MaThCryst

International Union of Crystallography
Commission on Mathematical and Theoretical Crystallography

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Facultad de Ciencias

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

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CRYSTALLOGRAPHIC POINT GROUPS I (basic facts)

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GROUP THEORY
(brief introduction)

Crystallographic symmetry operations

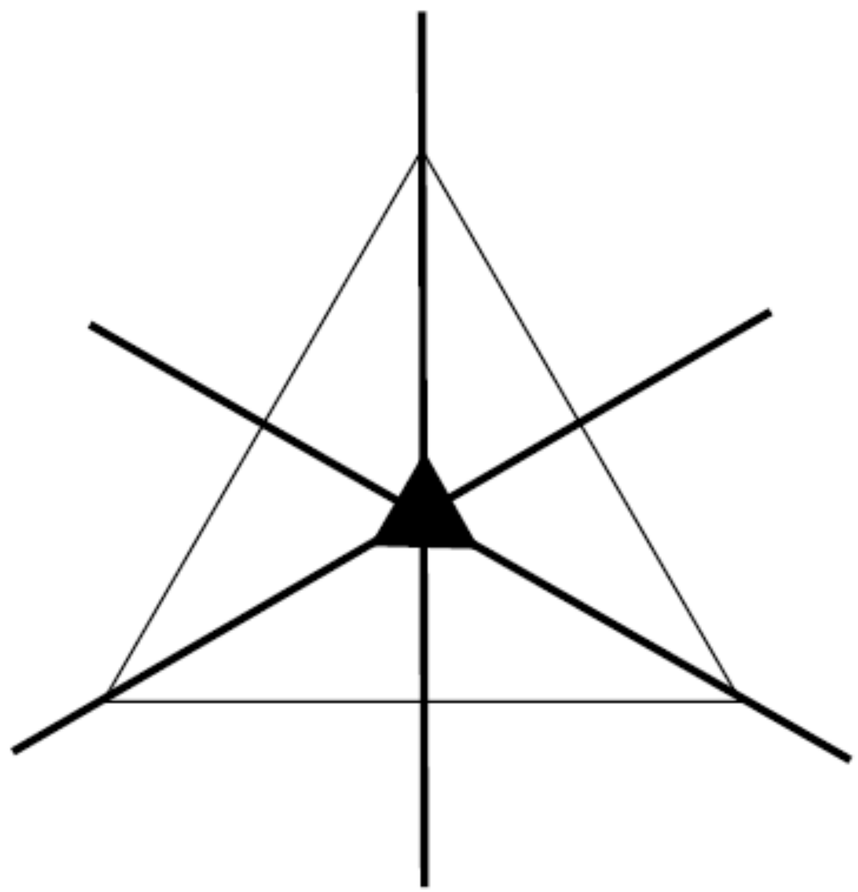
Symmetry operations of an object

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

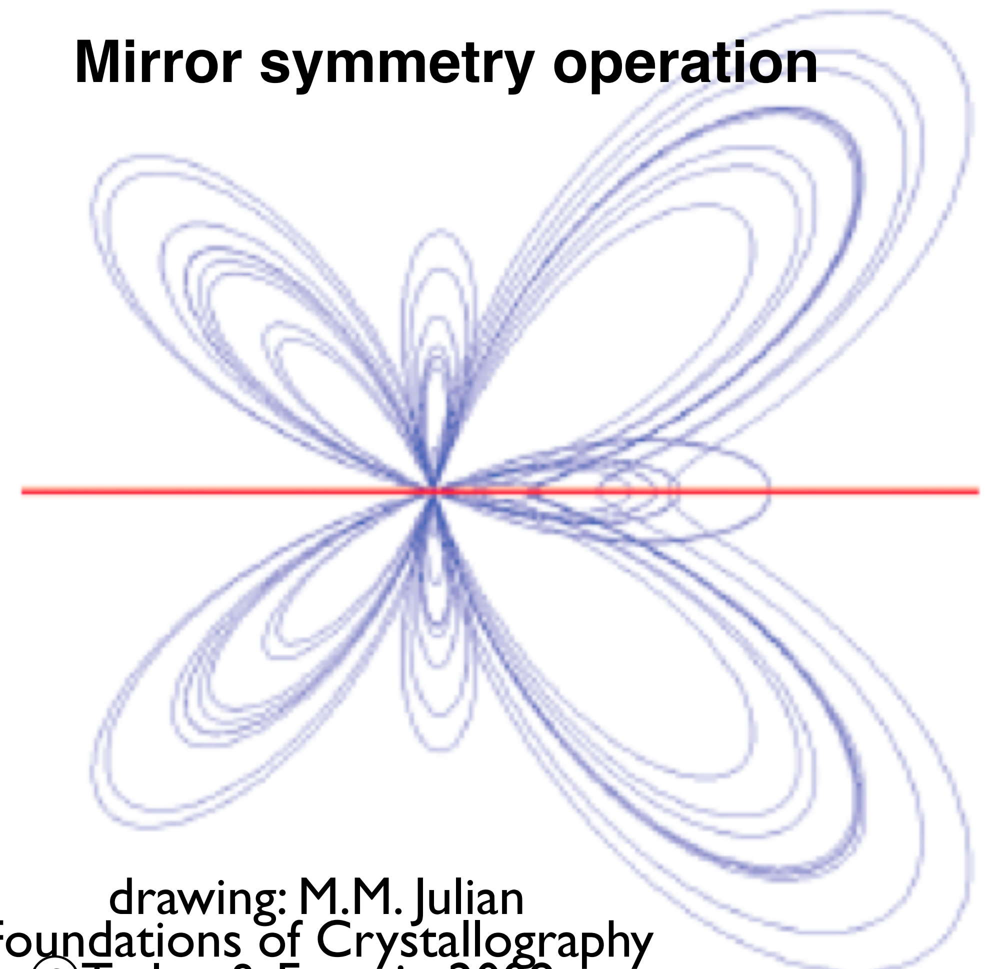
If the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.



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



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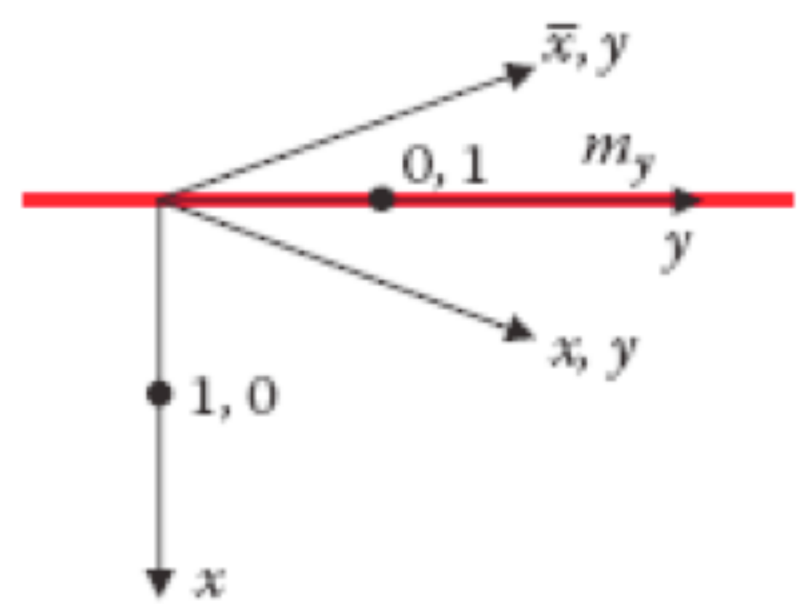
Mirror line m_y at 0,y



Matrix representation

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

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

Fixed points

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

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

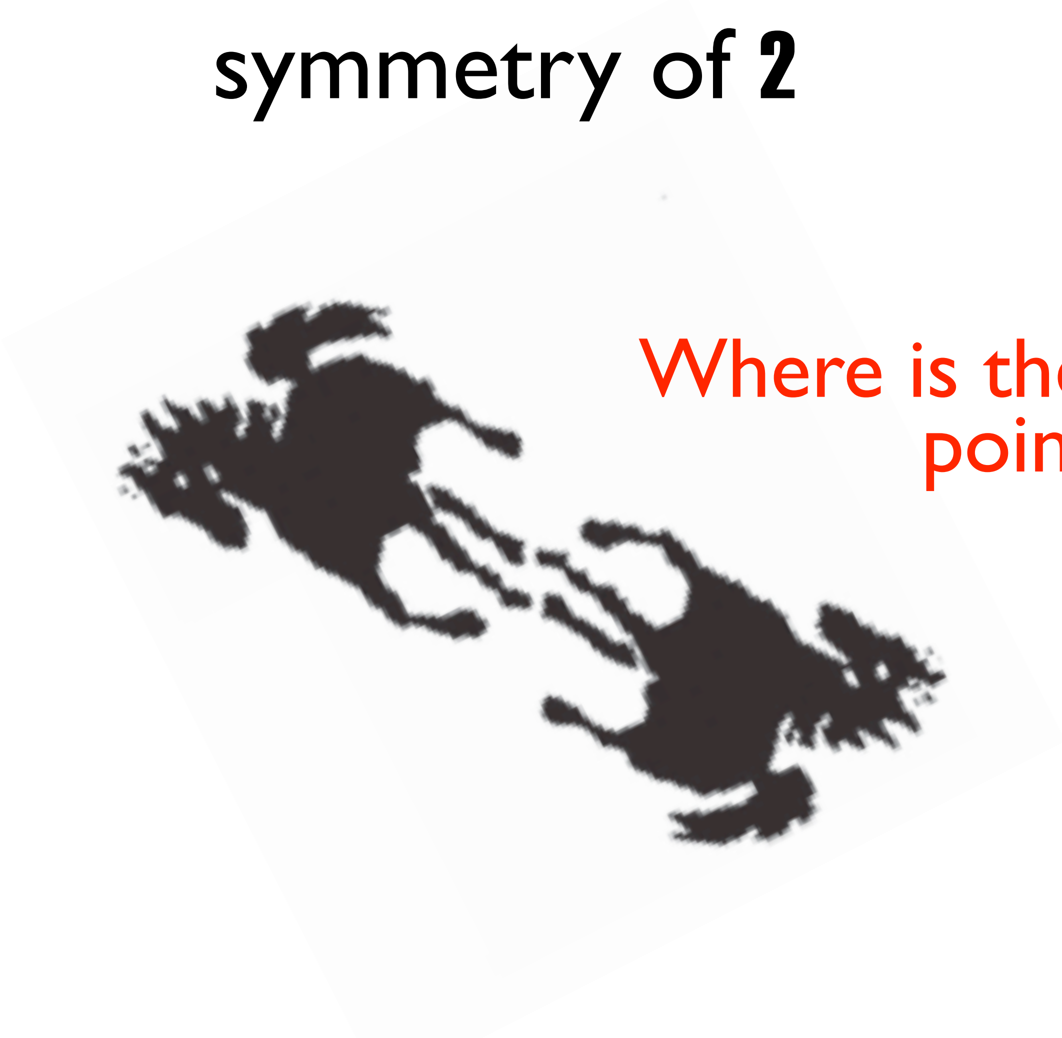
Group generators

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

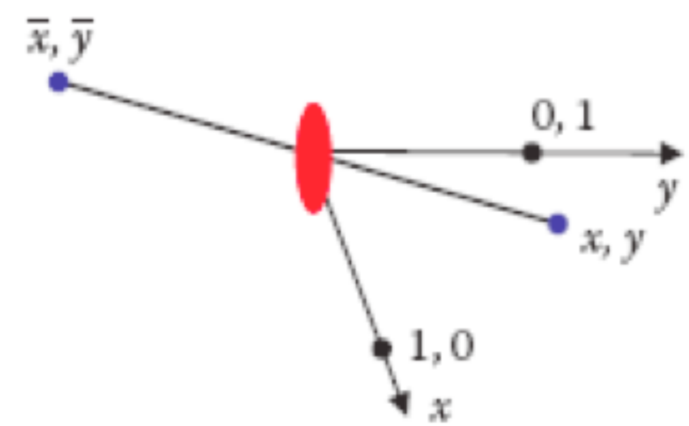
Point group **2** = {1,2}

Motif with symmetry of **2**



Where is the two-fold point?

drawing: M.M. Julian
Foundations of Crystallography



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

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

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

Crystallographic Point Groups in 2D

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

-group axioms?

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

Motif with symmetry of **2**

drawing: M.M. Julian
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-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?

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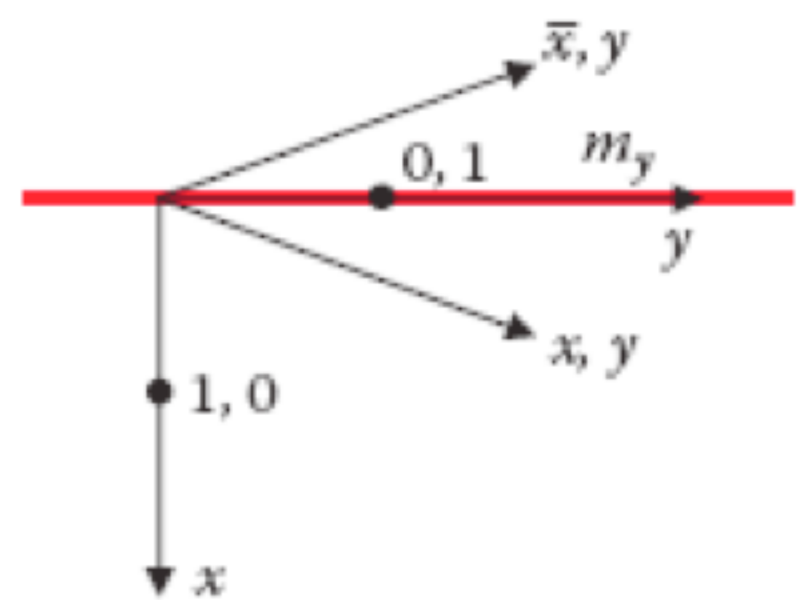
Mirror line m_y at 0,y



Matrix representation

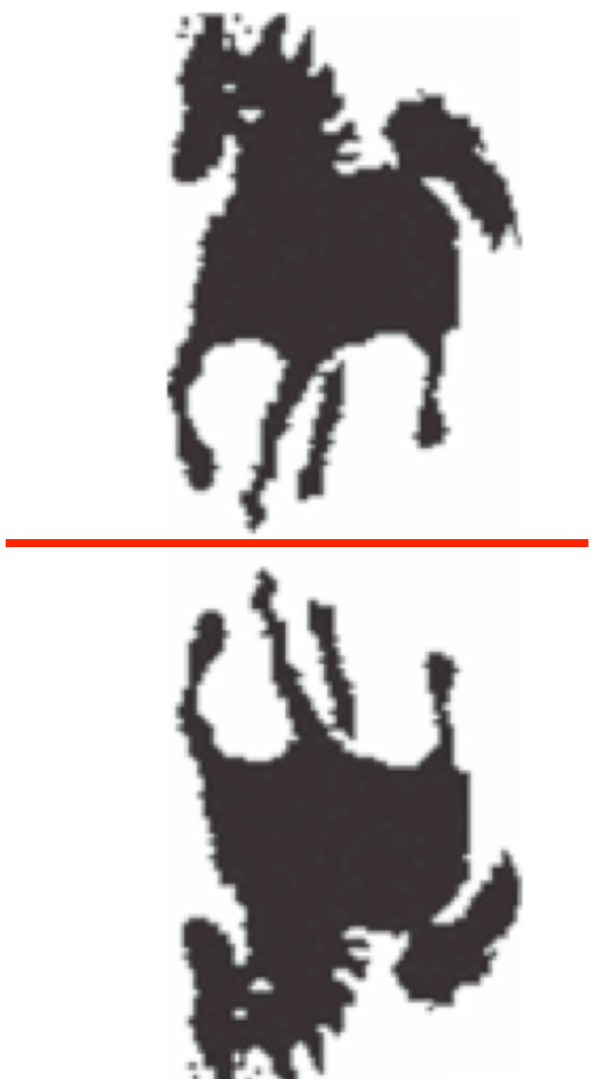
$$m_y \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ y \end{pmatrix} = \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

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

Crystallographic Point Groups in 2D

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

Motif with symmetry of **m**



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-group axioms?

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

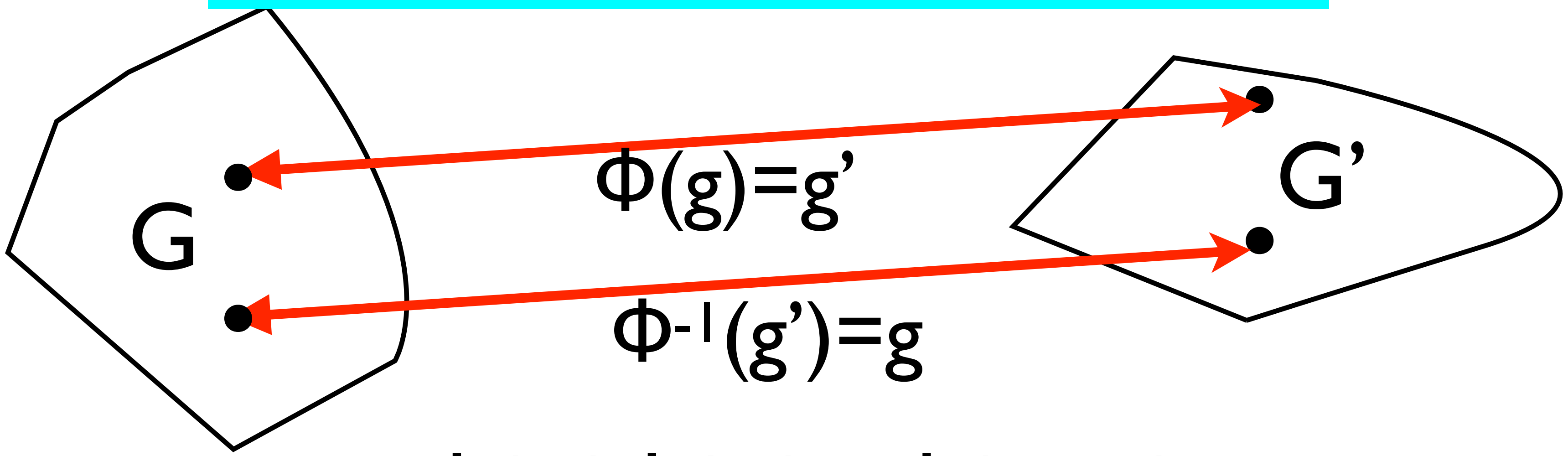
-order of **m**?

-multiplication table

$\times$	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}

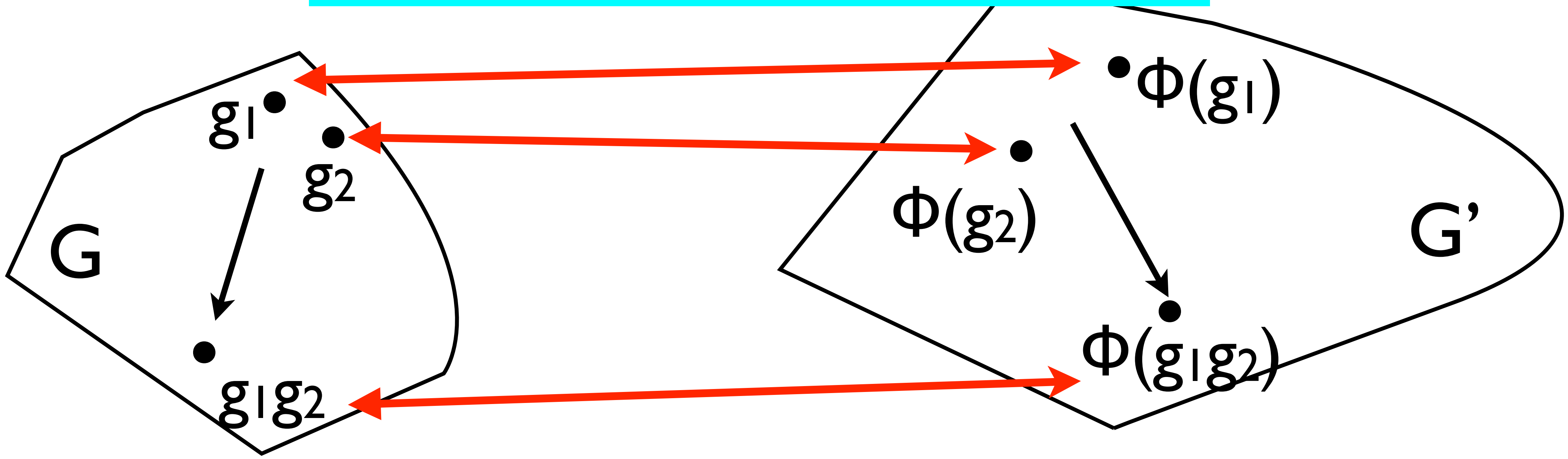
×	1	2
1	1	2
2	2	1

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

×	1	m_y
1	1	m_y
m_y	m_y	1

-groups with the same multiplication table

Isomorphic groups



$$\Phi(g)=g'$$

$$G=\{g\} \longleftrightarrow G'=\{g'\}$$

$$\Phi^{-1}(g')=g$$

$\Phi: G \longrightarrow G'$ $\quad \Phi^{-1}: G' \longrightarrow G$

homomorphic condition $\Phi(g_1)\Phi(g_2)= \Phi(g_1g_2)$

-groups with the same multiplication table

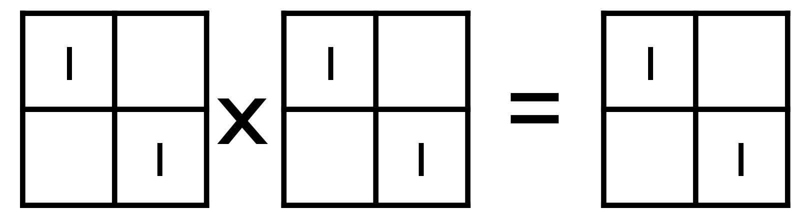
Crystallographic Point Groups in 2D

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

Motif with symmetry of **1**

drawing: M.M. Julian
Foundations of Crystallography

-group axioms?

1 x 1 = 

-order of **1**?

-multiplication table

×	1
1	1

-generators of **1**?

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

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

$$\begin{cases} x' = R_{11}x + R_{12}y \\ y' = R_{21}x + R_{22}y \end{cases}$$

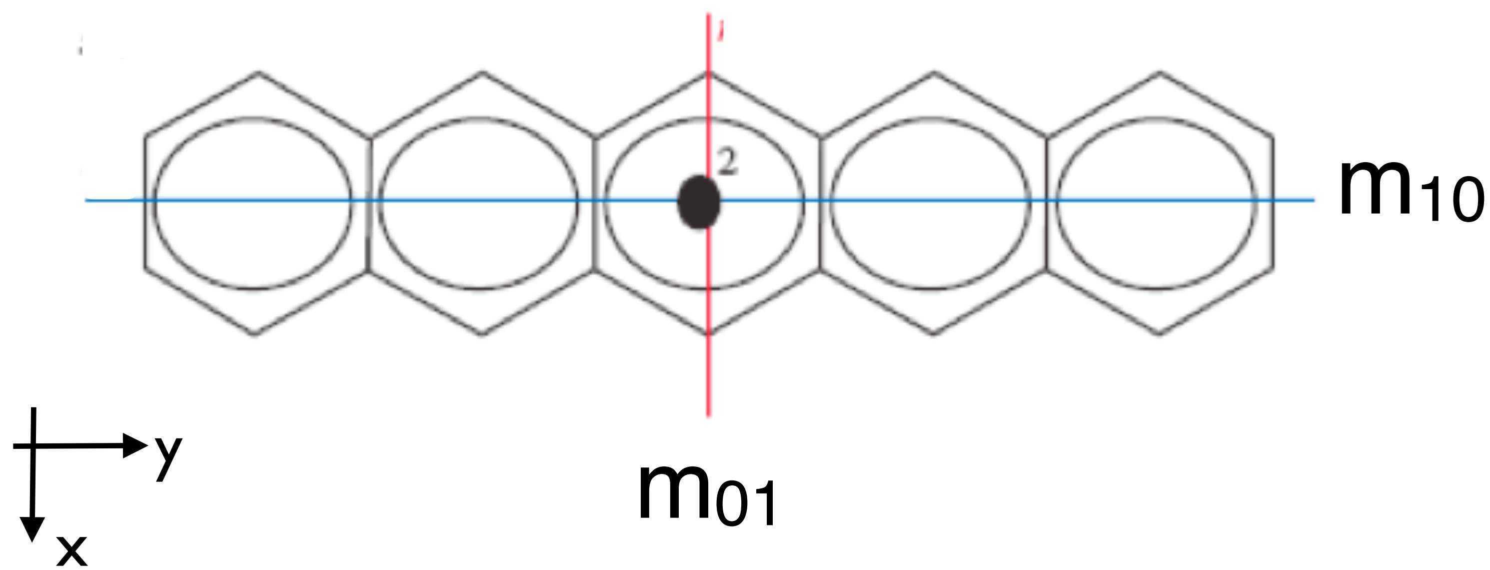
notation:

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

$$\begin{pmatrix} 0 & -1 \\ -1 & 1 \end{pmatrix} \longrightarrow \begin{cases} -y, -x+y \\ \bar{y}, \bar{x}+y \end{cases}$$

Problem 2.1

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



Determine:

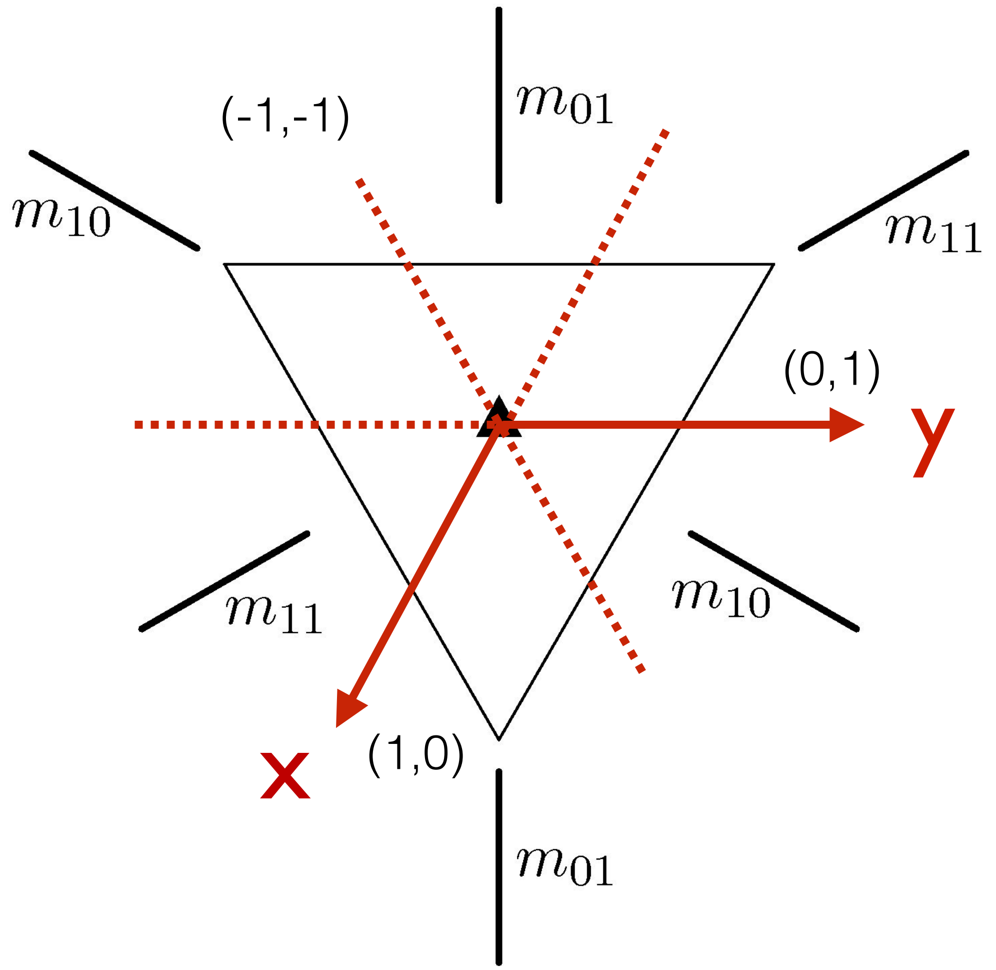
-symmetry operations:
matrix and (x,y) presentation

-generators

-multiplication table

Problem 2.3

Consider the symmetry group of the equilateral triangle. Determine:



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

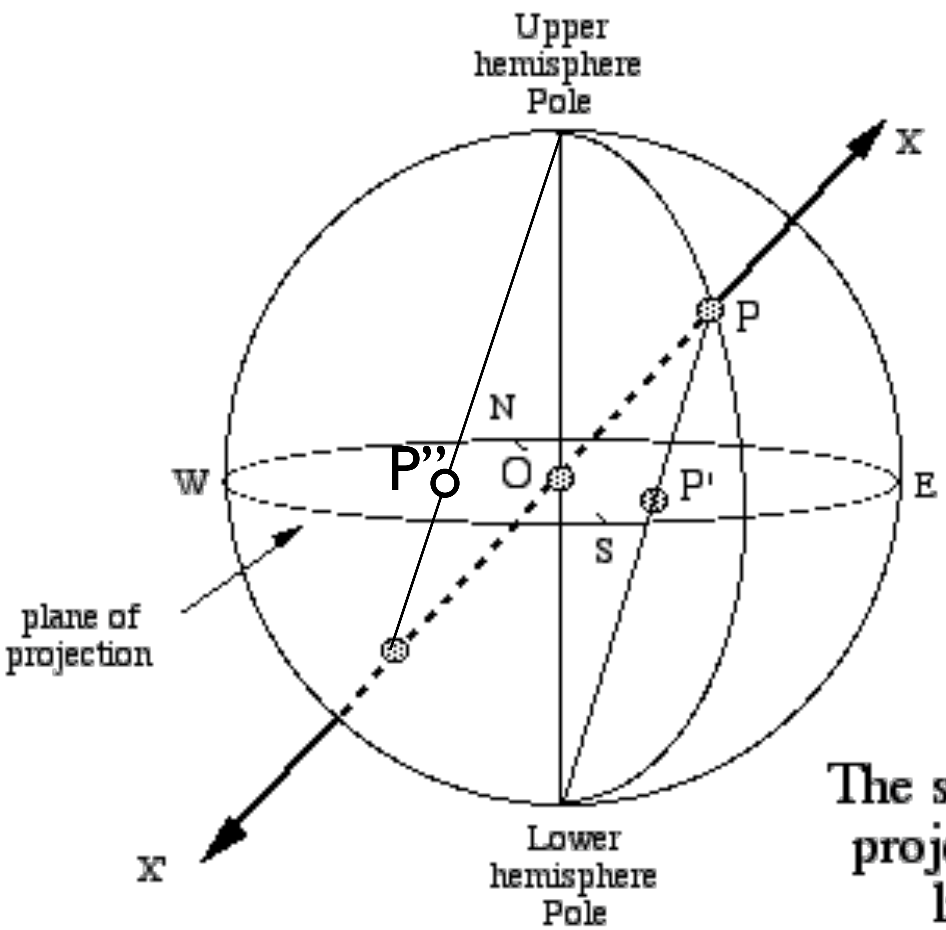
-generators

-multiplication table

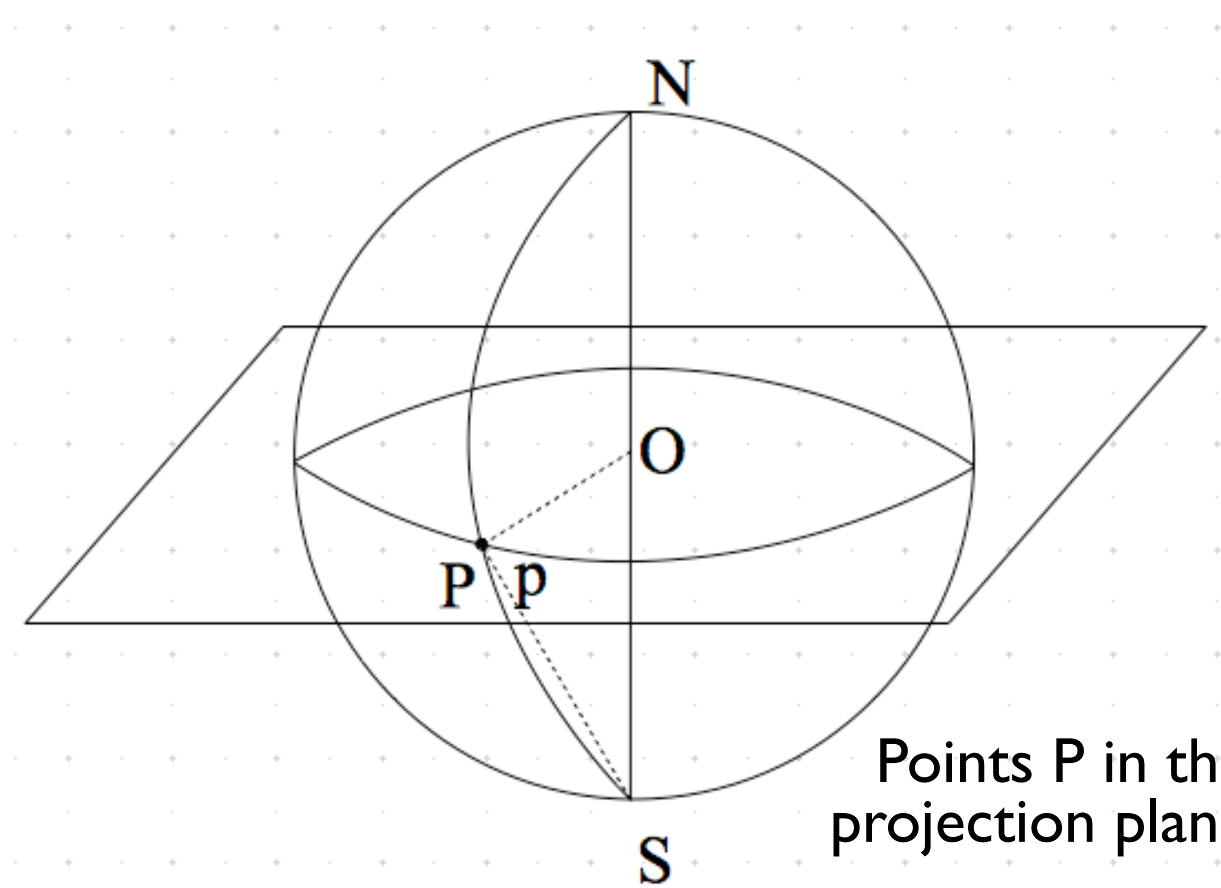
Visualization of Crystallographic Point Groups

- general position diagram
- symmetry elements diagram

Stereographic Projections



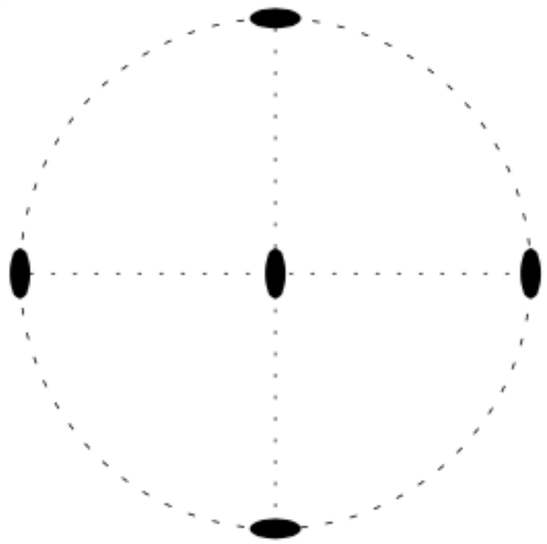
The stereographic projection of the line X-X'



Points P in the projection plane

Rotation axes

Symmetry-elements diagrams



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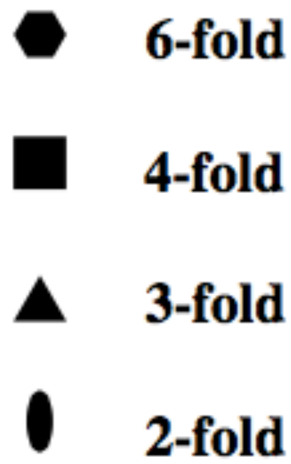
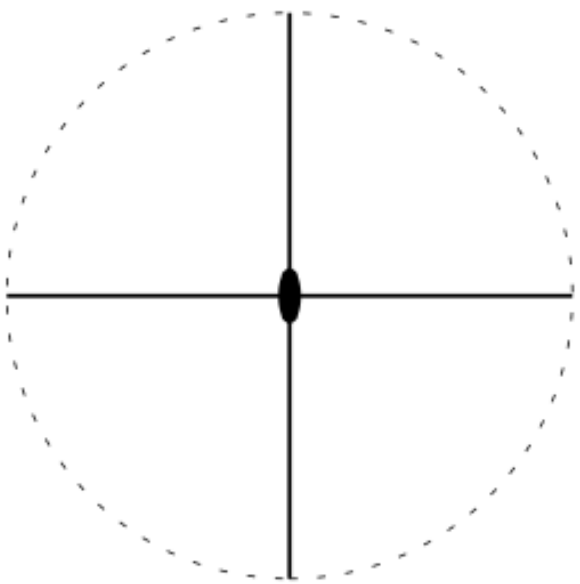
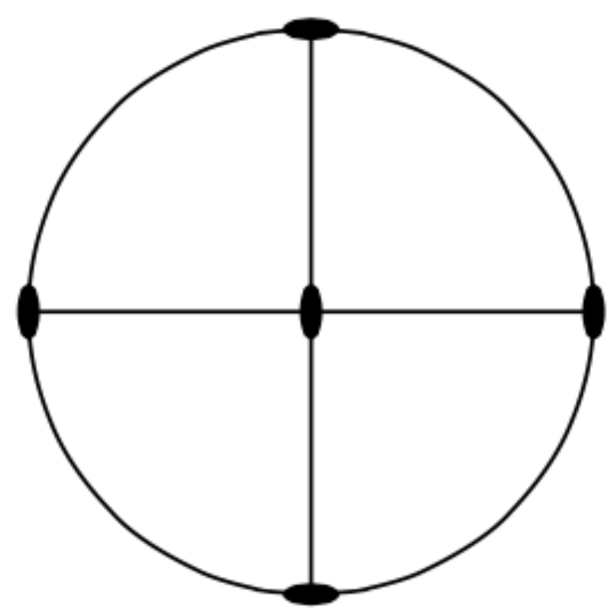


filled polygons with the same number of sides as the foldness of the axes

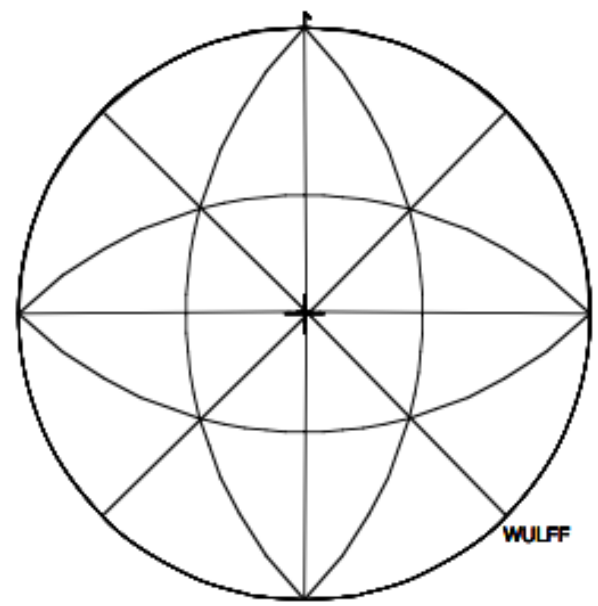
Mirror planes



2mm



2/m 2/m 2/m



Combinations of symmetry elements

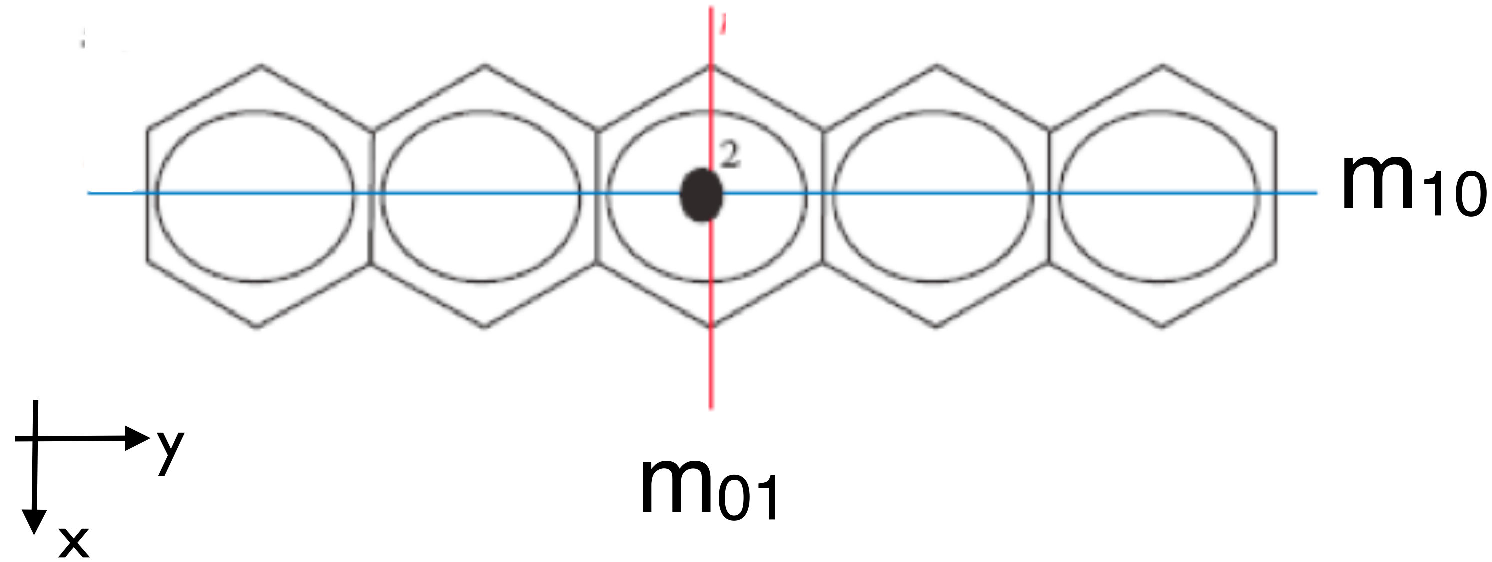
- **line of intersection of any two mirror planes must be a rotation axis**.

EXAMPLE

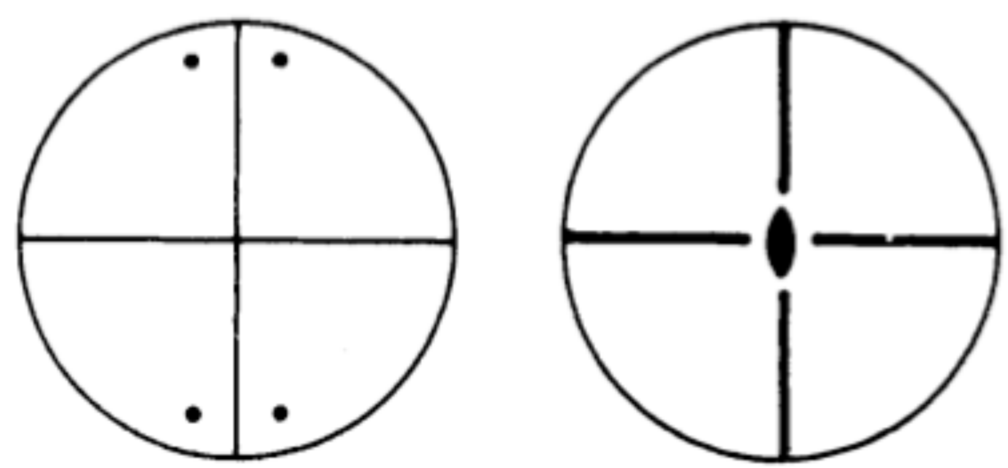
Stereographic Projections of ***mm2***

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

Molecule of pentacene



Stereographic projections diagrams

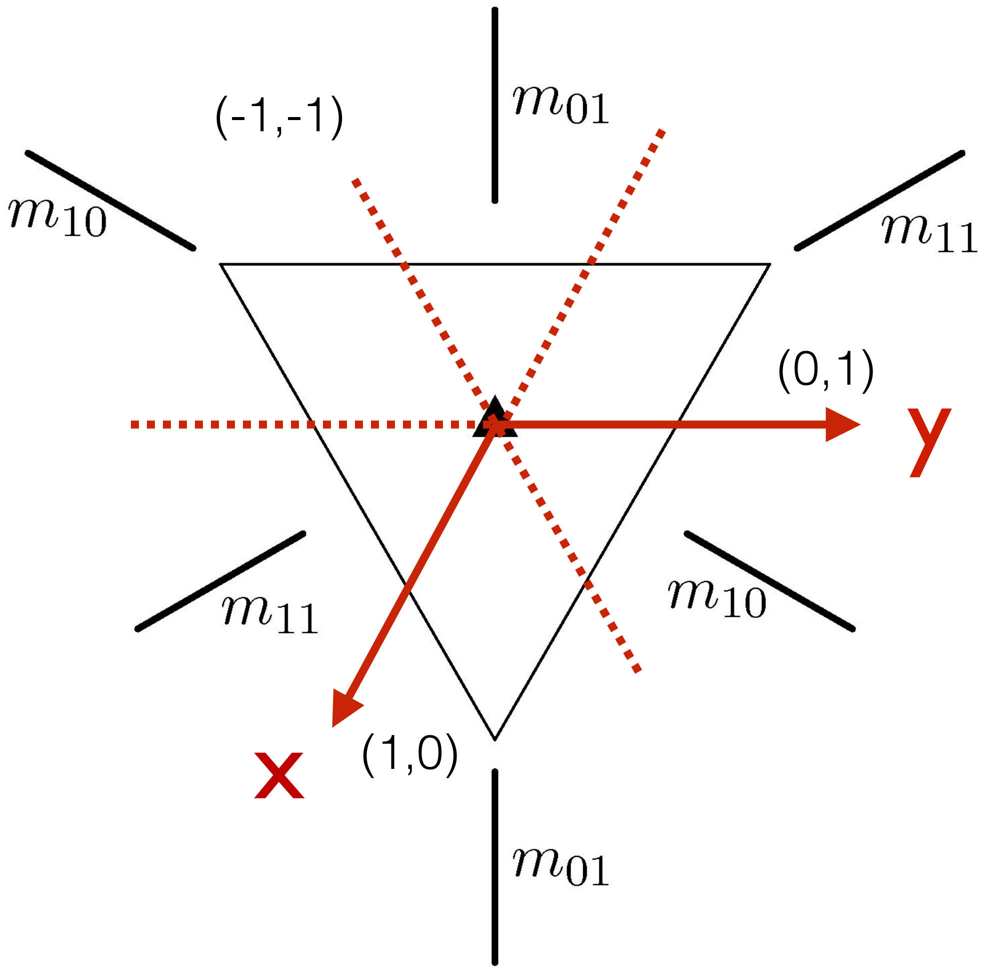


general position

symmetry elements

EXAMPLE

Stereographic Projections of *3m*



Point group **3m** =

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

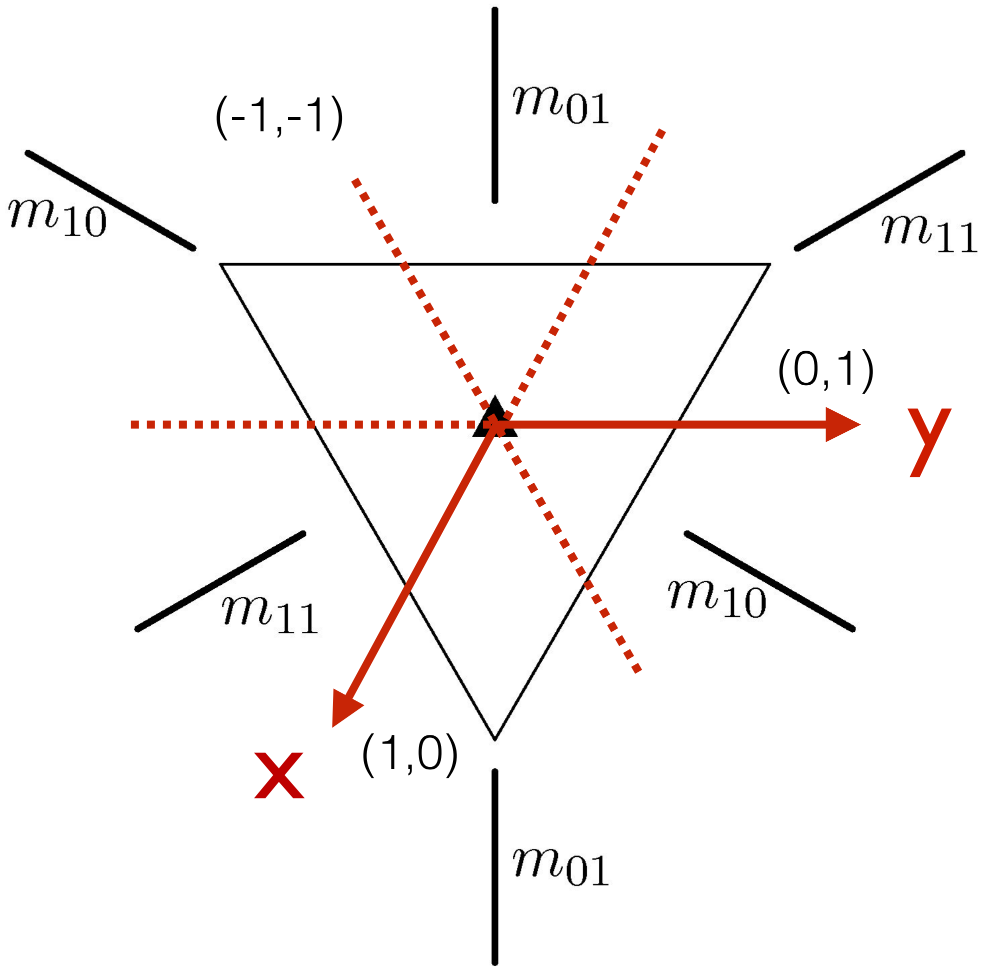
Stereographic projections diagrams

general position **?**

? symmetry elements

EXAMPLE

Stereographic Projections of ***3m***

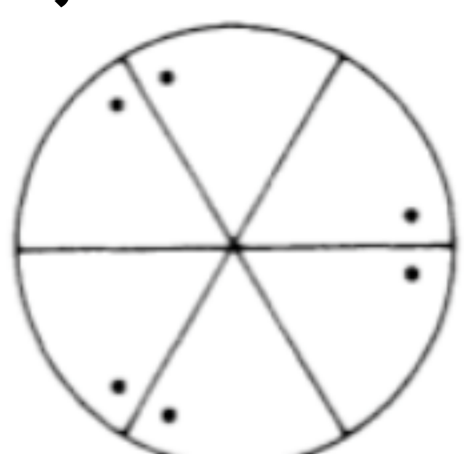


Point group **3m** =

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

Stereographic projections diagrams

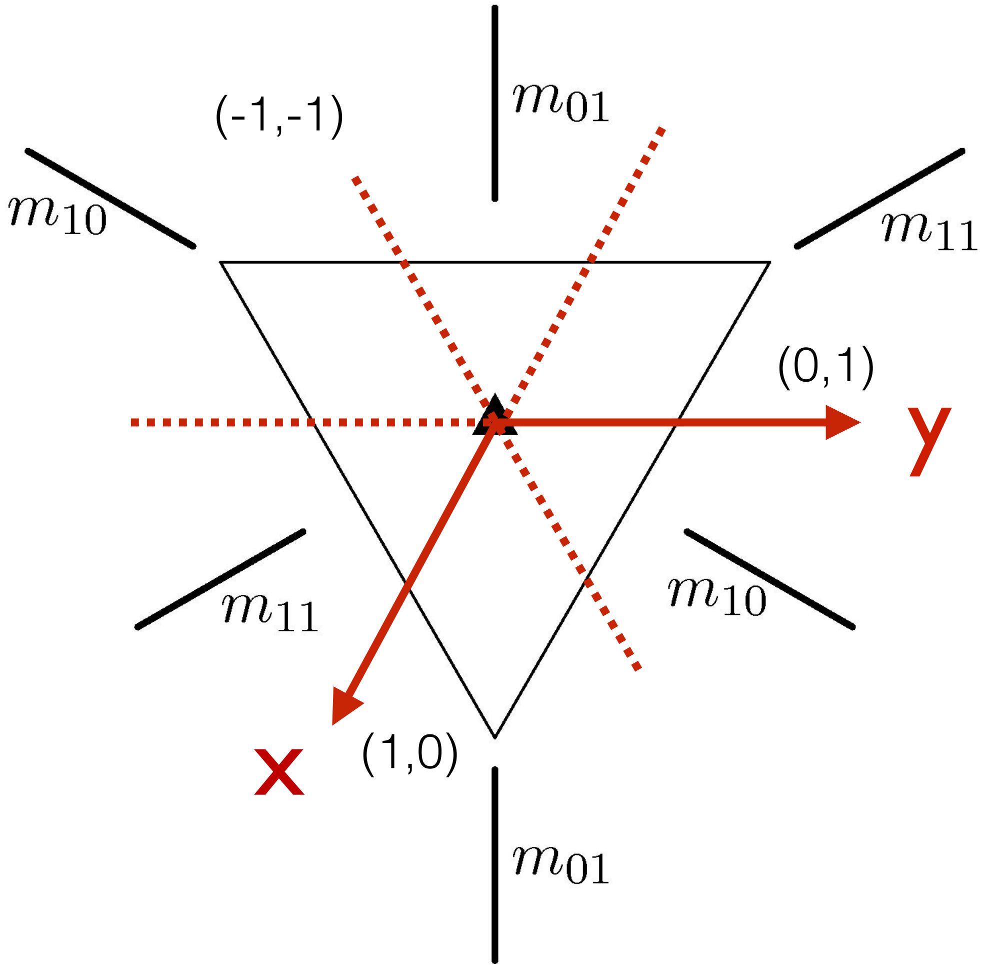
general position

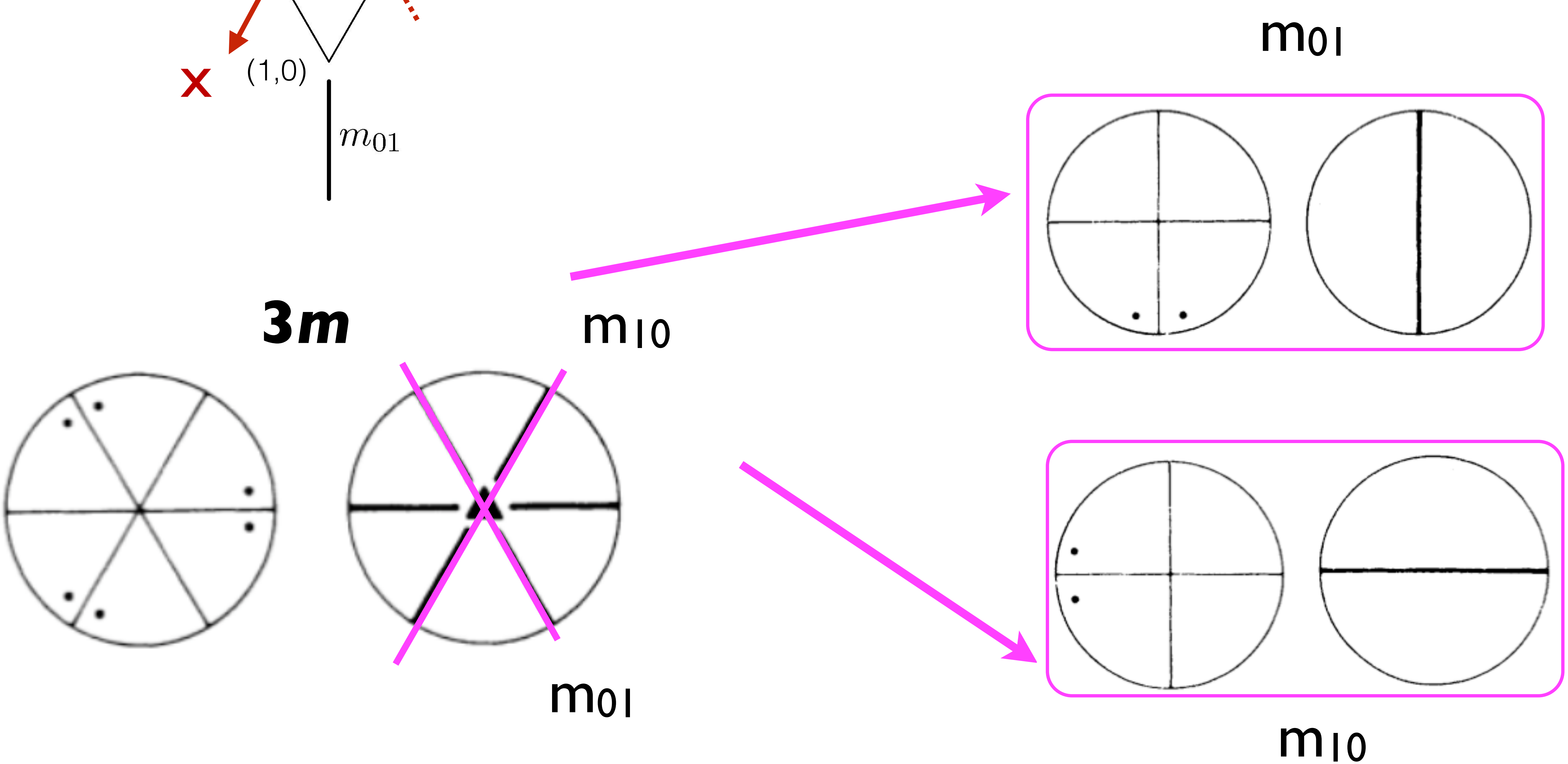


symmetry elements

Conjugate elements

$$m_{10} \overset{3^+}{\sim} m_{01}$$





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 $g_i \notin L(g_j)$

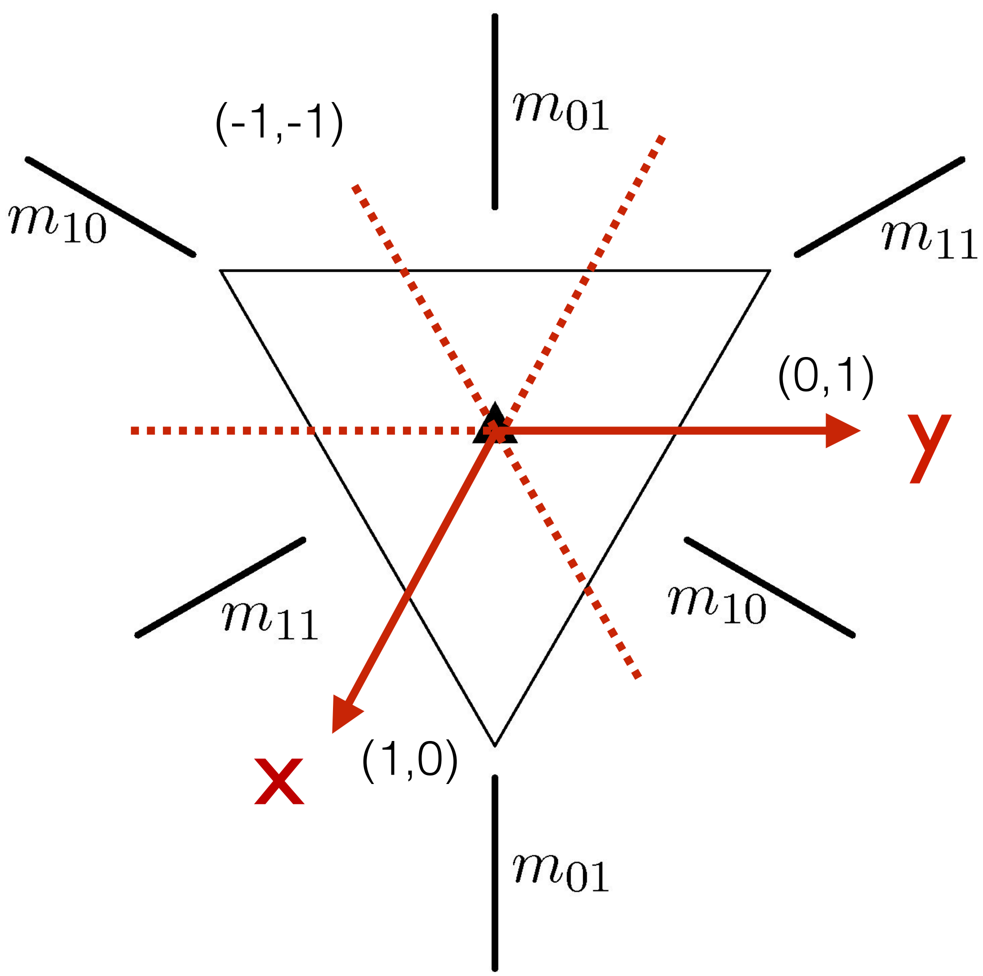
(ii) $|L(g_i)|$ is a divisor of $|G|$ (iii) $L(e)=\{e\}$

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

Problem 2.3 (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

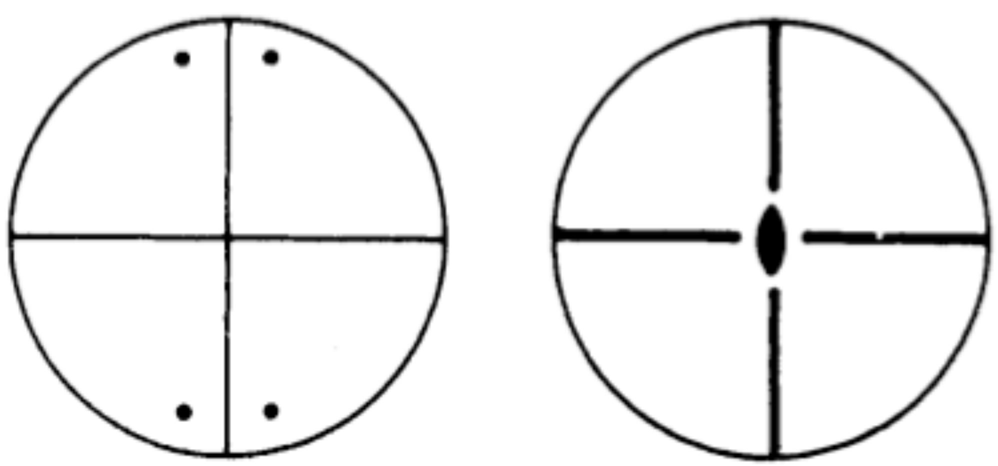
EXERCISES

Problem 2.1 (cont)

Distribute the symmetry elements of the group **mm2** = {1,2,m_{10},m_{01}} in classes of conjugate elements.

multiplication table

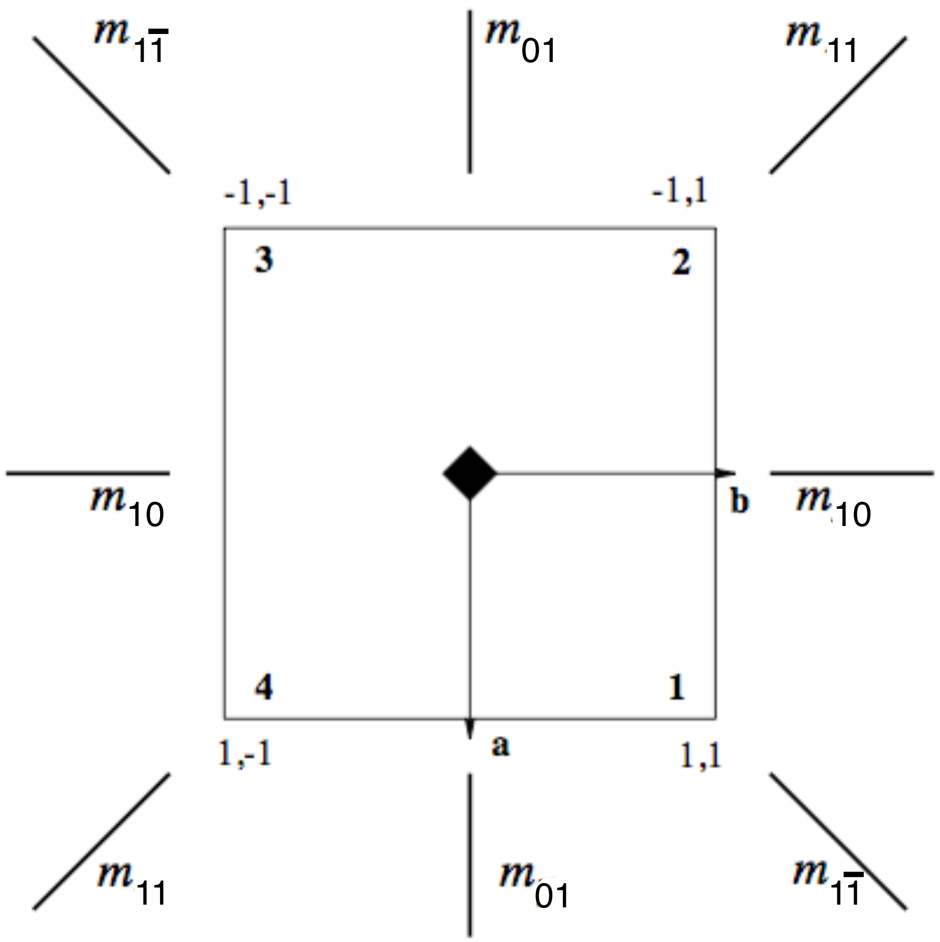
	1	2	m_{10}	m_{01}
1	1	2	m_{10}	m_{01}
2	2	1	m_{01}	m_{10}
m_{10}	m_{10}	m_{01}	1	2
m_{01}	m_{01}	m_{10}	2	1



stereographic projection

Problem 2.2

Consider the symmetry group of the square. Determine:



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

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

-generators

-multiplication table

-classes of conjugate elements

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

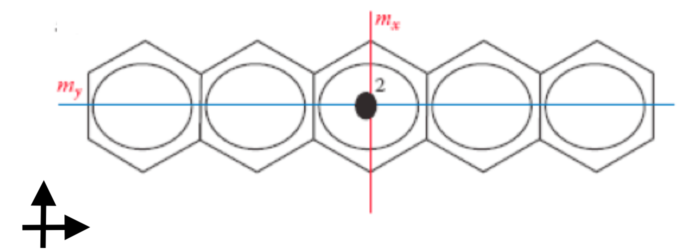
NO subgroup Z exists such that:

$H < Z < G$

Example

Subgroups of point groups

Molecule of pentacene



Subgroups of mm2

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

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

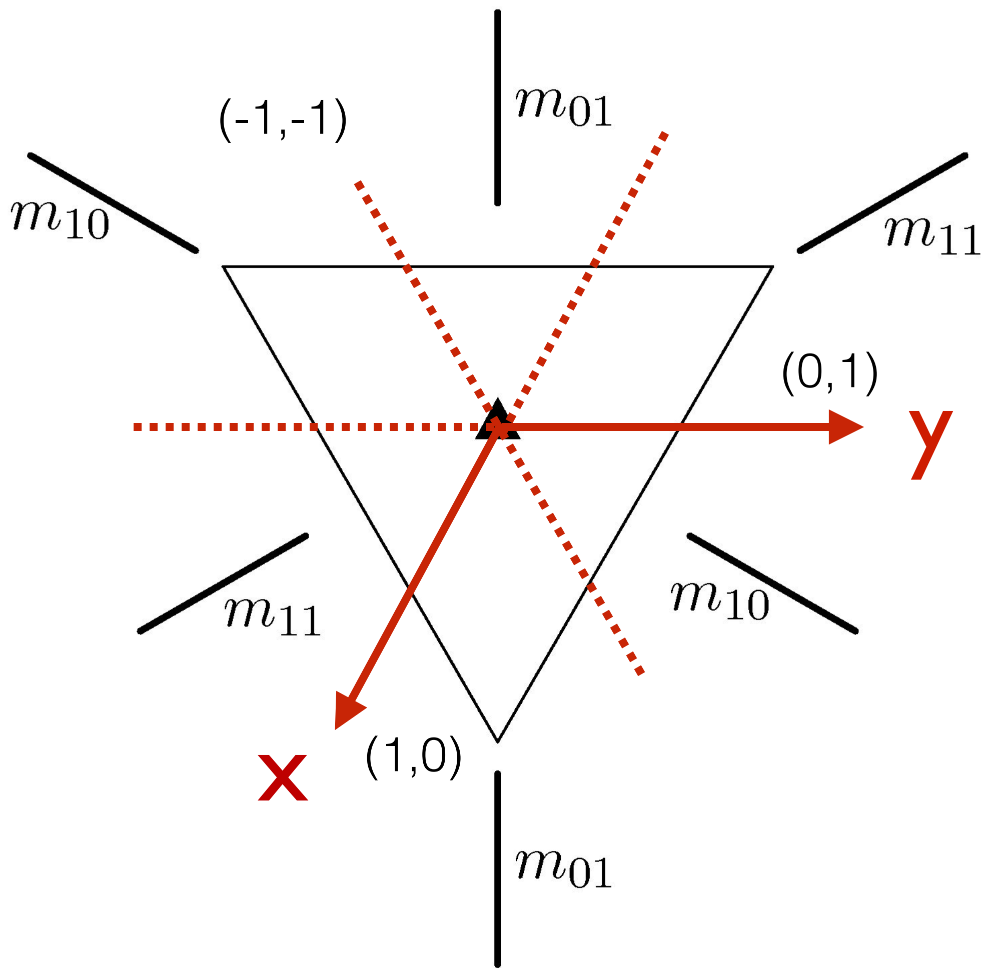
Subgroup graph

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

Problem 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: $G = H + g_2H + \ldots + g_mH$, $g_i \notin H$, m=index of H in G

right coset decomposition: $G = H + Hg_2 + \ldots + Hg_m$, $g_i \notin H$ m=index of H in G

Coset decomposition-properties

(i) $g_iH \cap g_jH = \{\varnothing\}$, 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

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

Theorem of Lagrange

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

then

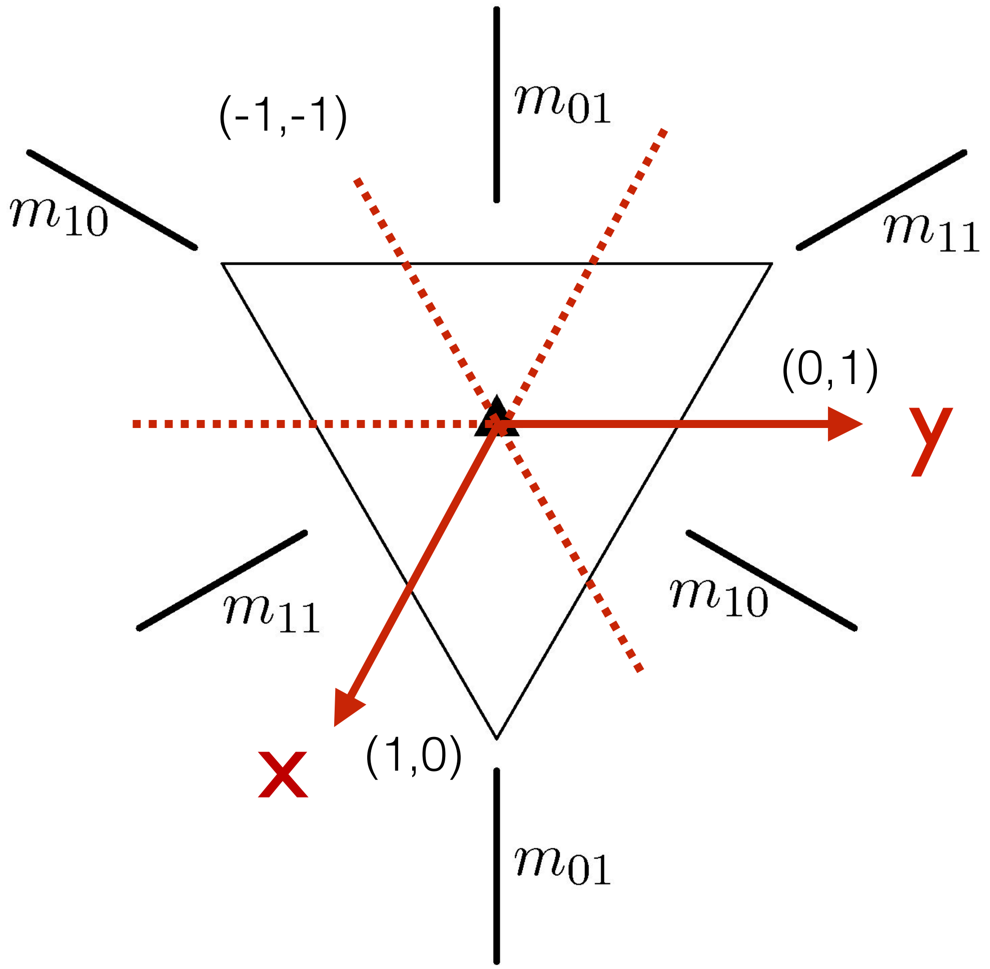
|H| is a divisor of |G|
and [i]=|G:H|

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

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

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

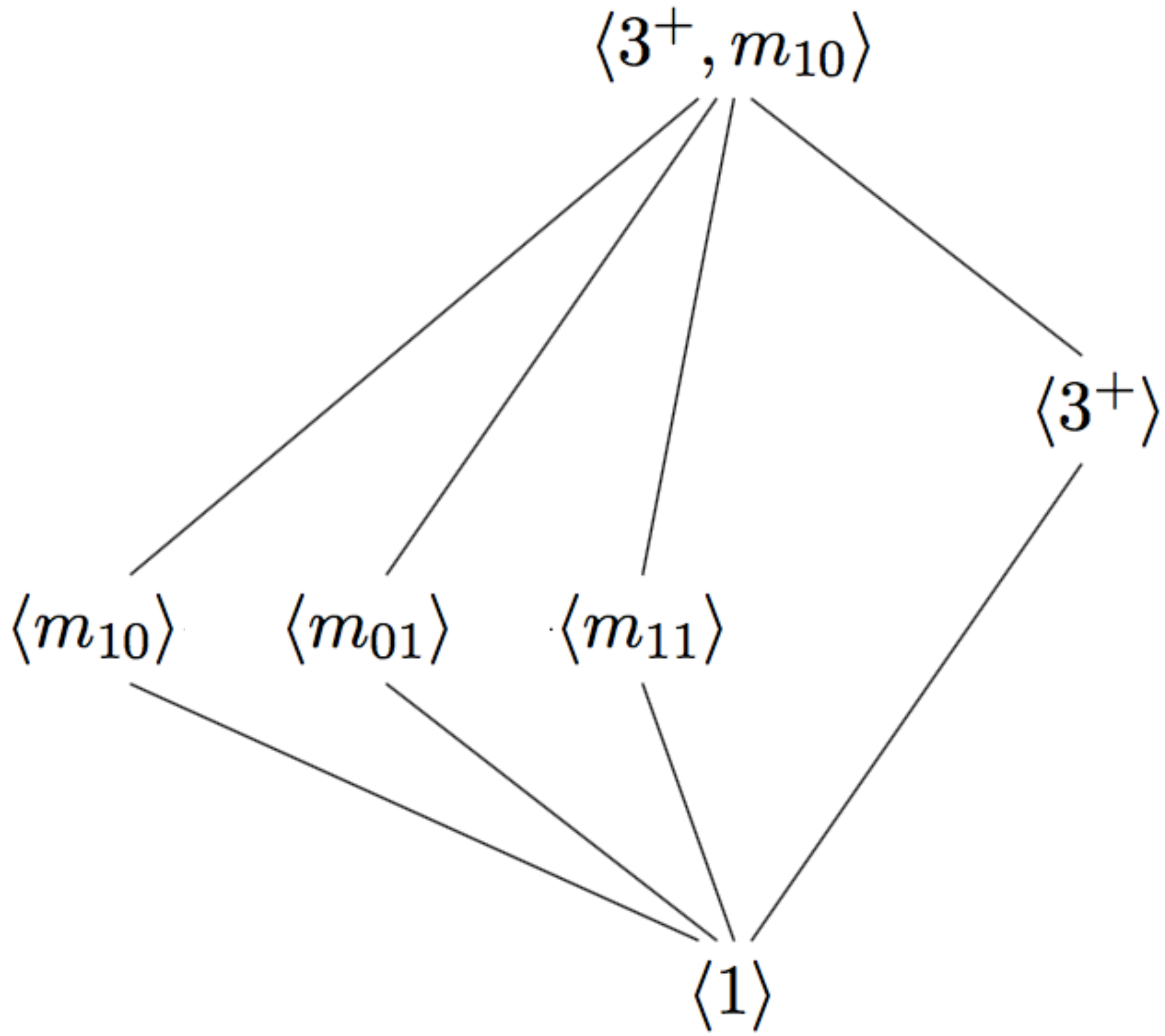
(iii) $|L(H)|$ is a divisor of $|G|/|H|$

Normal subgroup

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

Problem 2.5 (cont.)

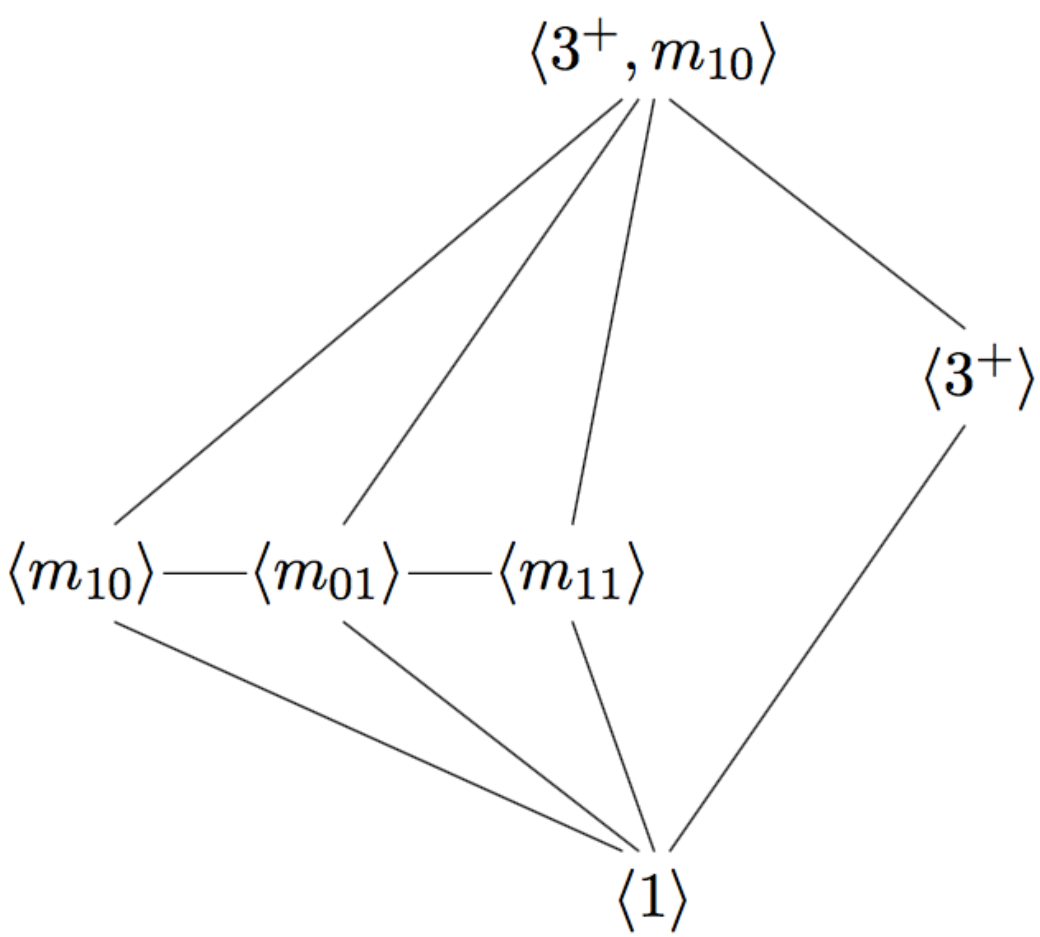
Consider the subgroups of ***3m*** and distribute them into classes of conjugate subgroups



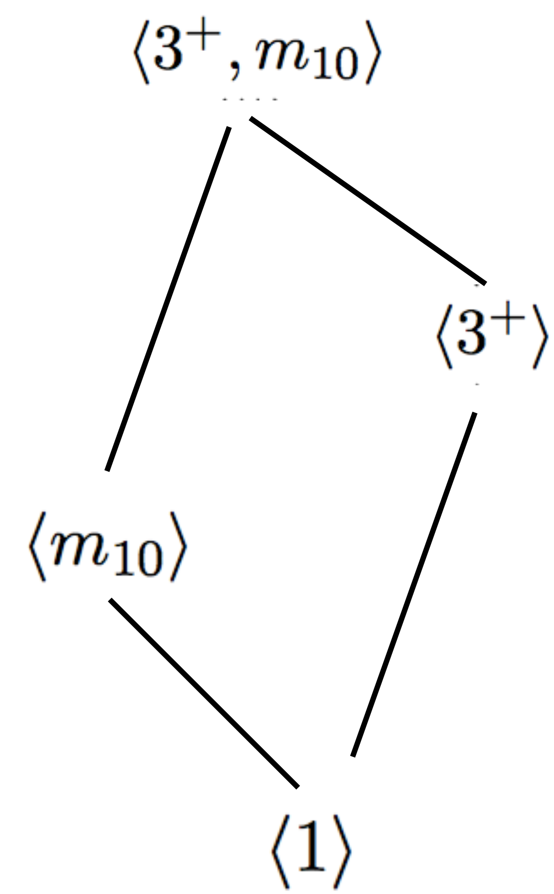
	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

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

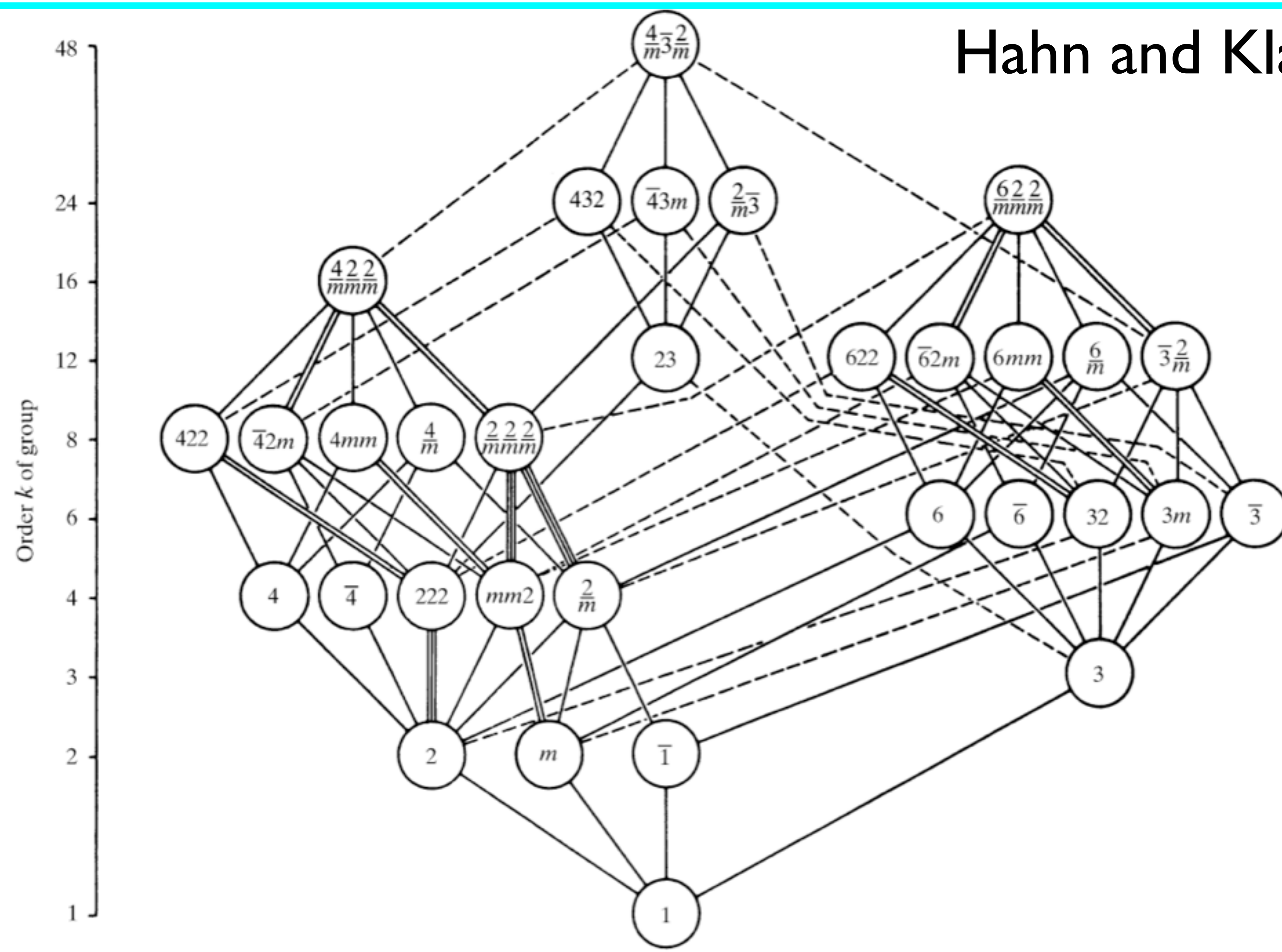


Fig. 10.1.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal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

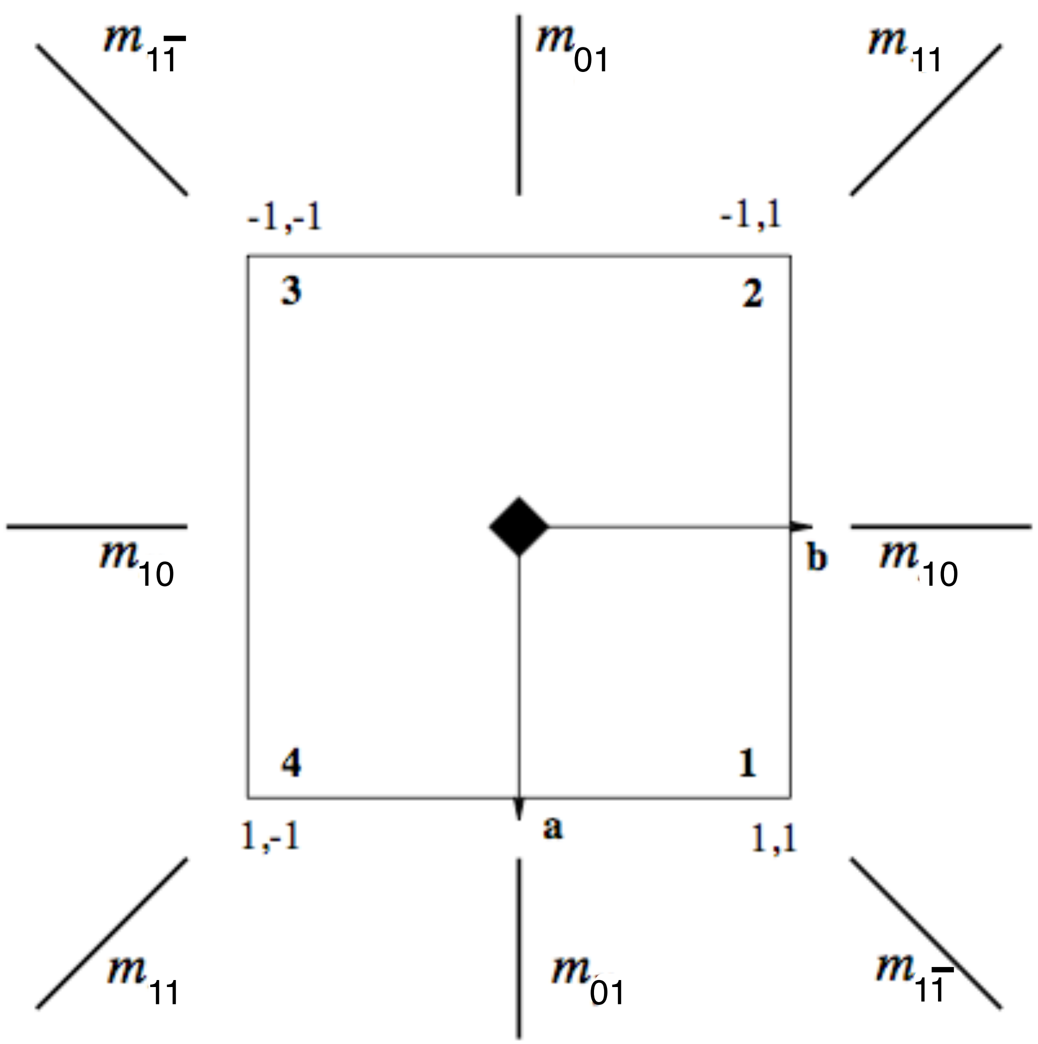
EXERCISES

Problem 2.4

(i) Consider the group of the square and determine its subgroups

(ii) Distribute the subgroups into classes of conjugate subgroups;

(iii) Construct the maximal-subgroup graph of ***4mm***



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

EXERCISES

Problem 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?

FACTOR GROUP

Factor group

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

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

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:

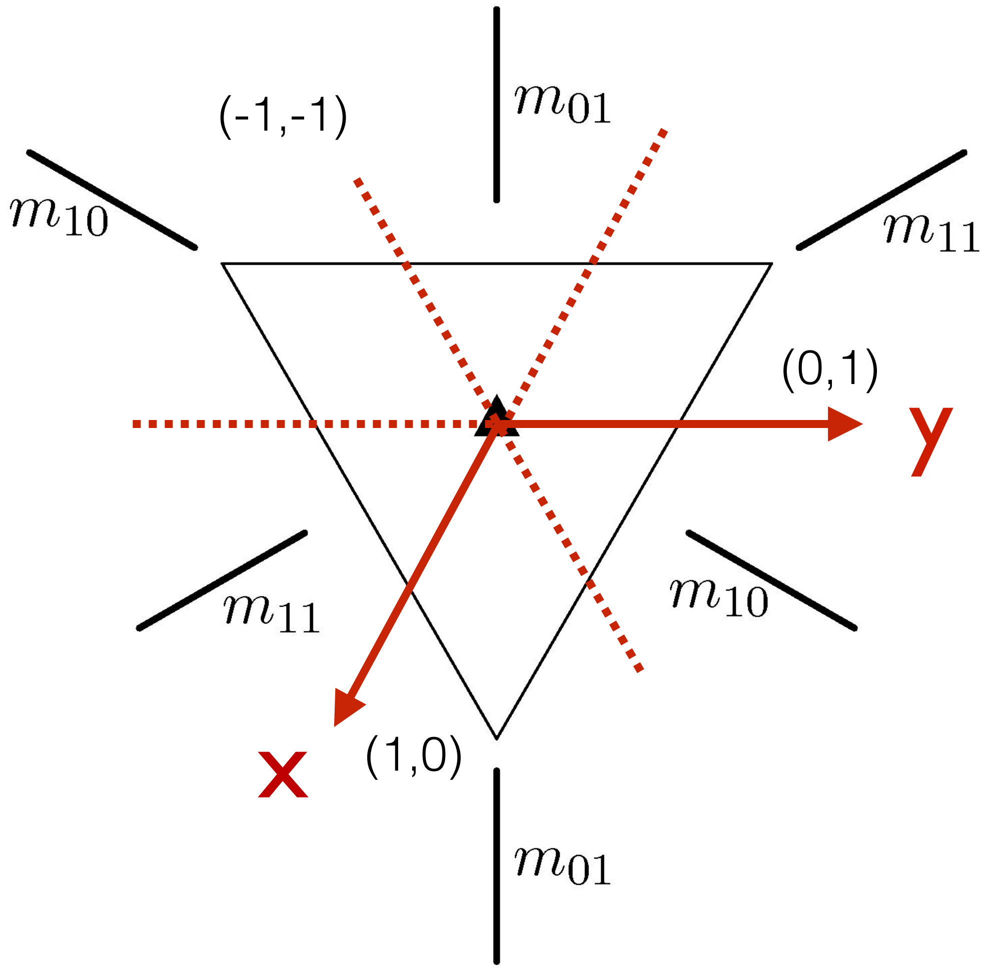
(i) $(g_iH)(g_jH) = g_{ij}H$

(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***

Consider the subgroup ***3***={1,3^+,3^-} of ***3m***

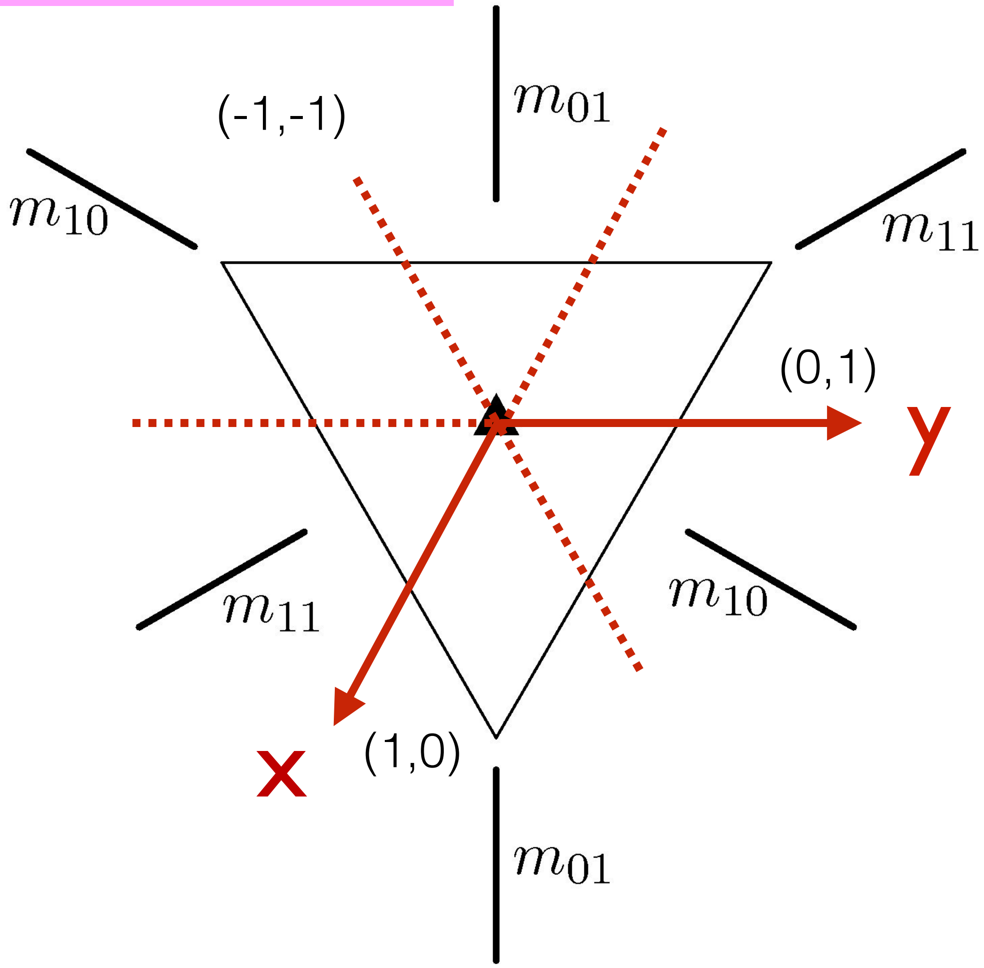
(i) Show that the cosets of the decomposition ***3m***:***3*** fulfil the group axioms and form a factor group

(ii) Construct the multiplication table of the factor group

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

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

E A

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

(ii) factor group and multiplication table

	E	A
E	E	A
A	A	E

Problem 2.6 (cont)

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

(3) Show that the cosets of the decomposition ***4mm***:{e,2} fulfil 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

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

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_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

$S_o = 1 = \{1\}$

Multiplicity: $|P|$

Special position X_o

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

Multiplicity: $|P|/|S_o|$

Site-symmetry groups: oriented symbols

Example

General and special Wyckoff positions

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

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

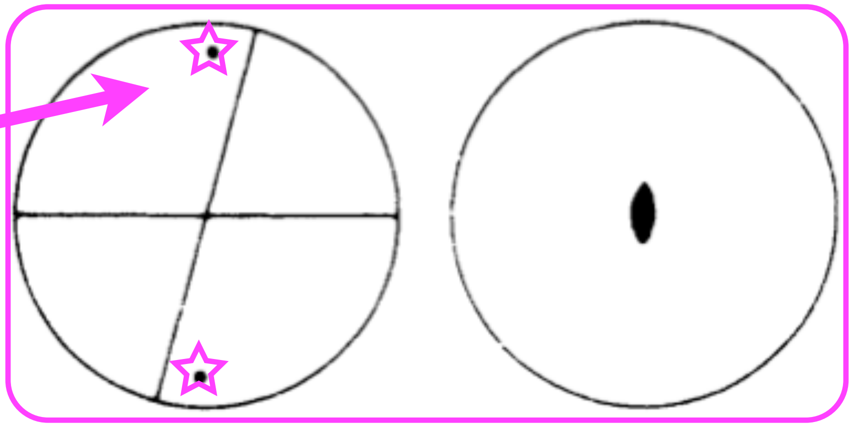
$S_o = \mathbf{2}$

$WX_o = X_o$

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

Multiplicity: $|P|/|S_o|$

2	b	1	(x,y,z) (-x,-y,z)
1	a	2	(0,0,z)



Example

General and special Wyckoff positions

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

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

S_o = **mm2**

$WX_o = X_o$

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

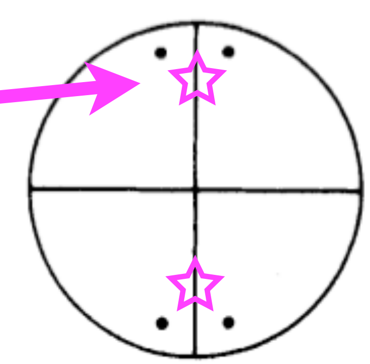
$$m_y: \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$$

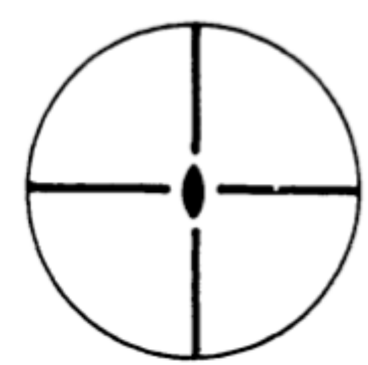
4 d 1 (x,y,z) (-x,-y,z) (x,-y,z) (-x,y,z)

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

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

1 a mm2 (0,0,z)





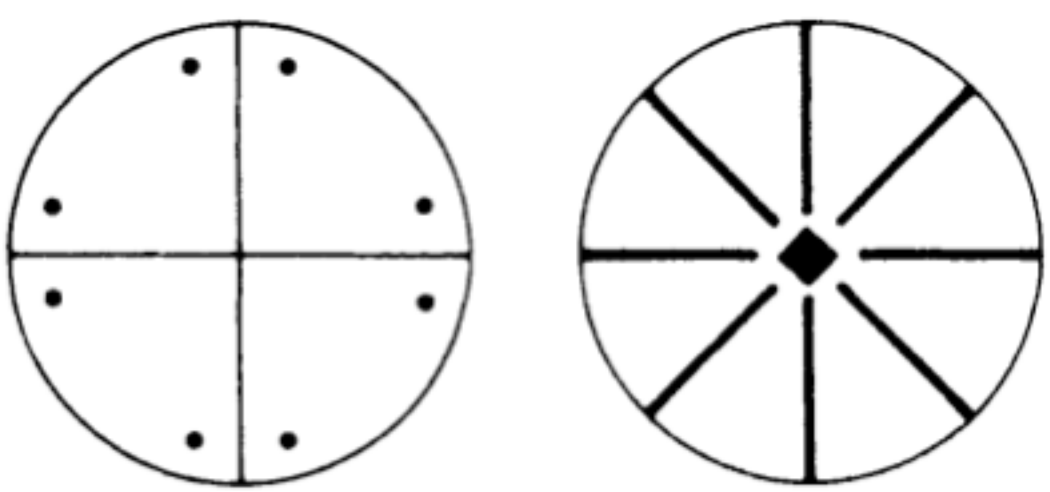
EXERCISES

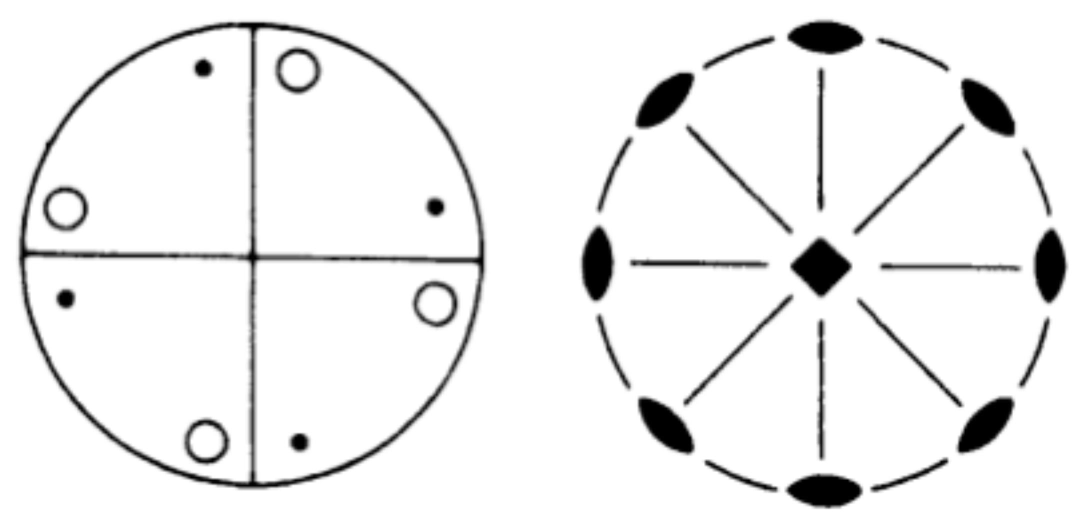
Problem 2.8

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



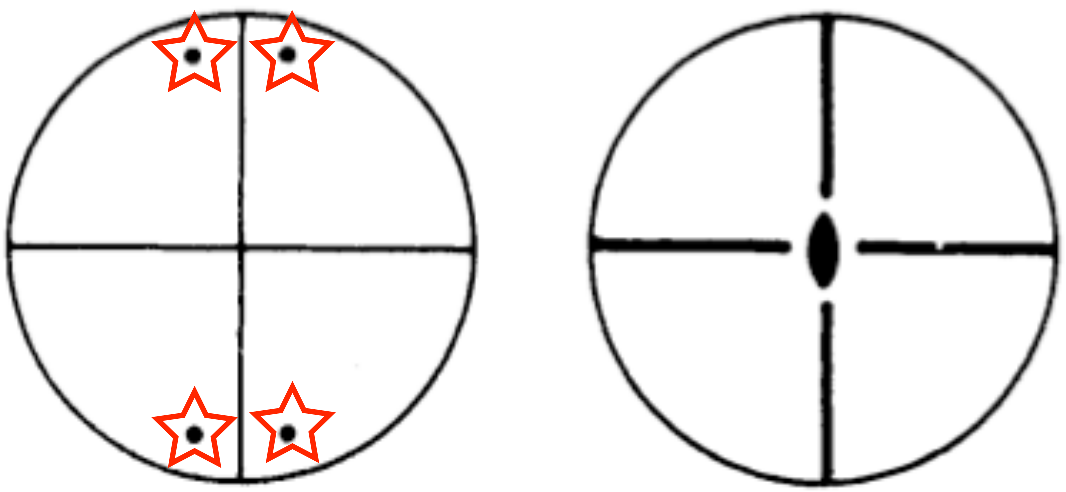


EXAMPLE

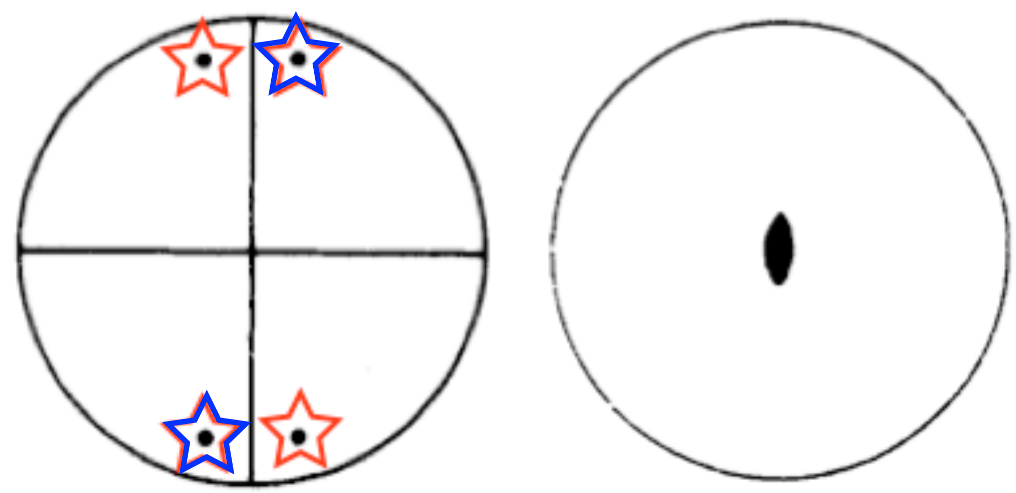
Wyckoff positions splitting schemes

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

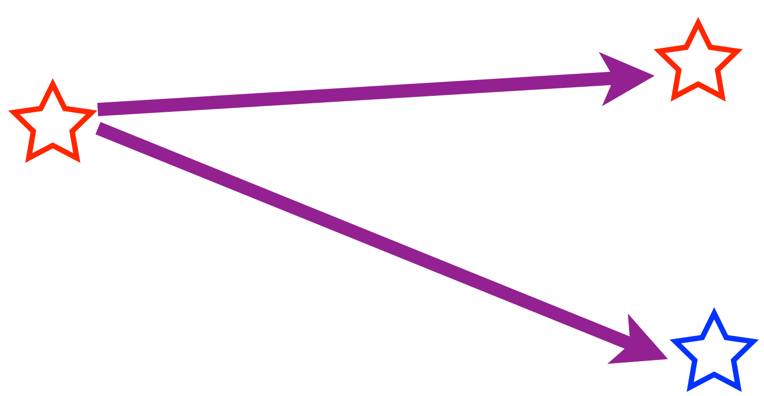
mm2



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=$-x_2,-y_2,z_2$

EXERCISES

Problem 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