline 0 \\ \hline 0 \\ \hline z \\ \hline \end{array}$$

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

2 c m.. (0,y,z) (0,-y,z)

2 b .m. (x,0,z) (-x,0,z)

1 a mm2 (0,0,z)



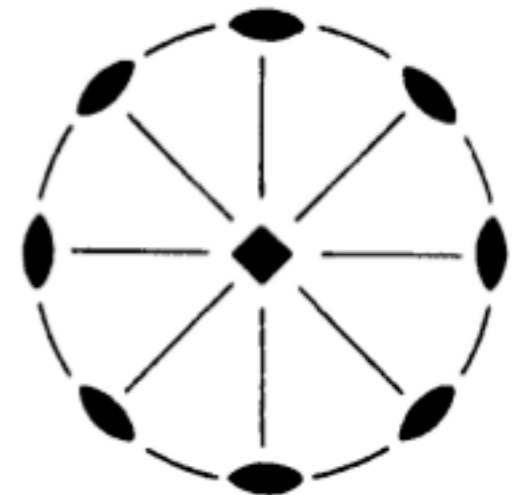
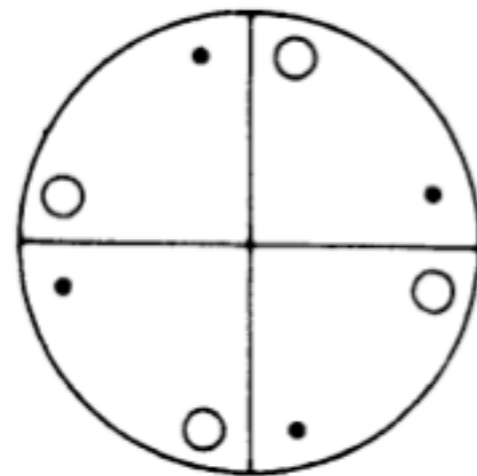
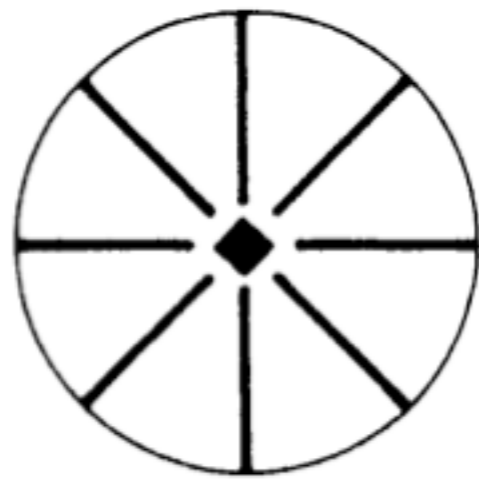
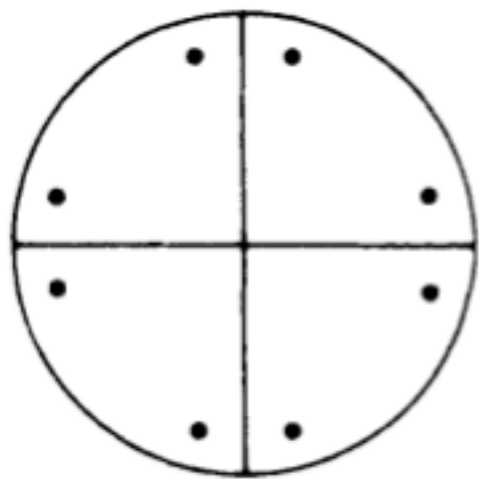
EXERCISES

Problem 2.2.8

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

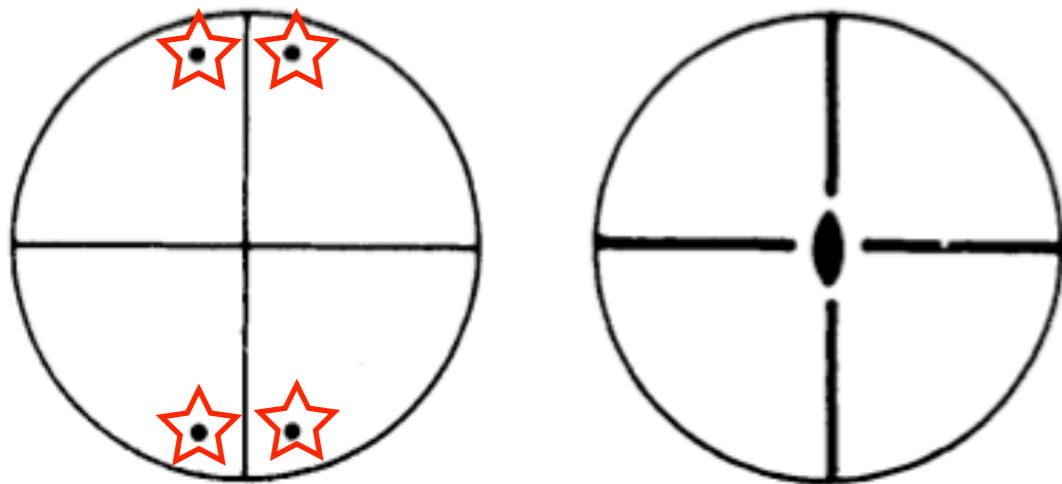


Wyckoff positions splitting schemes

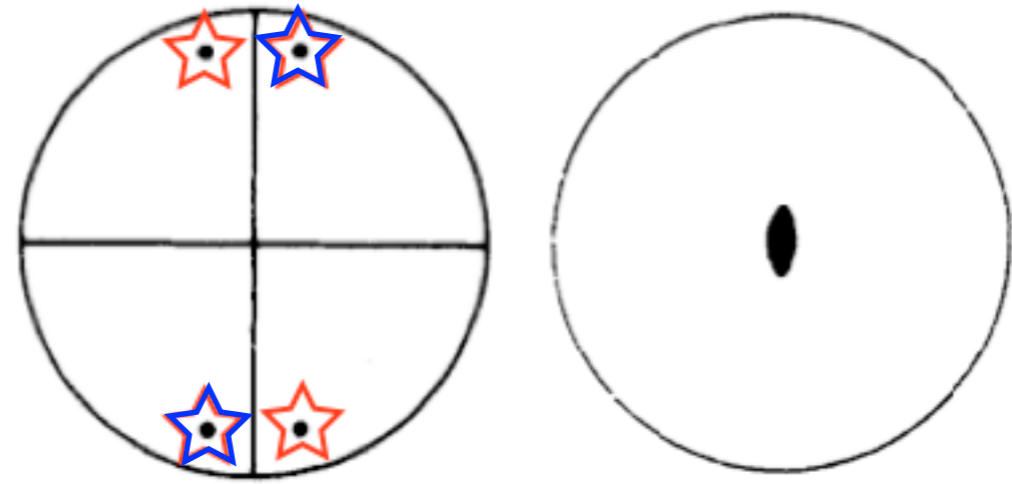
EXAMPLE

Group-subgroup pair $mm2 \supset 2$, $[i]=2$

$mm2$



2



4 d |

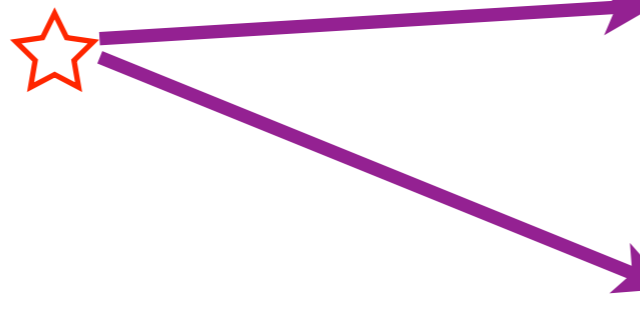
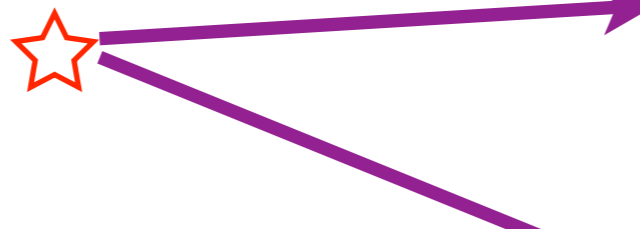
(x, y, z)
 $(-x, -y, z)$
 $(x, -y, z)$
 $(-x, y, z)$



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



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



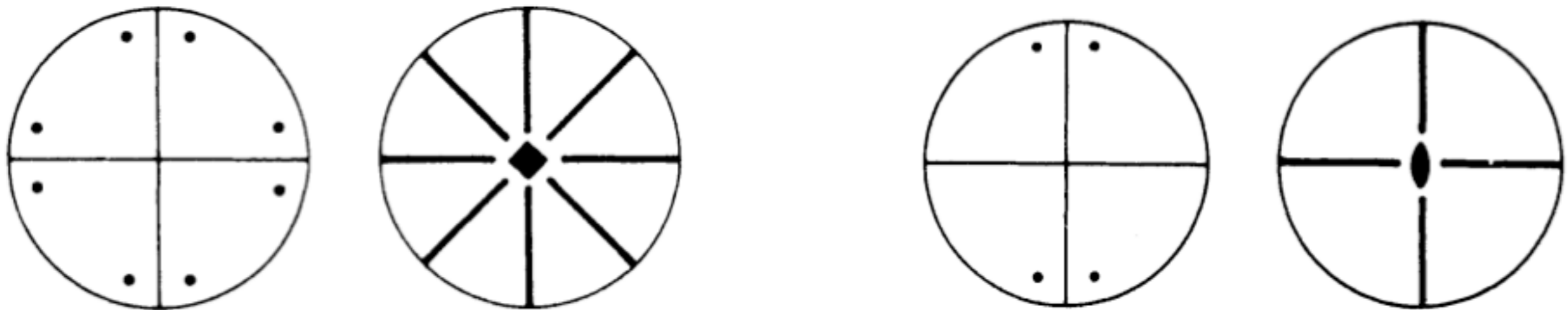
EXERCISES

Problem 2.2.9

Consider the general and special Wyckoff positions of the symmetry group of the square **4mm** and those of its subgroup **mm2** of index 2.

Determine the splitting schemes of the general and special Wyckoff positions for **4mm** $>$ **mm2**.

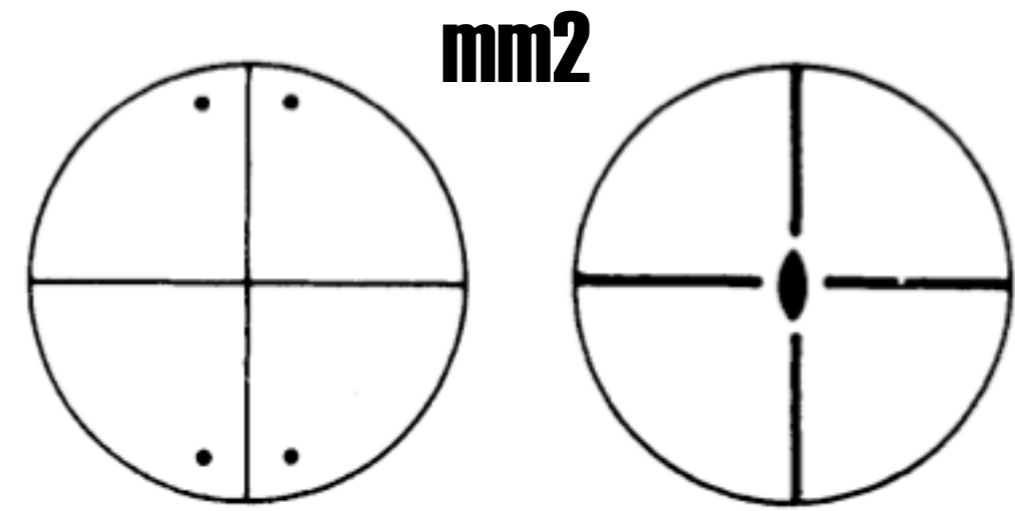
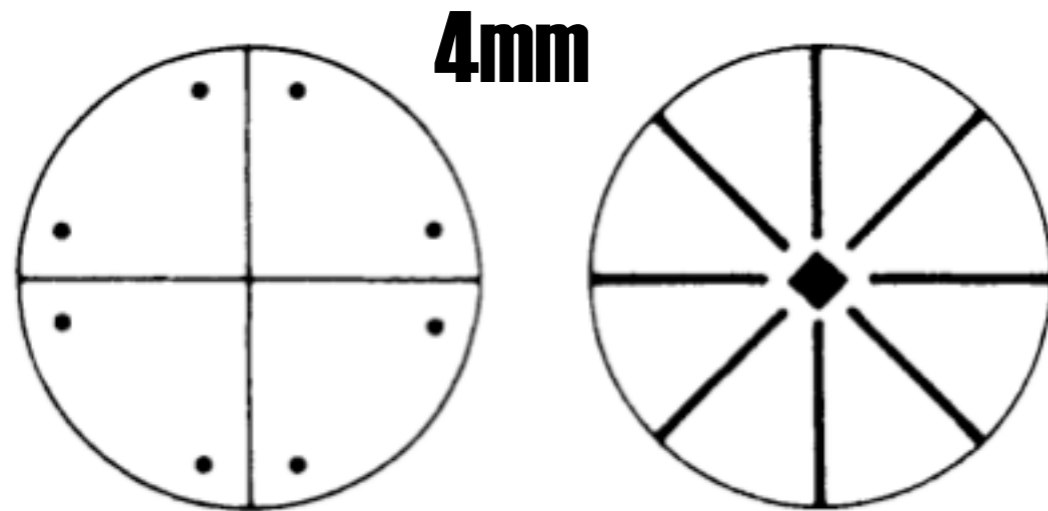
Hint: The stereographic projections could be rather helpful



Problem 2.2.9

SOLUTION

General and Special Wyckoff positions



8 d l (x,y,z) $(-x,-y,z)$ $(-y,x,z)$ $(y,-x,z)$
 $(x,-y,z)$ $(-x,y,z)$ $(-y,-x,z)$ (y,x,z)
 4 c .m. $(x,0,z)$ $(-x,0,z)$ $(0,x,z)$ $(0,-x,z)$
 4 b ..m (x,x,z) $(-x,-x,z)$ $(-x,x,z)$ $(x,-x,z)$
 1 a 4mm $(0,0,z)$

4 d l (x,y,z) $(-x,-y,z)$ $(x,-y,z)$ $(-x,y,z)$
 2 c m.. $(0,y,z)$ $(0,-y,z)$
 2 b .m. $(x,0,z)$ $(-x,0,z)$
 1 a mm2 $(0,0,z)$