Lecture Course
GROUP THEORY AND TOPOLOGY

Donostia - San Sebastian

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GROUP THEORY
(few basic facts)

1. Crystallographic symmetry operations

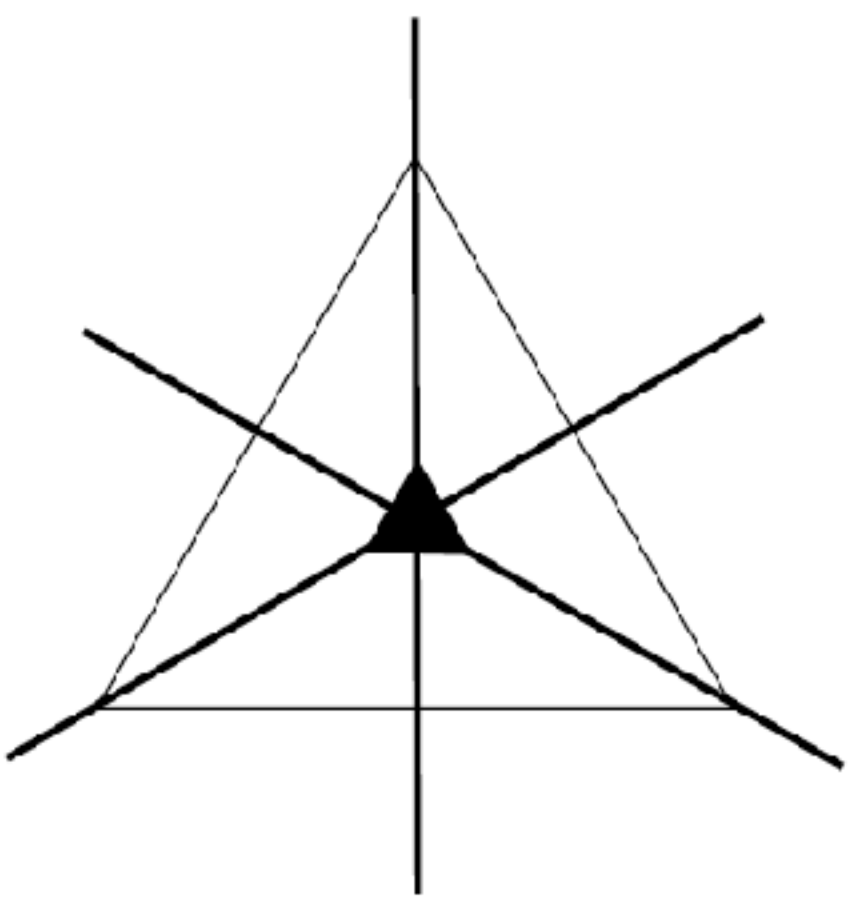
Symmetry operations of an object

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

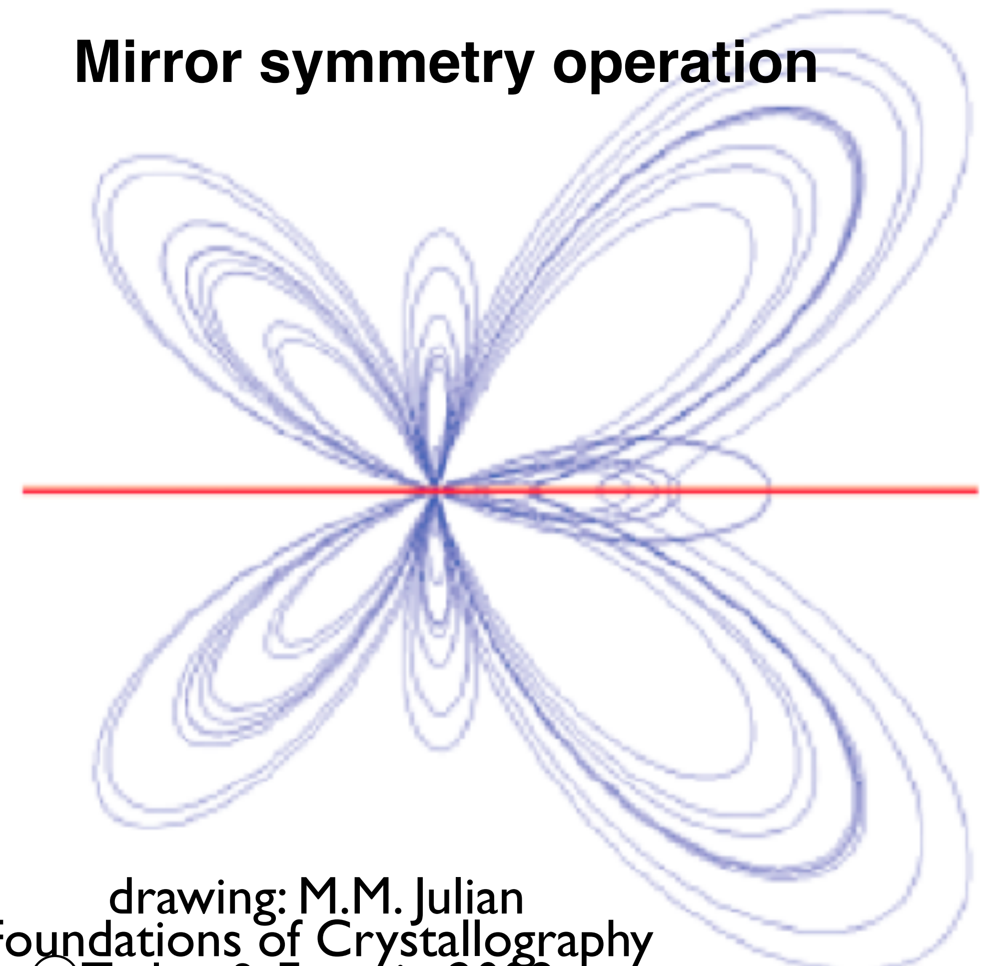
If the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.



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.

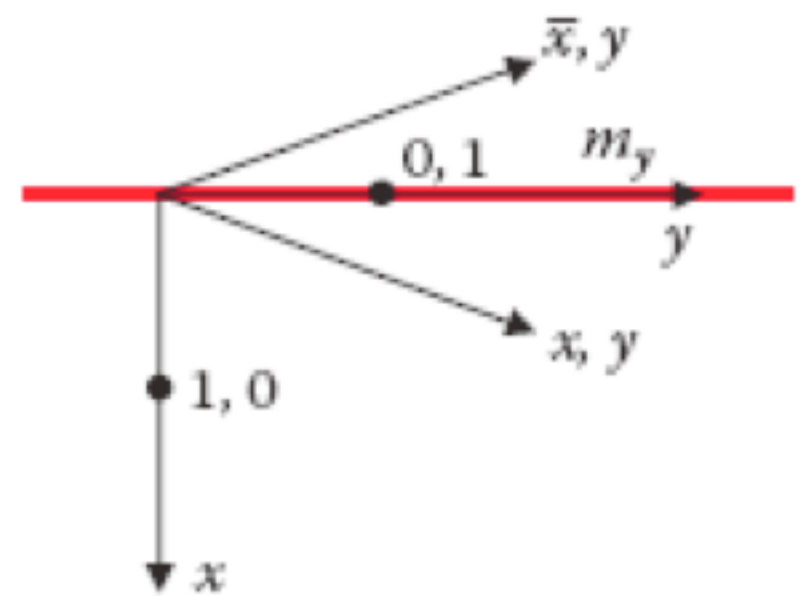
Symmetry operations in the plane
Matrix representations

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Matrix representation

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

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

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:**

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

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

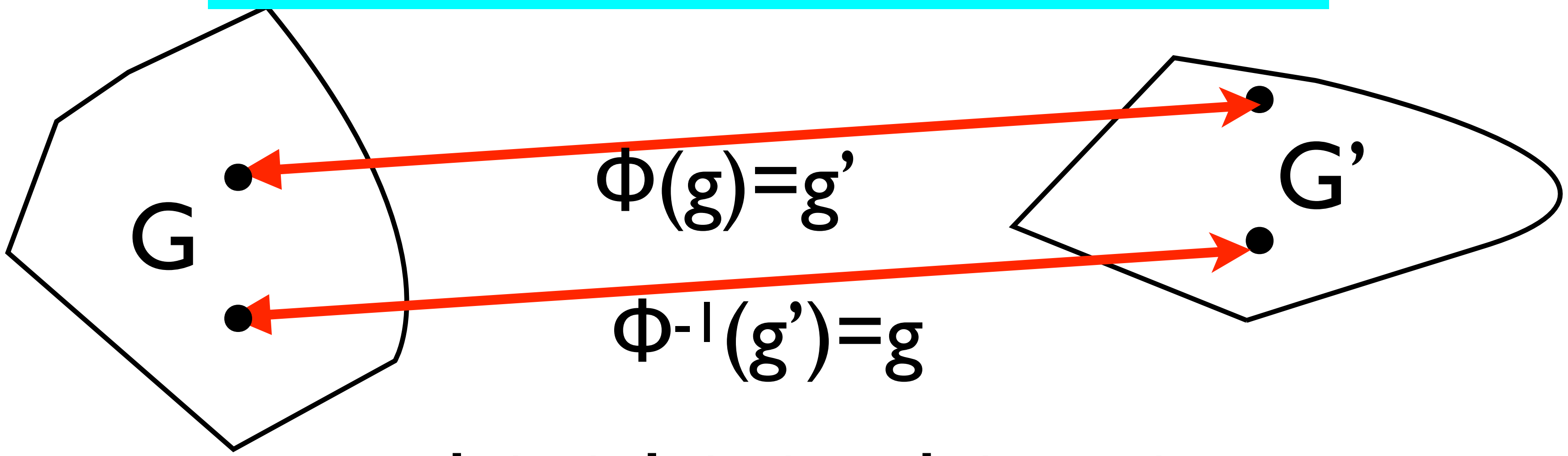
Multiplication table

	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

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}

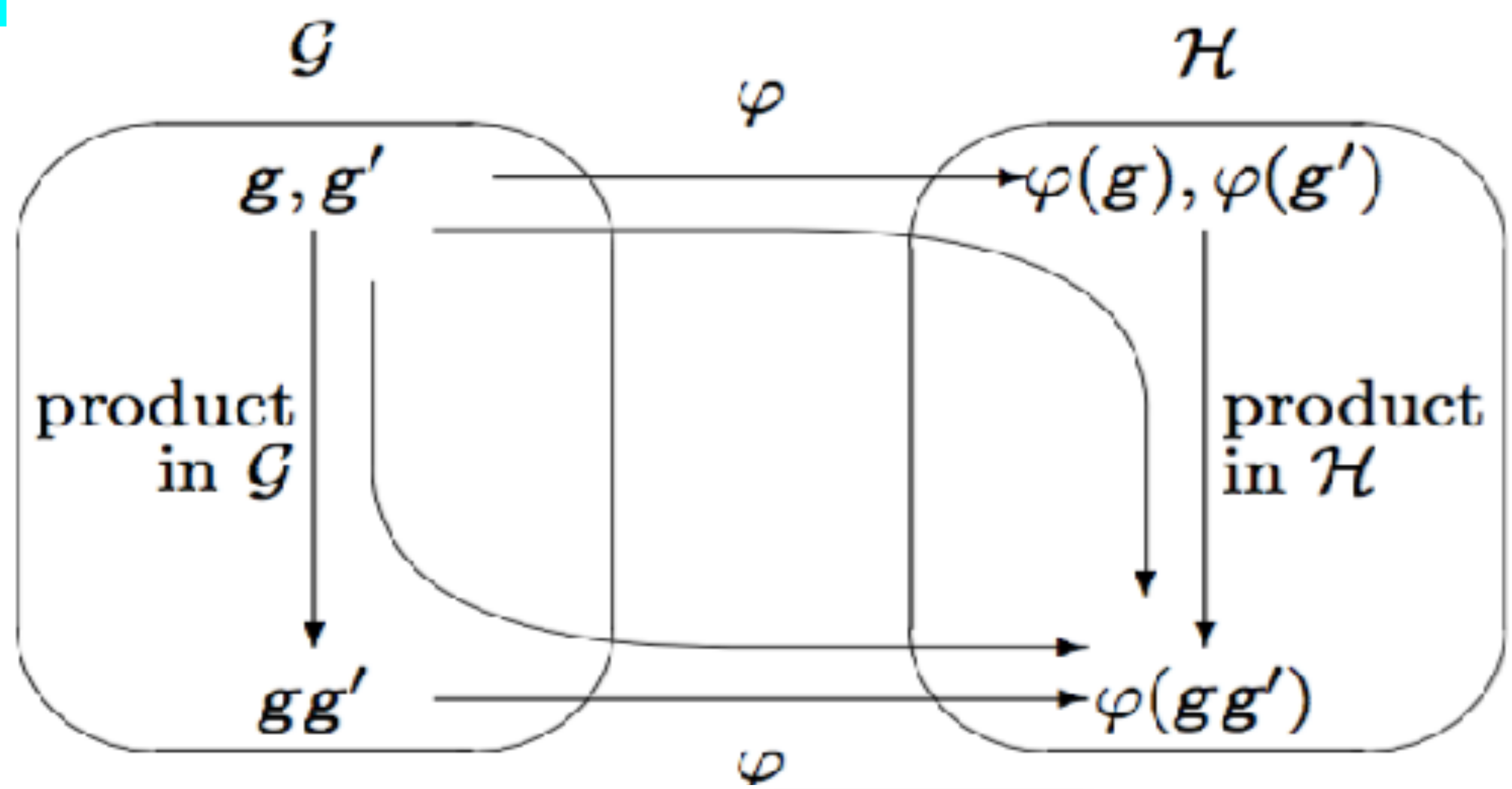
×	1	m_y
1	1	m_y
m_y	m_y	1

-groups with the same multiplication table

Homomorphism

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

homomorphic condition $\varphi(gg') = \varphi(g)\varphi(g')$ for all $g, g' \in \mathcal{G}$



The set $\{g \in \mathcal{G} \mid \varphi(g) = e\}$ is called the *kernel* of φ, denoted by $\ker(\varphi)$

The set $\varphi(\mathcal{G}) = \{\varphi(g) \mid g \in \mathcal{G}\}$ is called the *image* of φ, denoted by $\mathrm{im}(\varphi)$

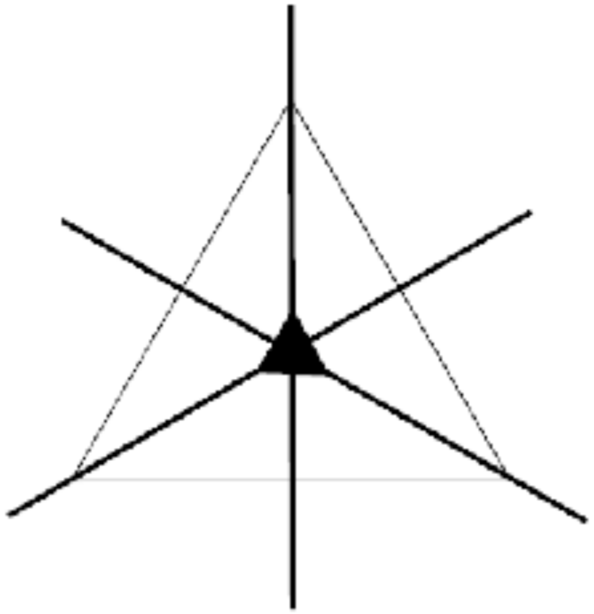
homomorphism for which $\ker(\varphi) = \{e\}$ is called *injective* or a *monomorphism*,
homomorphism for which $\mathrm{im}(\varphi) = \mathcal{H}$ is called *surjective* or an *epimorphism*.

isomorphism

homomorphism which is both injective and surjective is called *bijective*

Exercise 1.1

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

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

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

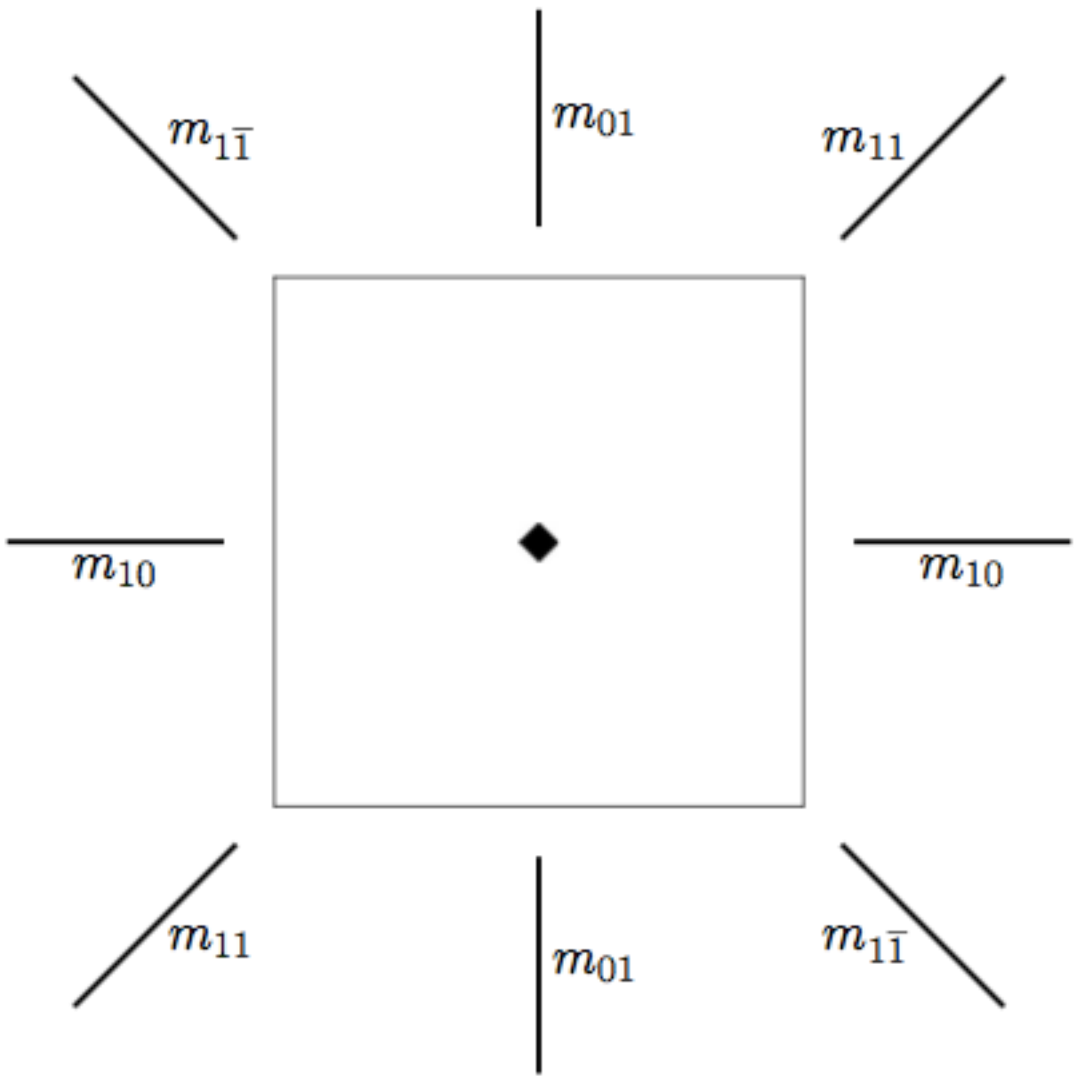
notation:

-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 1.2

Consider the symmetry group of the square. Determine:



symmetry operations: matrix and (x,y) presentation

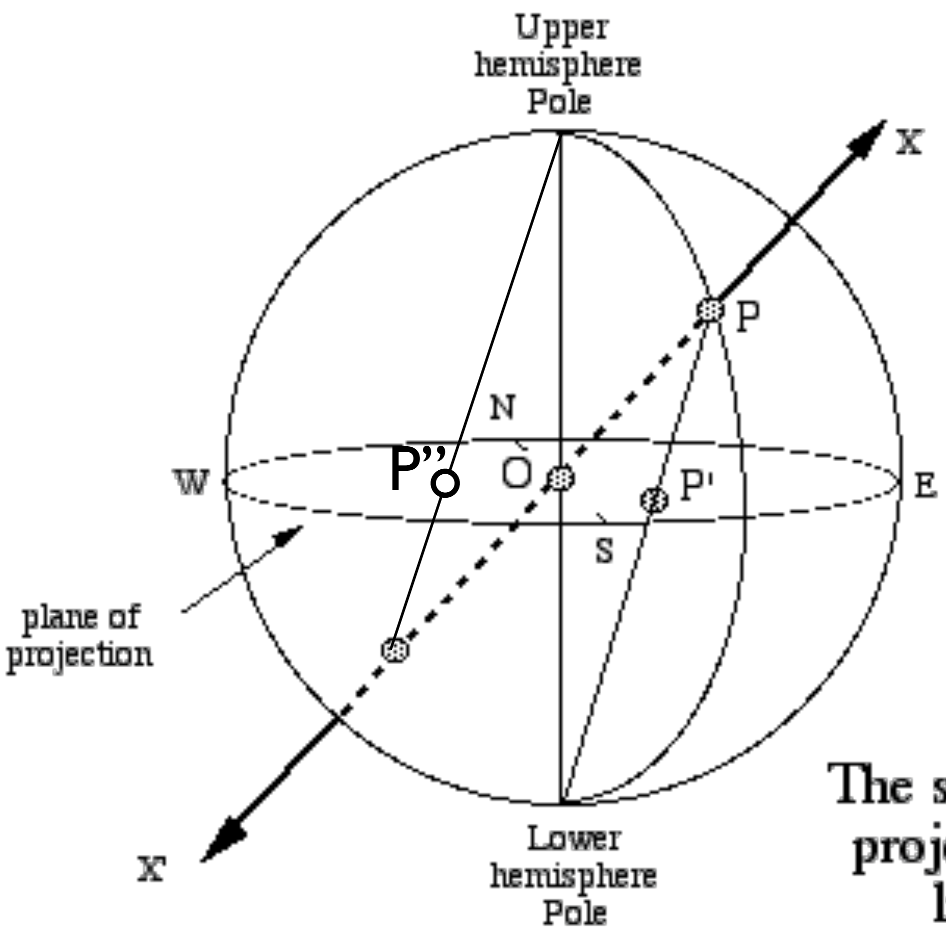
generators

multiplication table

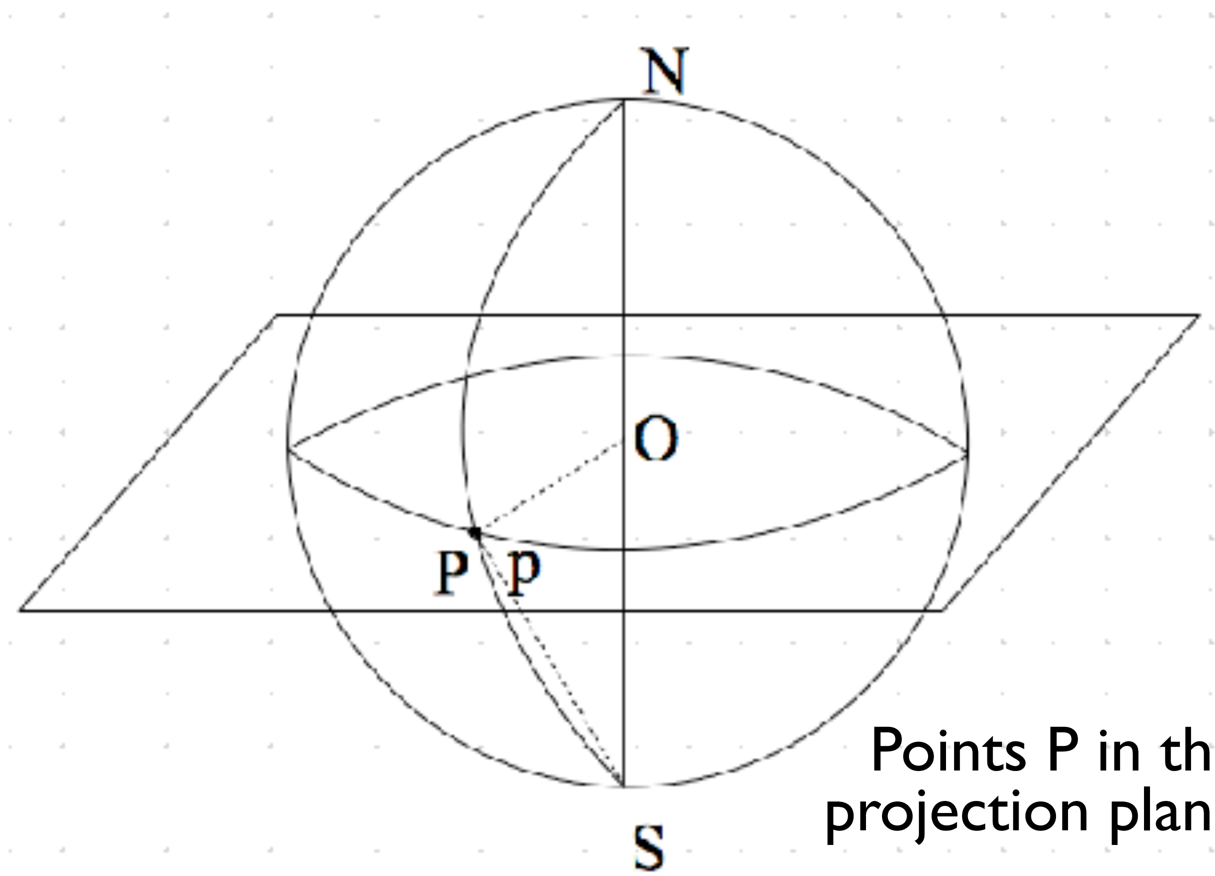
Visualization of Crystallographic Point Groups (3D)

- general position diagram
- symmetry elements diagram

Stereographic Projections



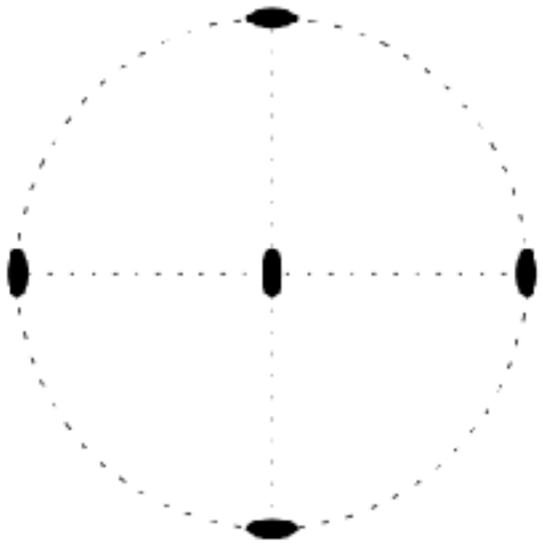
The stereographic projection of the line X-X'



Points P in the projection plane

Symmetry-elements diagrams

Rotation axes



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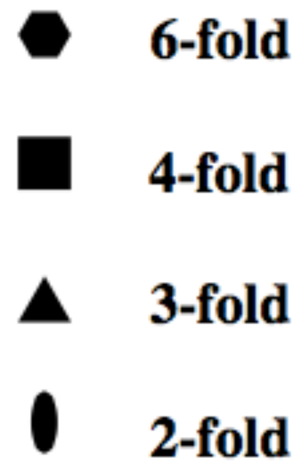
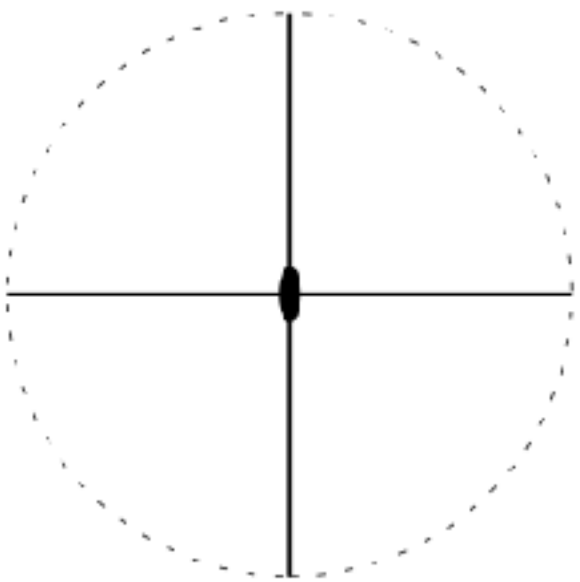
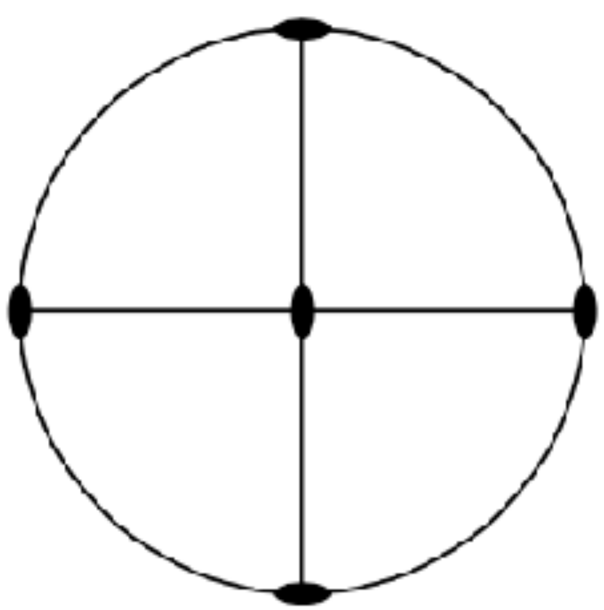


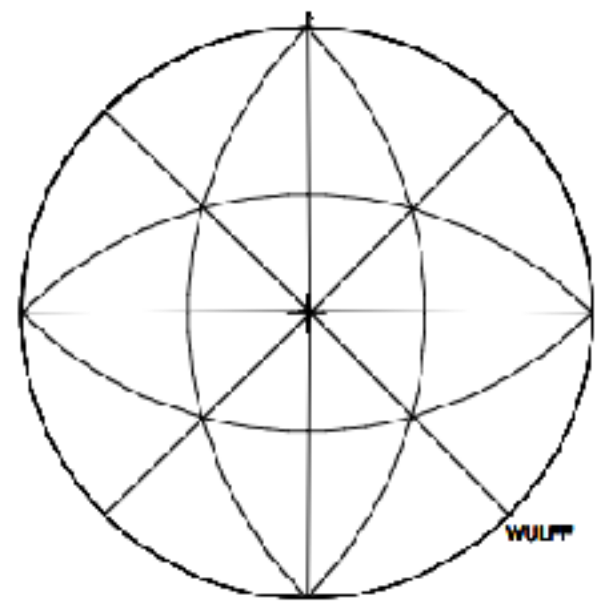
Mirror planes



2mm



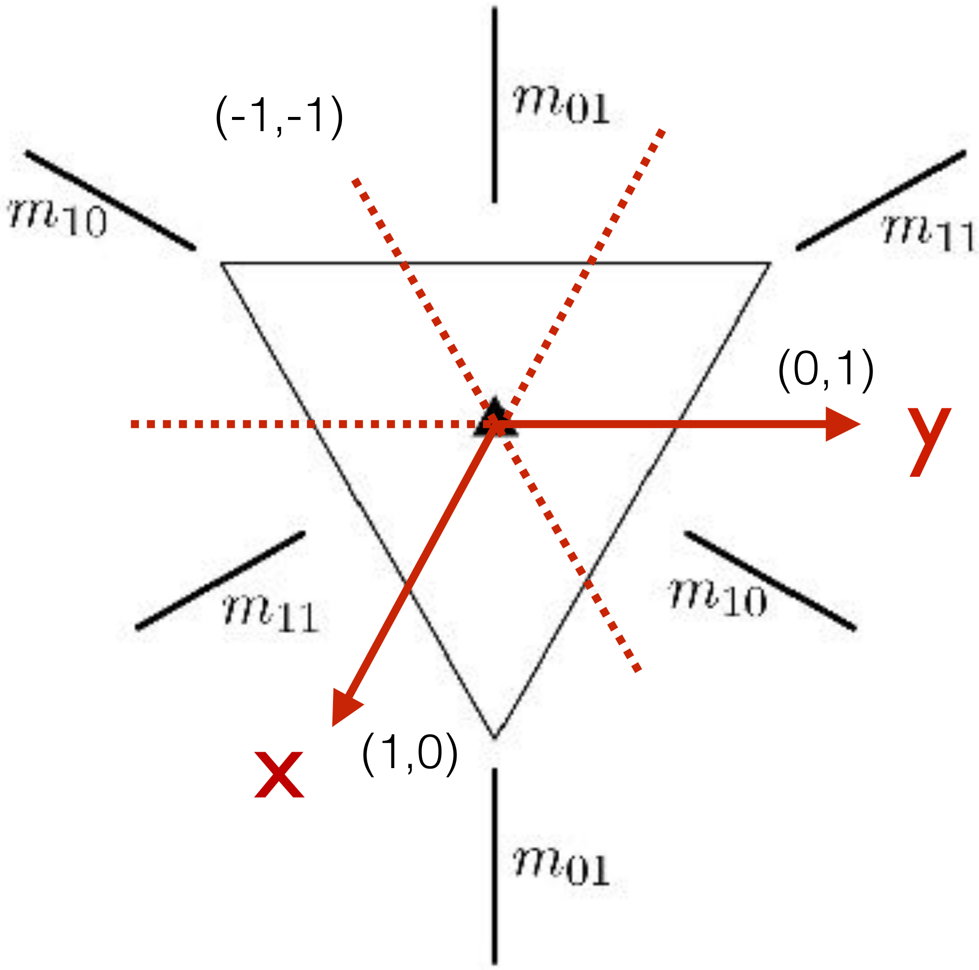
2/m 2/m 2/m



Combinations of symmetry elements

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

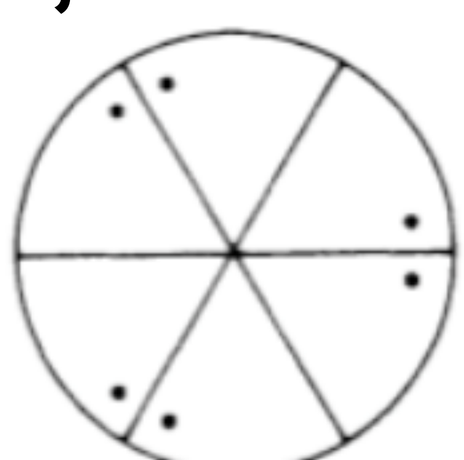
Stereographic Projections of *3m*



Point group **3m** = $\{1, 3^+, 3^-, m_{10}, m_{01}, m_{11}\}$

Stereographic projections diagrams

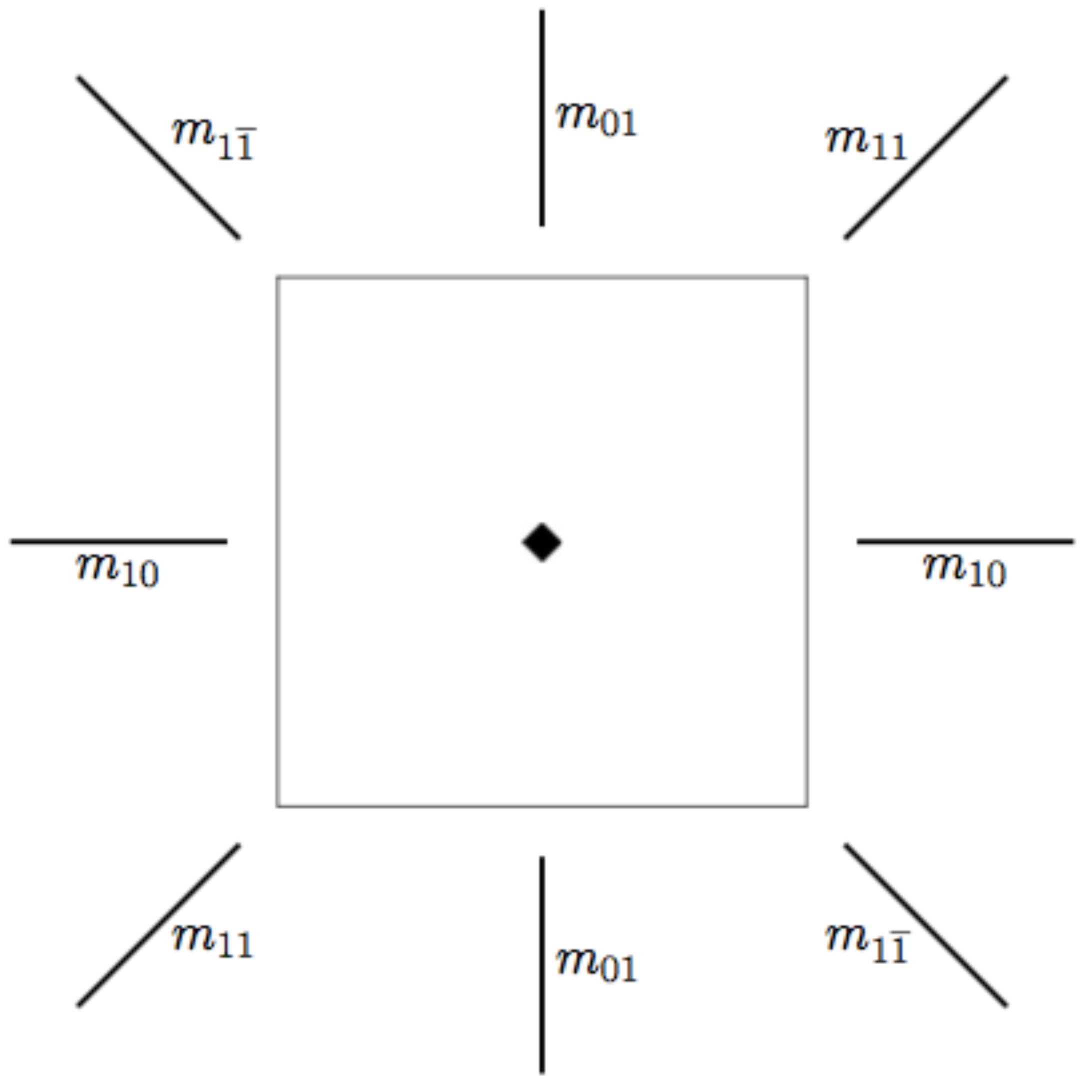
general position



symmetry elements

Problem 1.2 (cont.)

Stereographic Projections of ***4mm***



general position diagram

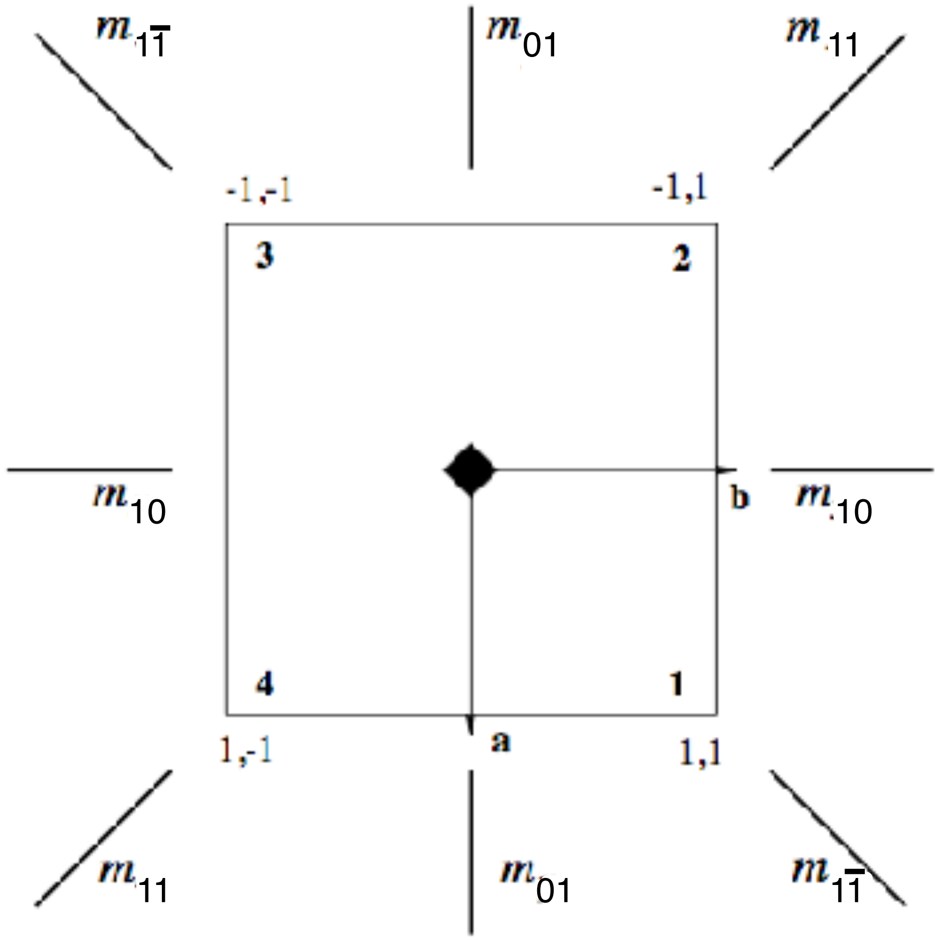
?

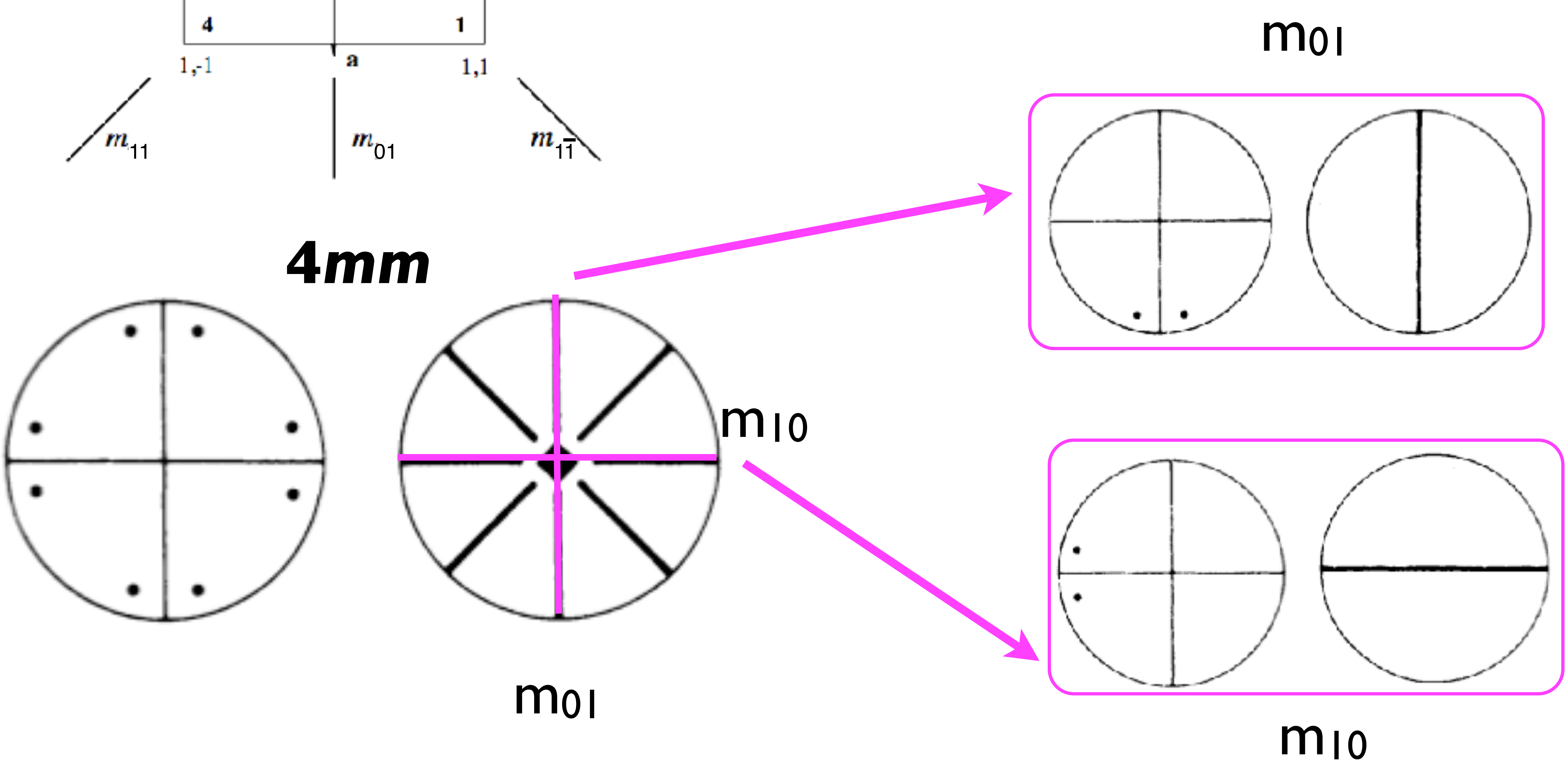
symmetry elements diagram

?

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 $|G|$

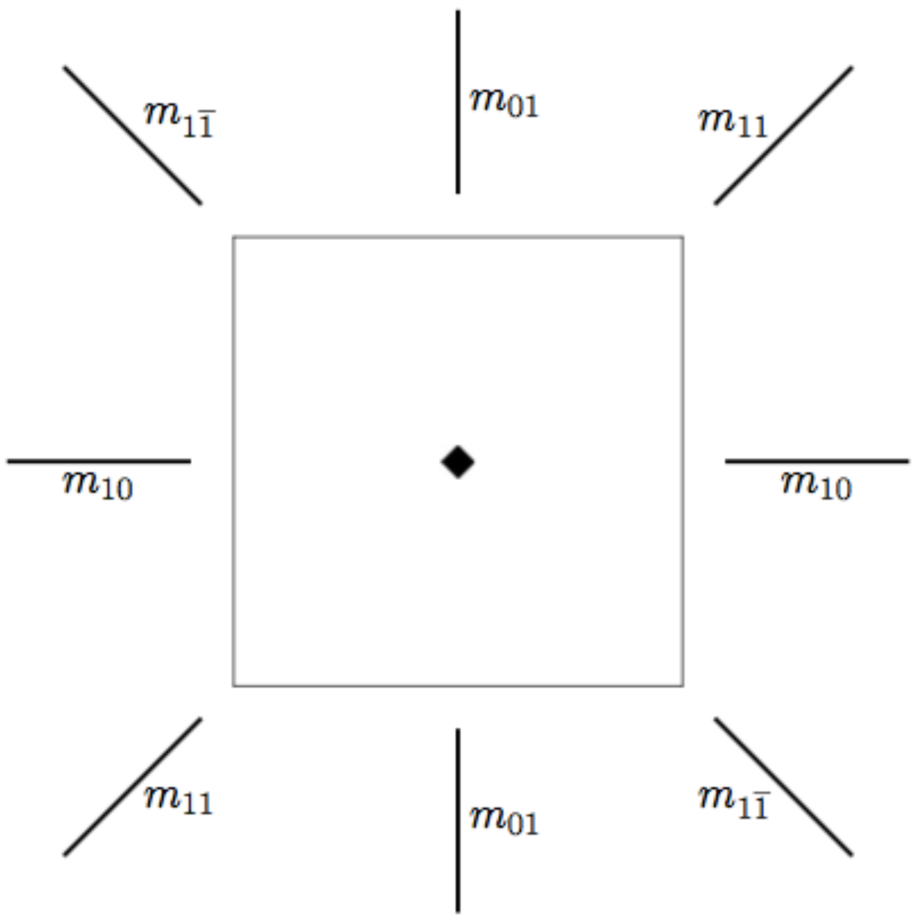
(iii) $L(e)=\{e\}$

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

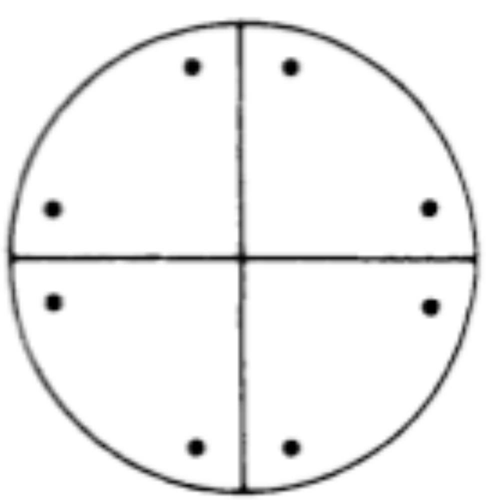
Problem 1.2 (cont.)

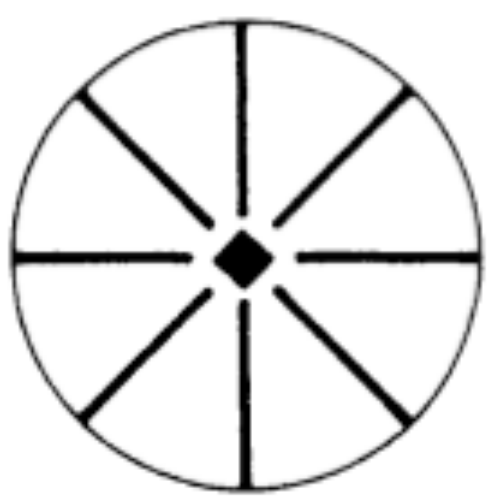
Classes of conjugate elements

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 $\exists\, g$: $g^{-1} g_i g = g_k$

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

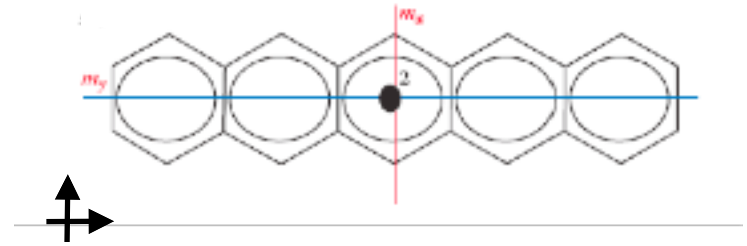
Index of the subgroup H in G: $[i]=|G|/|H|$
(order of G)/(order of H)

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**

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

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

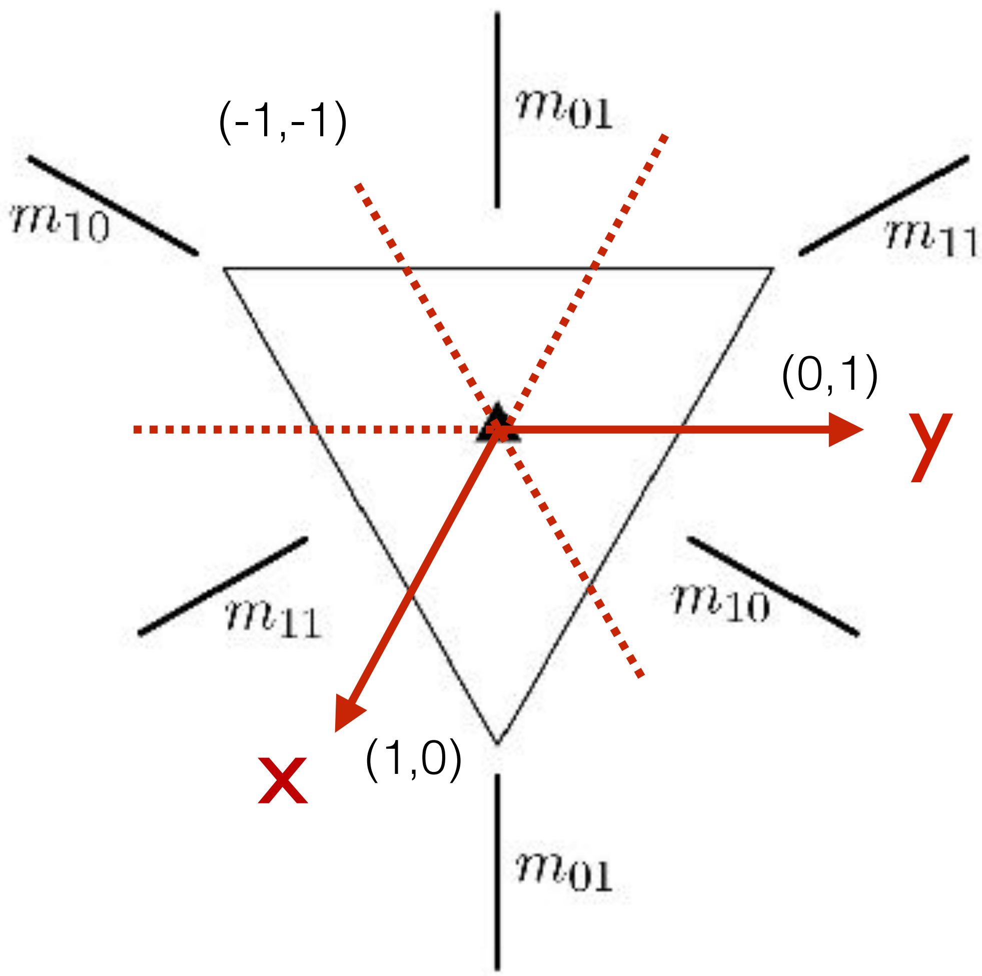
Subgroup graph

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

Problem 1.3

(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 $g_j = 1, \ldots, [i]$

Theorem of Lagrange

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

then

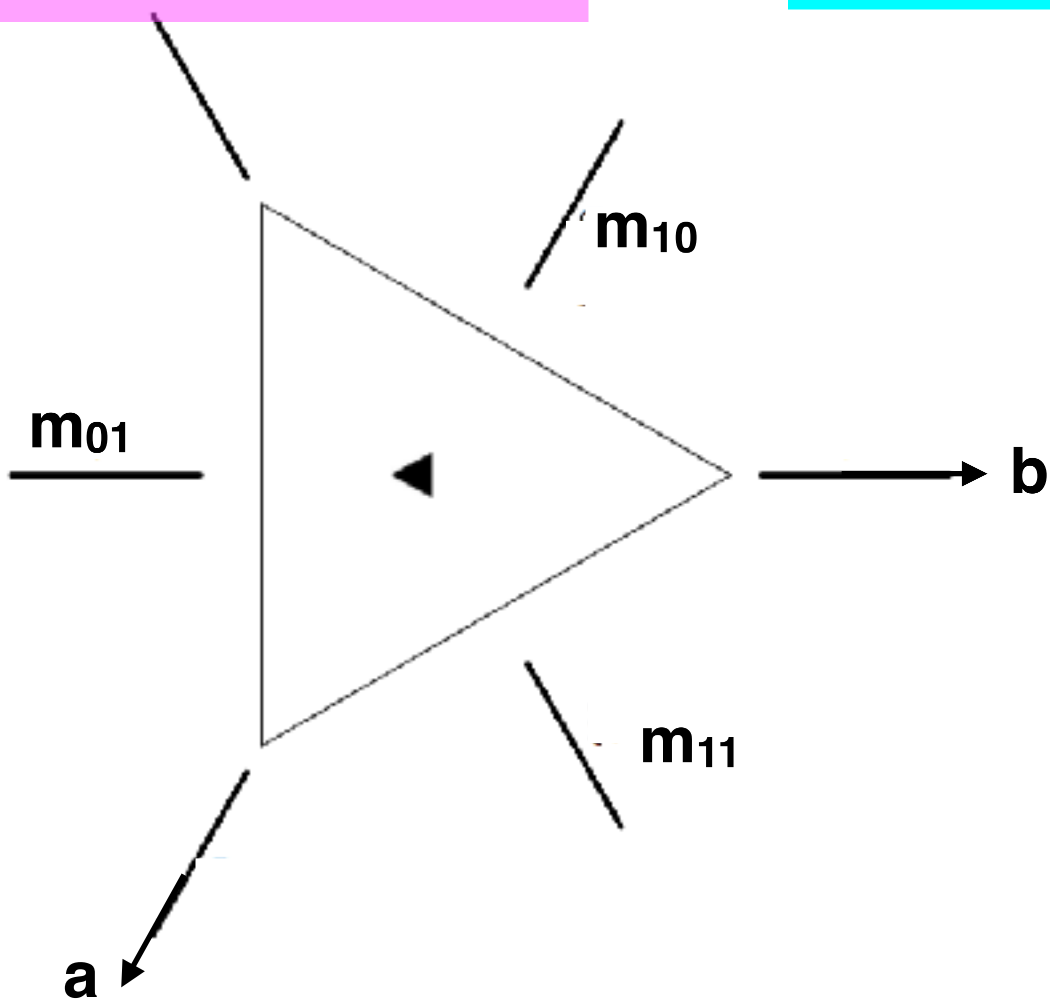
$|H|$ is a divisor of $|G|$
and $[i]=|G:H|$

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 1.4

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 $H_1 \cong H_2$

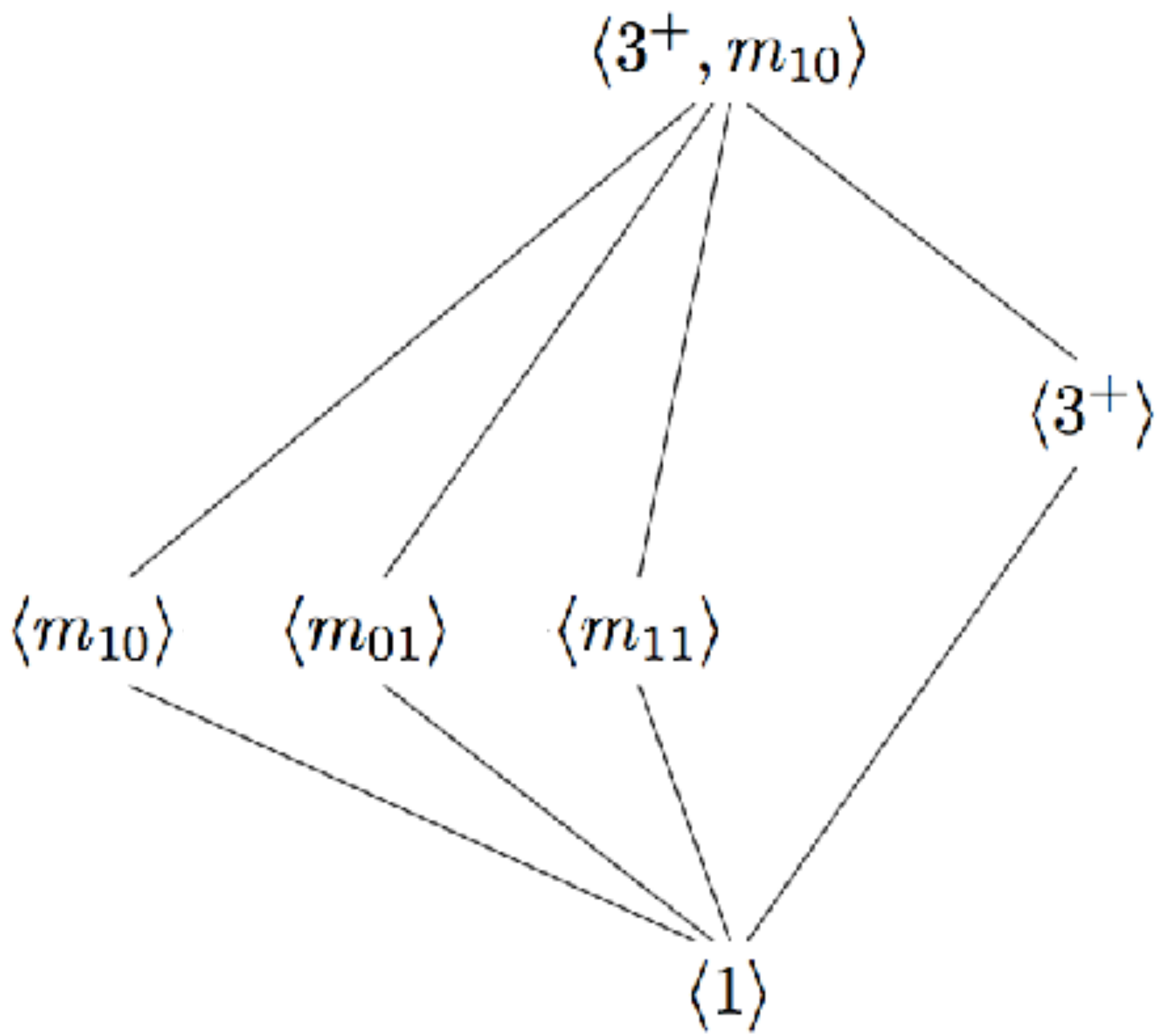
(iii) $|L(H)|$ is a divisor of $|G|/|H|$

Normal subgroup

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

Problem 1.3 (cont.)

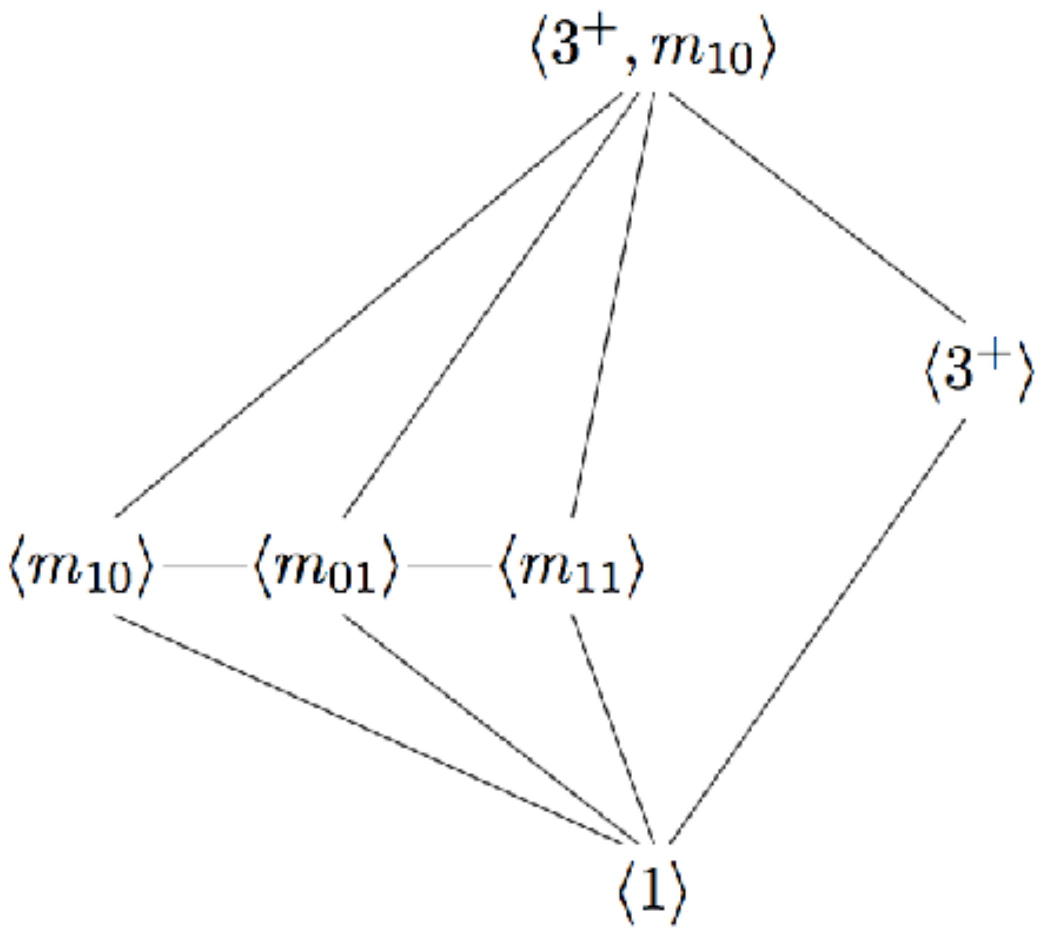
Consider the subgroups of 3m and distribute them into classes of conjugate subgroups



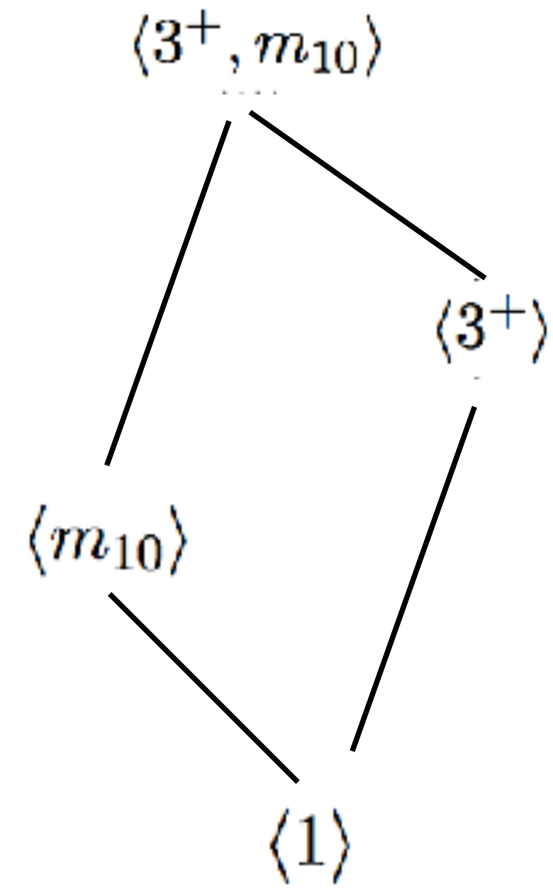
	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

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

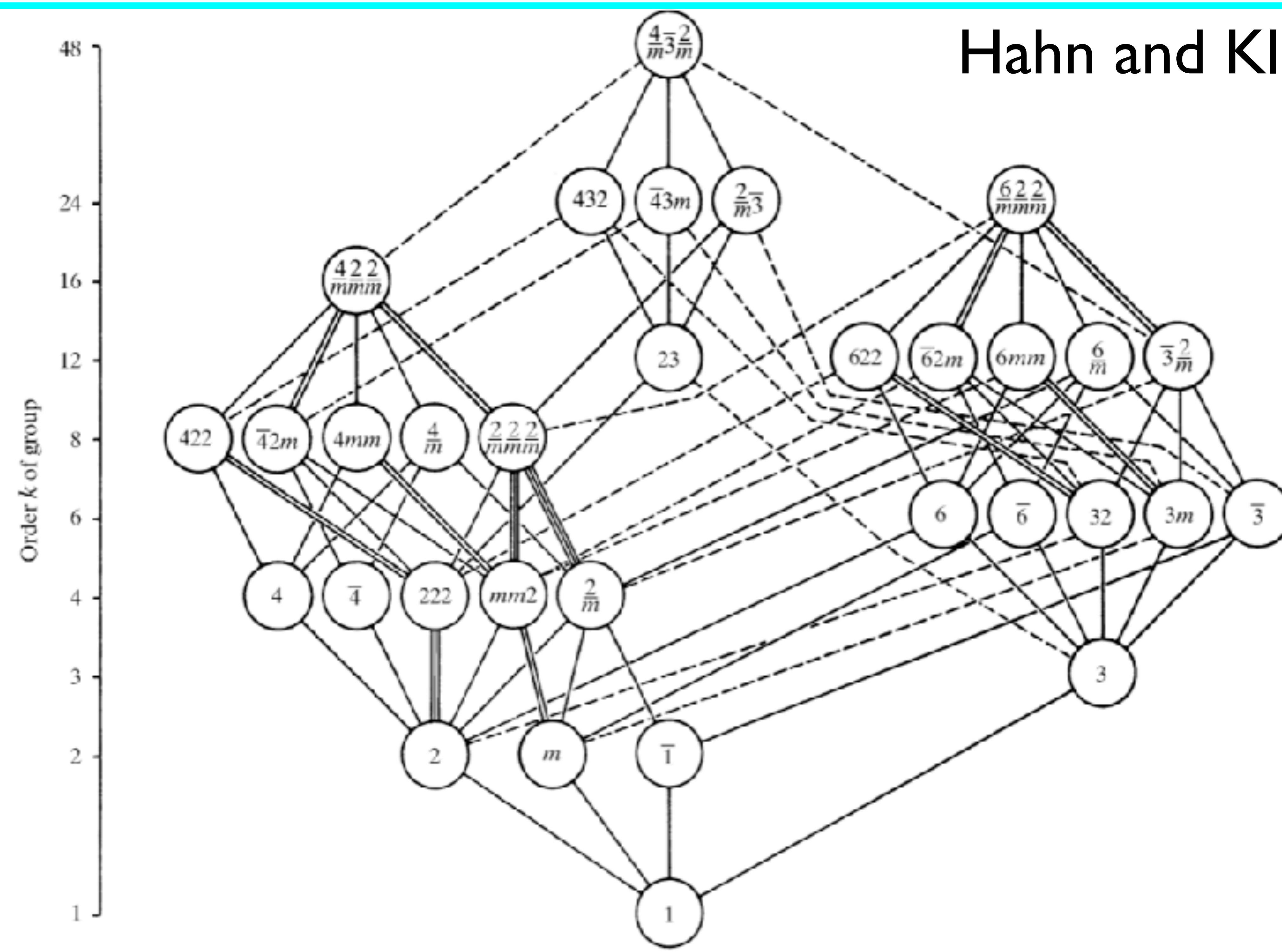


Fig. 10.1.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal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

FACTOR GROUP

Factor group

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

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

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

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

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

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

group axioms:

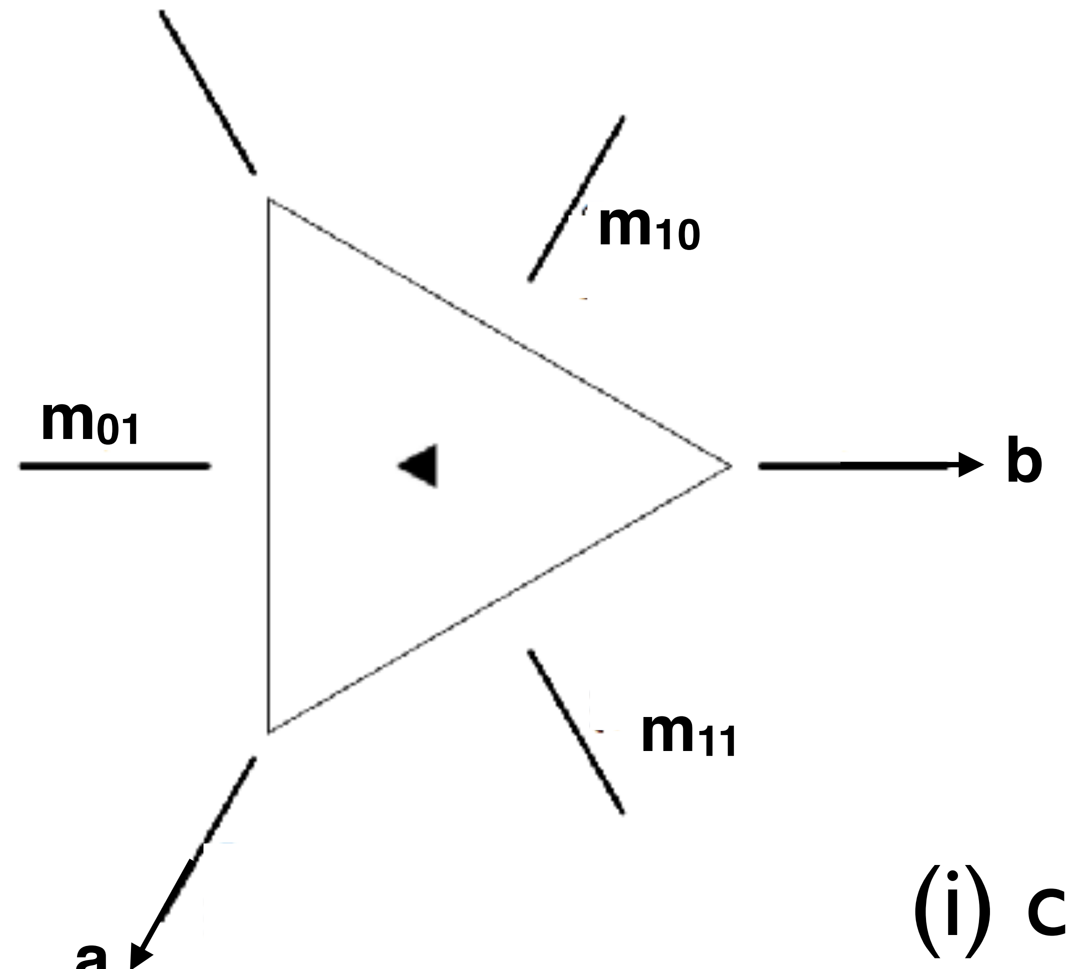
(i) $(g_iH)(g_jH) = g_{ij}H$

(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 1.5

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

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_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 $X_o=(0,0,z)$

$S_o = \mathbf{2}$

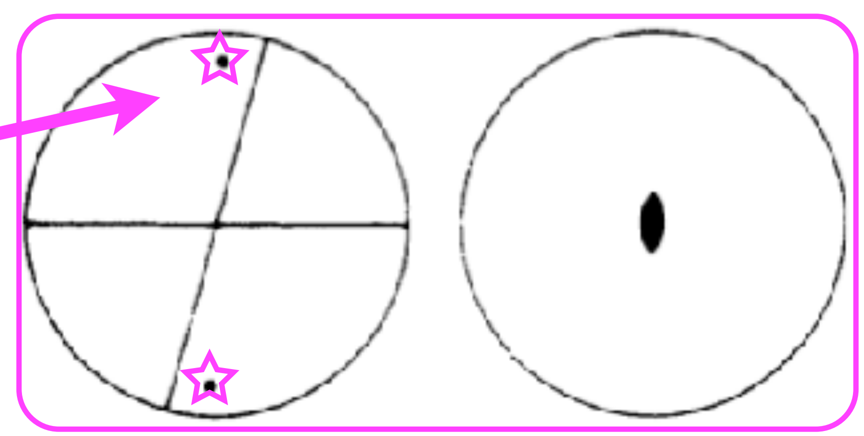
$WX_o = X_o$

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

Multiplicity: $|P|/|S_o|$

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

1 a 2 (0,0,z)



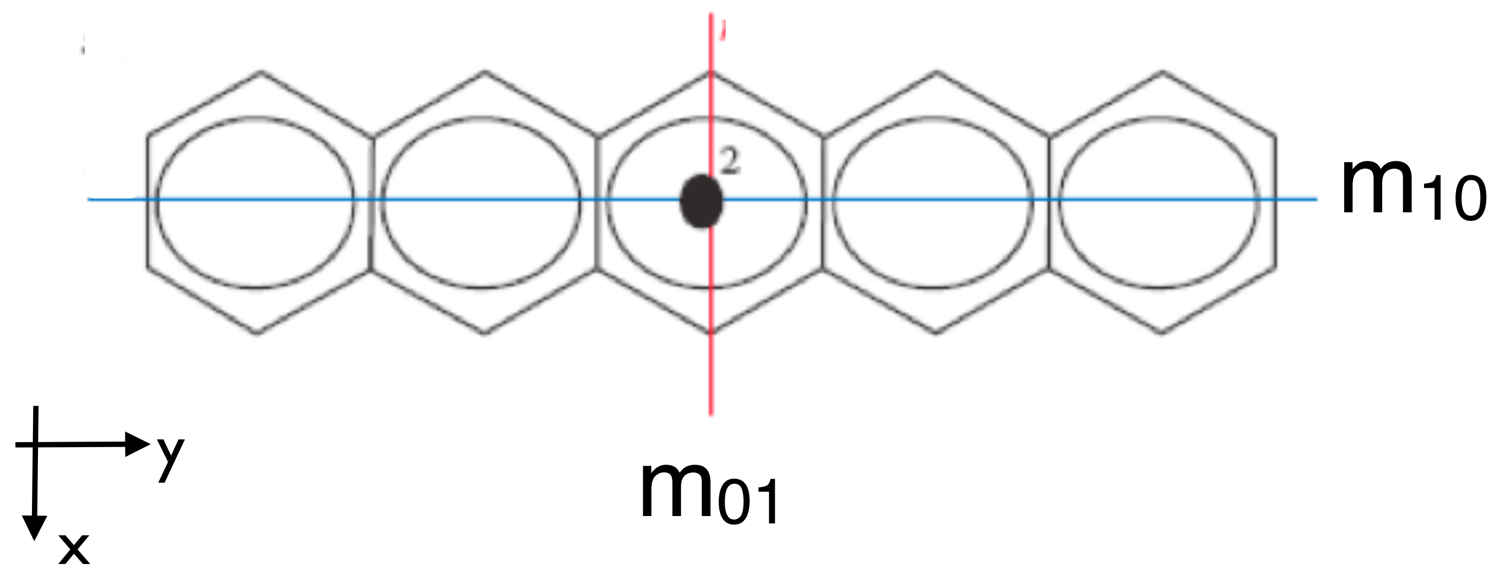
Problem 1.6

General and special Wyckoff positions

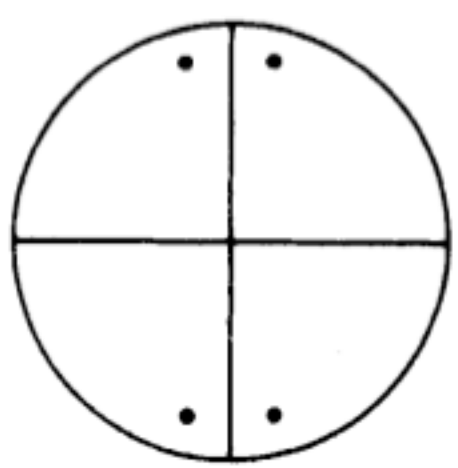
Determine the general and special Wyckoff positions of the group **mm2**

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

Molecule of pentacene



Stereographic projections diagrams



general position

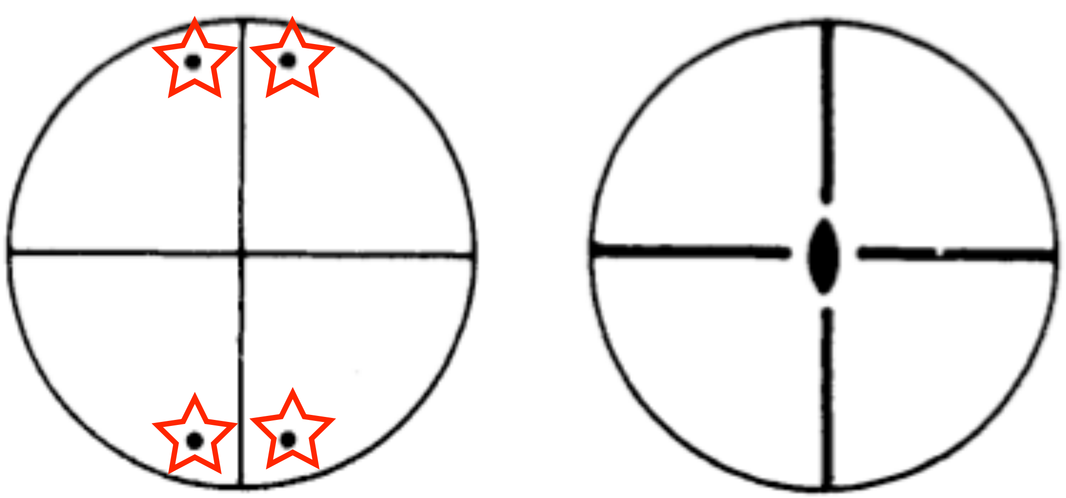
symmetry elements

Group-subgroup relations

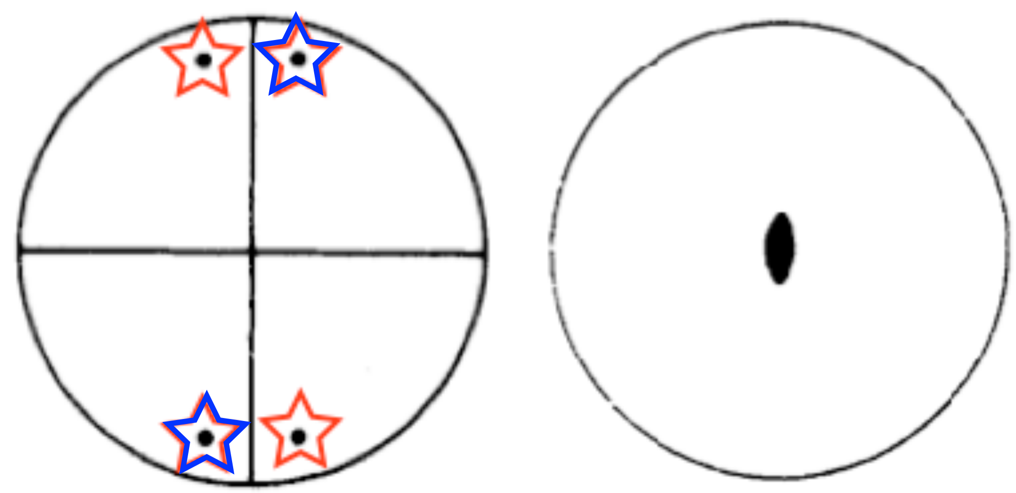
Wyckoff positions splitting schemes

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
$-x,y,z = -x_2,-y_2,z_2$

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

Crystallographic symmetry operations

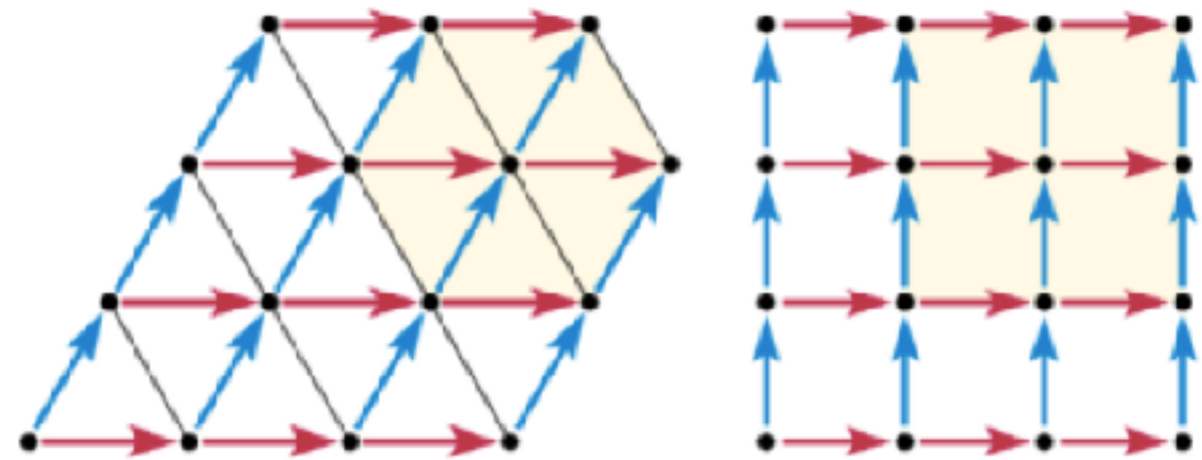
Crystallographic restriction theorem

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

Matrix proof:

Rotation with respect to orthonormal basis

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



Rotation with respect to lattice basis

R: integer matrix

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

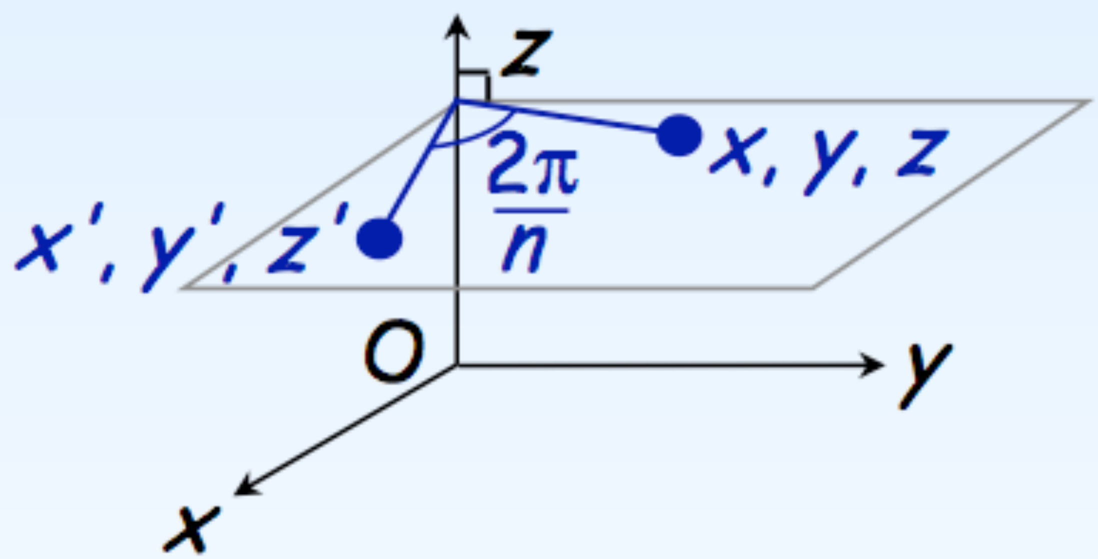
$\mathrm{Tr}\, R = 2\cos\theta =$ integer

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

Symmetry operations in 3D
Rotations

Rotation (around an axis)

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



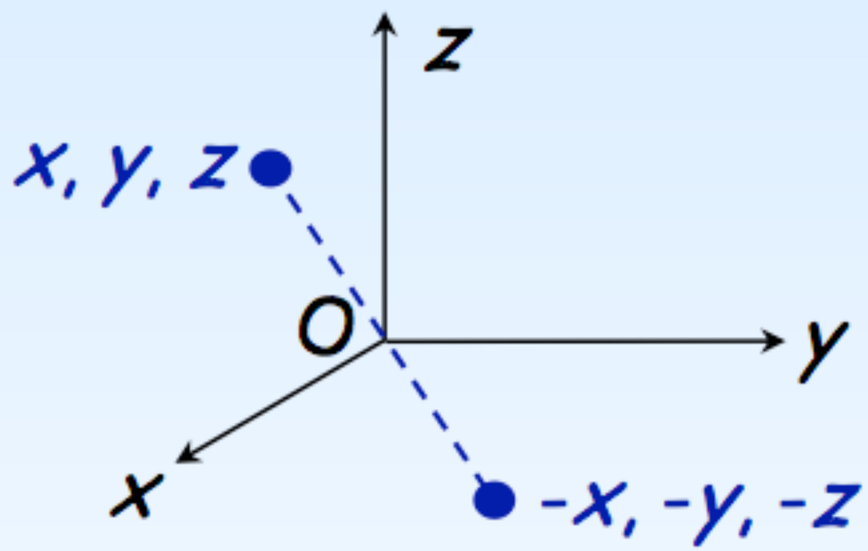
n

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

Det = +1

Symmetry operations in 3D
Rotoinvertions

Inversion (through a point)



$\boxed{\bar{1}}$

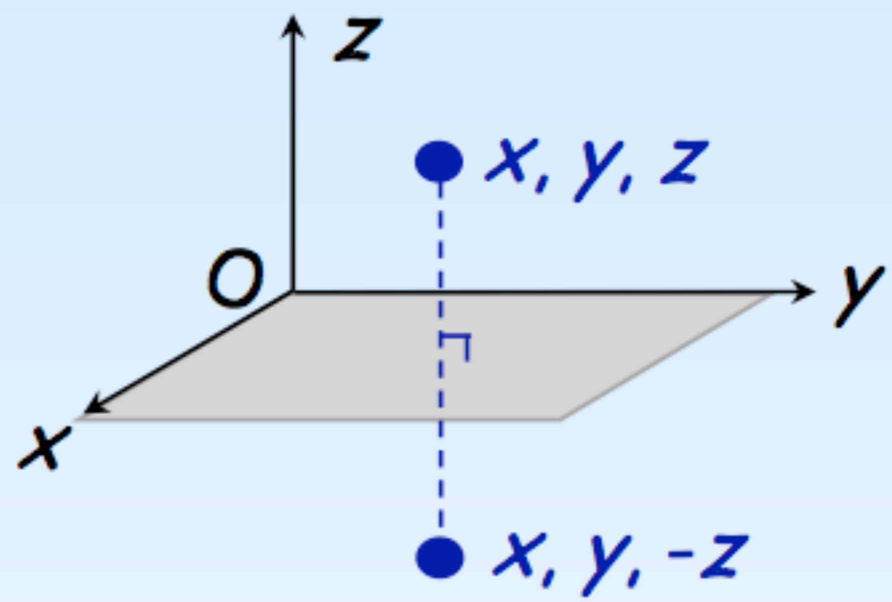
a crystal which has the inversion symmetry is called centrosymmetrical.

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

Det = -1

Symmetry operations in 3D
Rotoinvertions

Reflection (through a mirror plane)



m

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

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

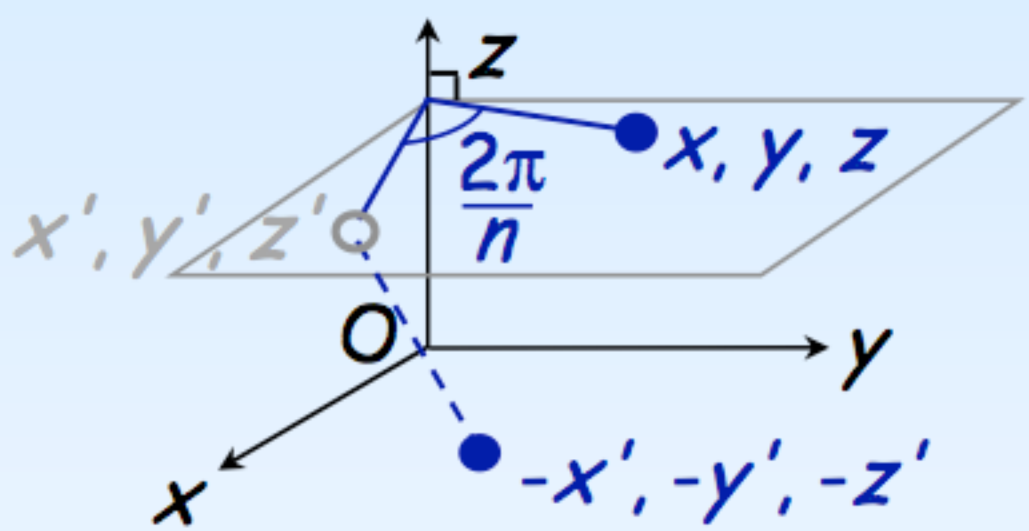
Det = -1

Symmetry operations in 3D
Rotoinversions

Roto-inversion

(around an axis and through a point)

Rotation followed by an inversion



$\bar{n}$

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

Det = -1

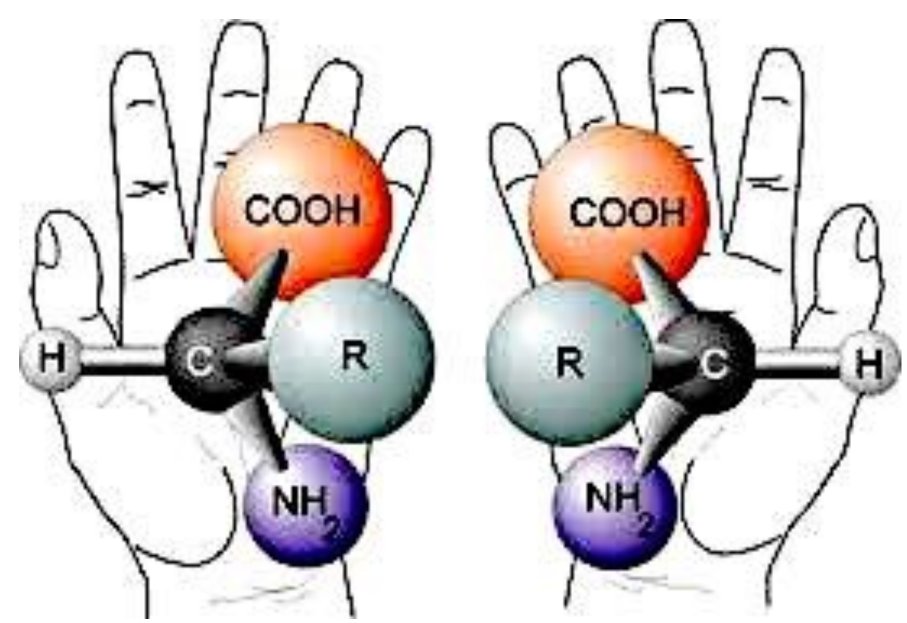
Crystallographic Point Groups in 3D

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

chirality preserving

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

chirality non-preserving



Crystallographic Point Groups in 3D

System used in this volume	Point group — International symbol — Short	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$\bar{3}$)

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

Crystal systems and Crystallographic point groups

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

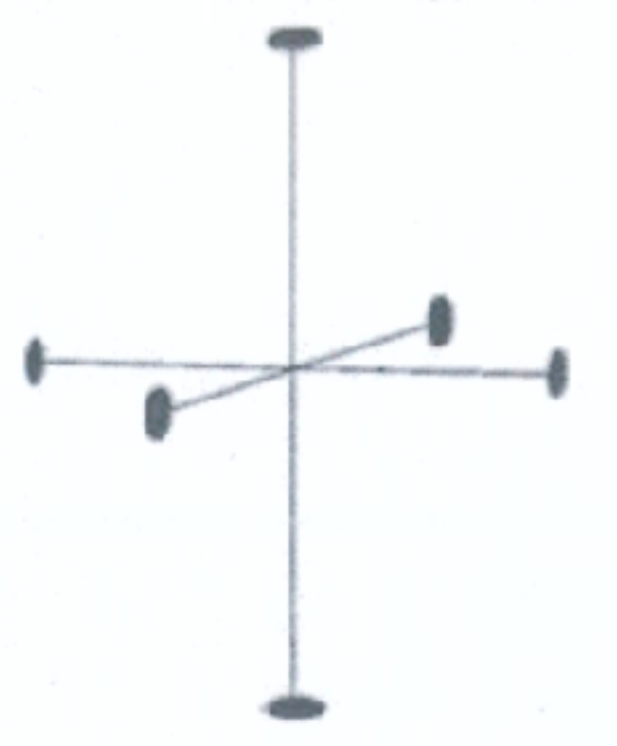
Crystal system	Crystallographic point groups†	Restrictions on cell parameters	primary	secondary	ternary
Trigonal	3, $\boxed{\bar{3}}$ $32, 3m$, $\boxed{\bar{3}m}$	$a = b$ $\alpha = \beta = 90^\circ,\ \gamma = 120^\circ$			
		$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell)	[111]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

Rotation Crystallographic Point Groups in 3D

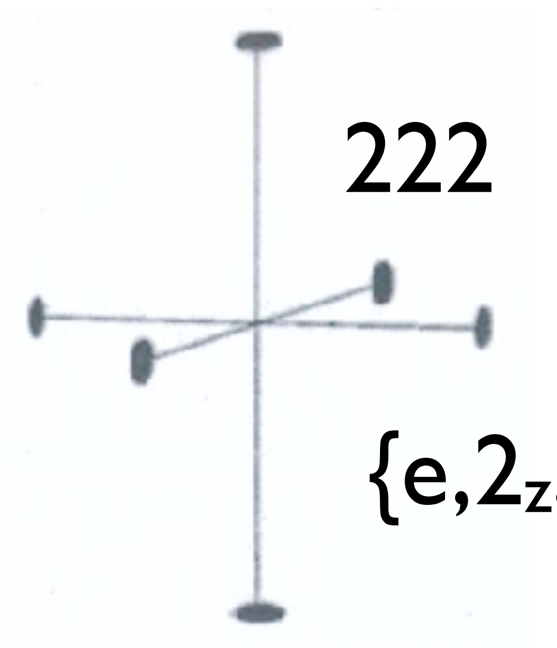
Cyclic: 1(C_1), 2(C_2), 3(C_3), 4(C_4), 6(C_6)

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

Cubic: 23 (T), 432 (O)

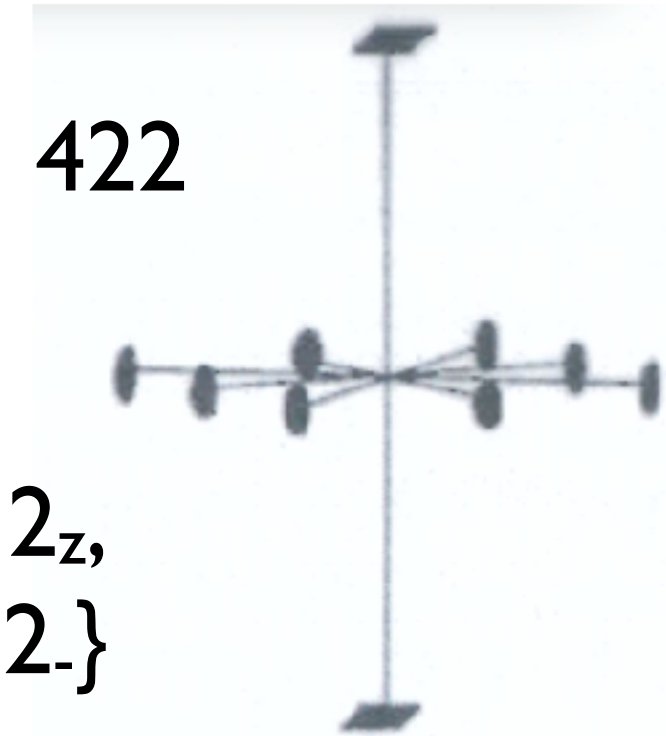


Dihedral Point Groups



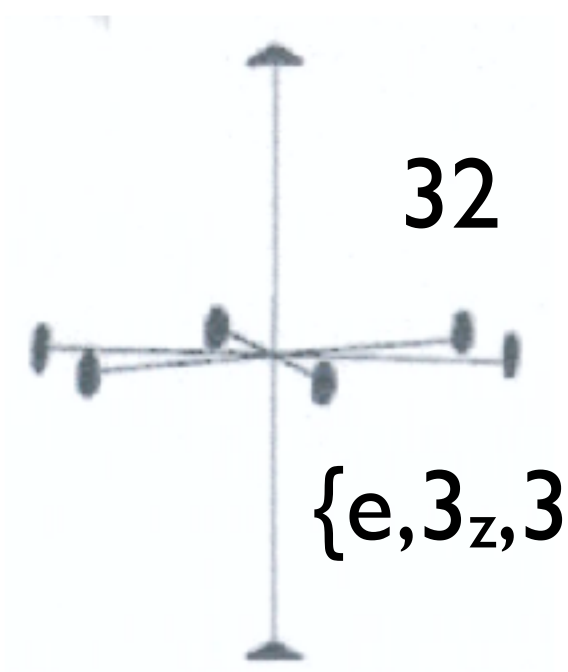
222

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



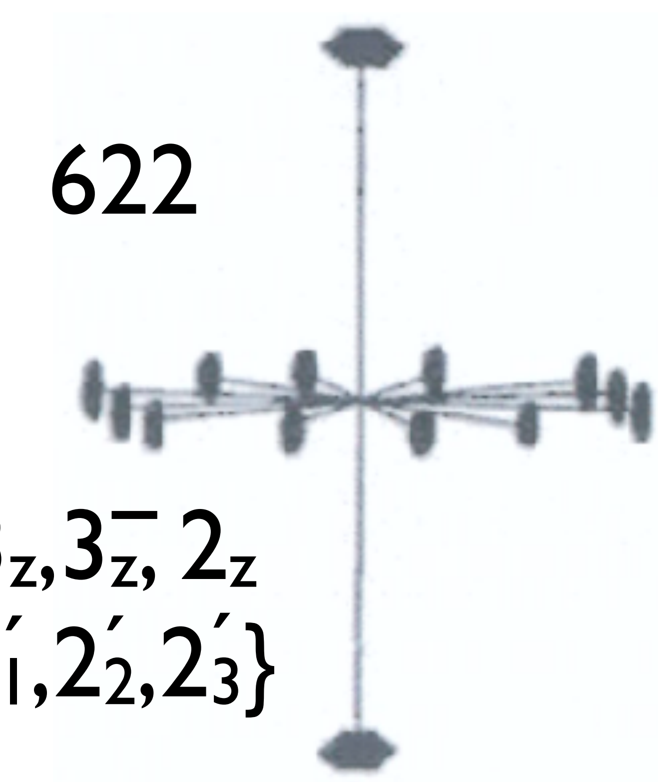
422

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



32

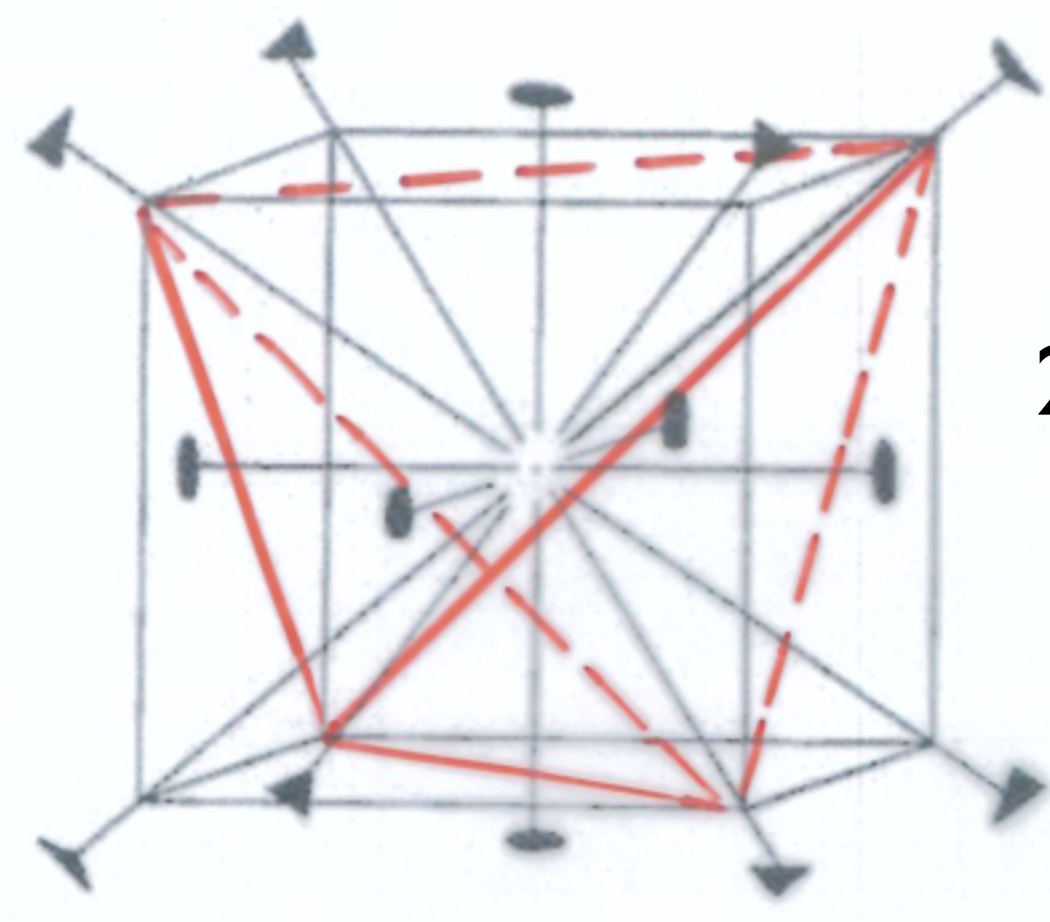
$\{e, 3_z, 3_{\bar{z}}, 2_1, 2_2, 2_3\}$



622

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

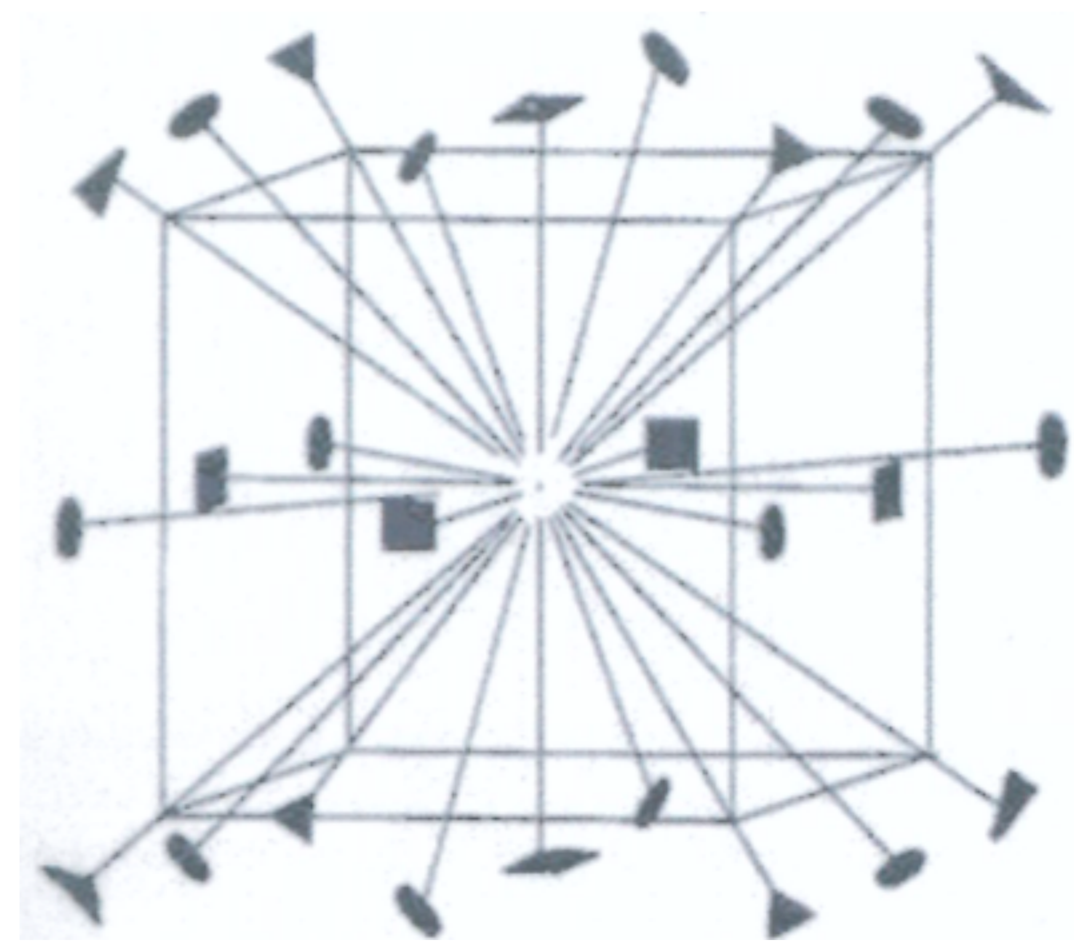
Cubic Rotational Point Groups



23 (T)

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

432(O)



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

Direct-product groups

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

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

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

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

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

Centro-symmetrical groups

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

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

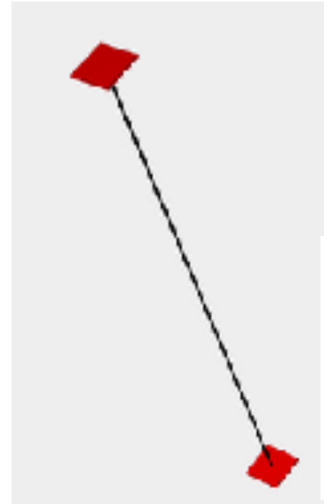
$\{1,2_{001},m_{100},m_{010}\}\otimes \{1,\bar{1}\}=$

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

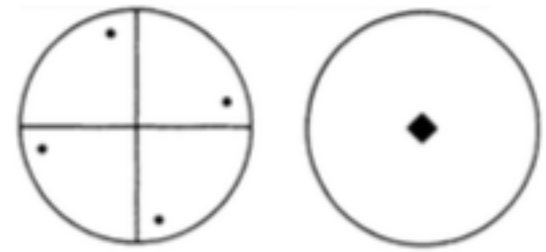
$\{1,2_{001},m_{100},m_{010},\bar{1},m_{001},2_{100},2_{010}\}=2/m2/m2/m$ or mmm

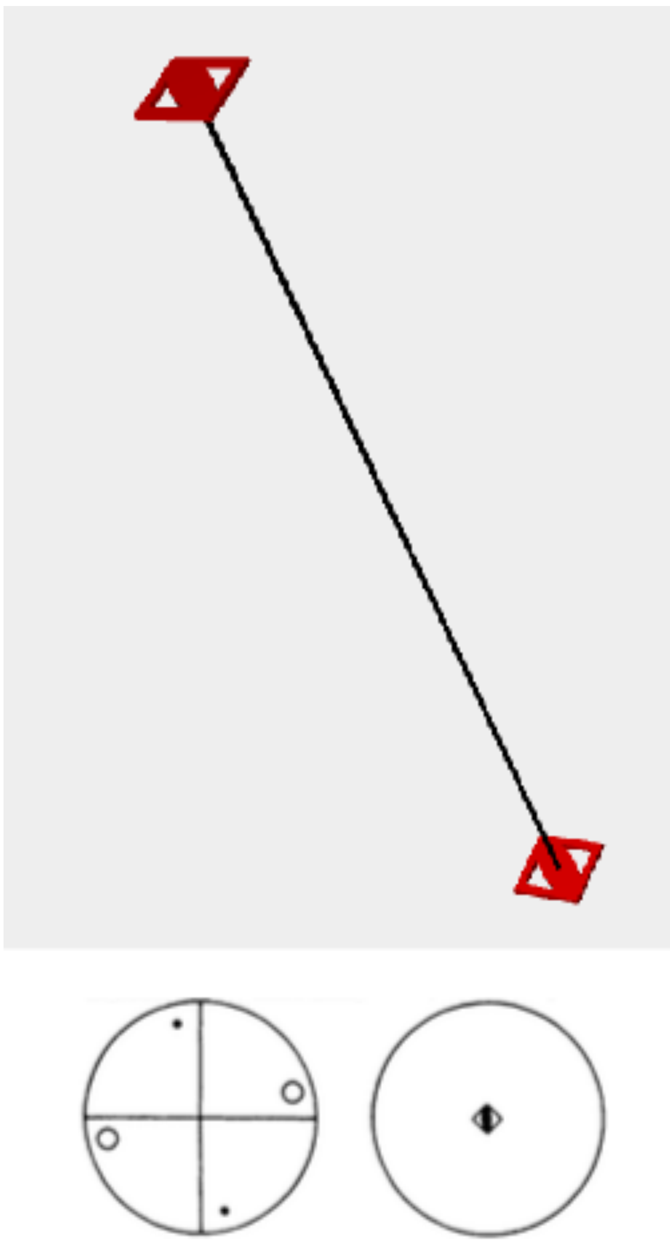
Crystallographic Point Groups

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

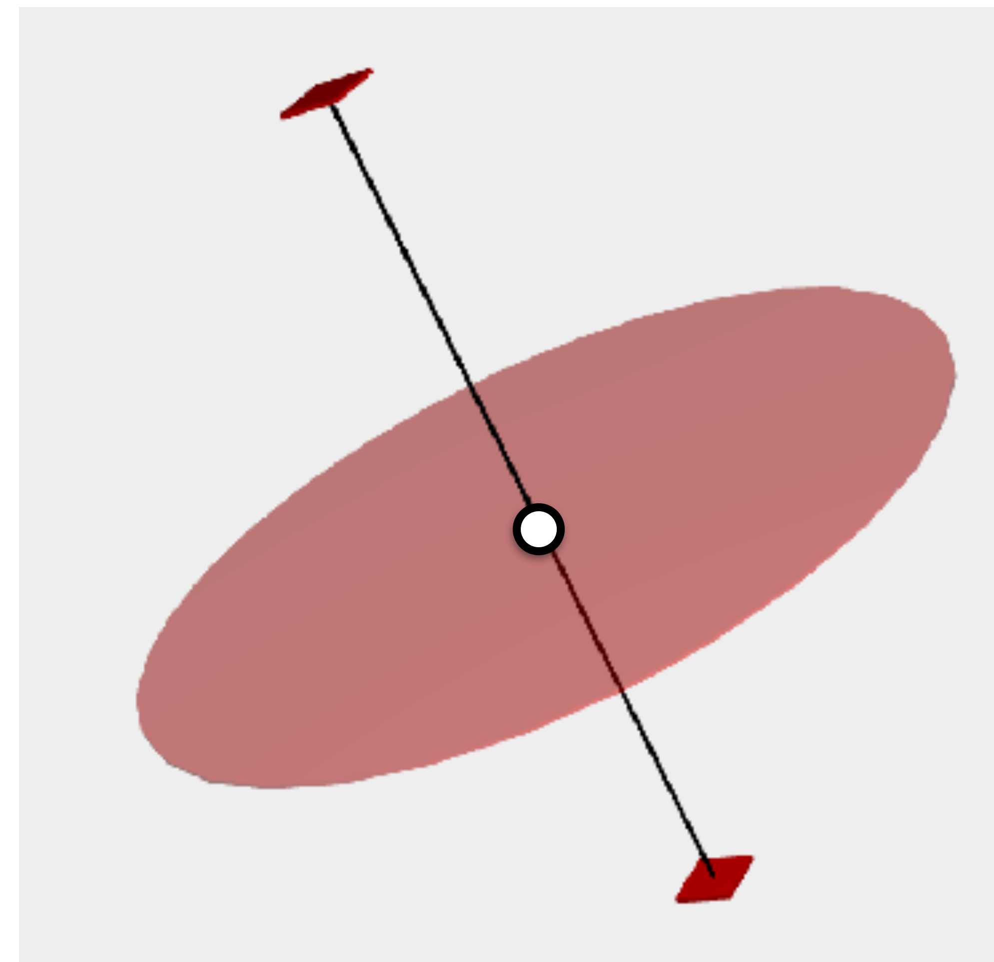


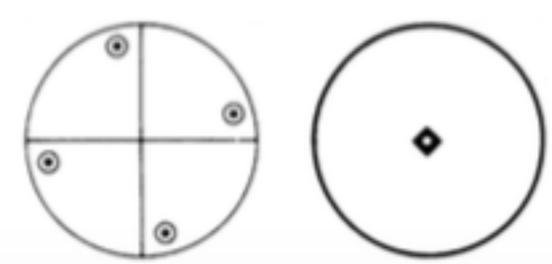
4 (C_4)





4(2) 4 (S_4)



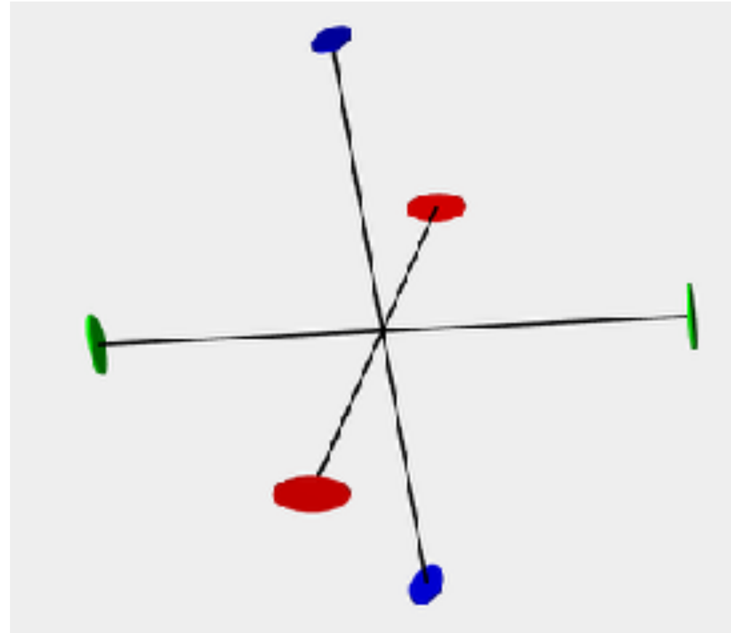


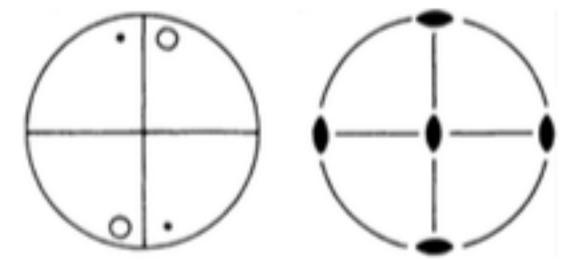
$4+\overline{1}.4=4/m$ (C_{4h})

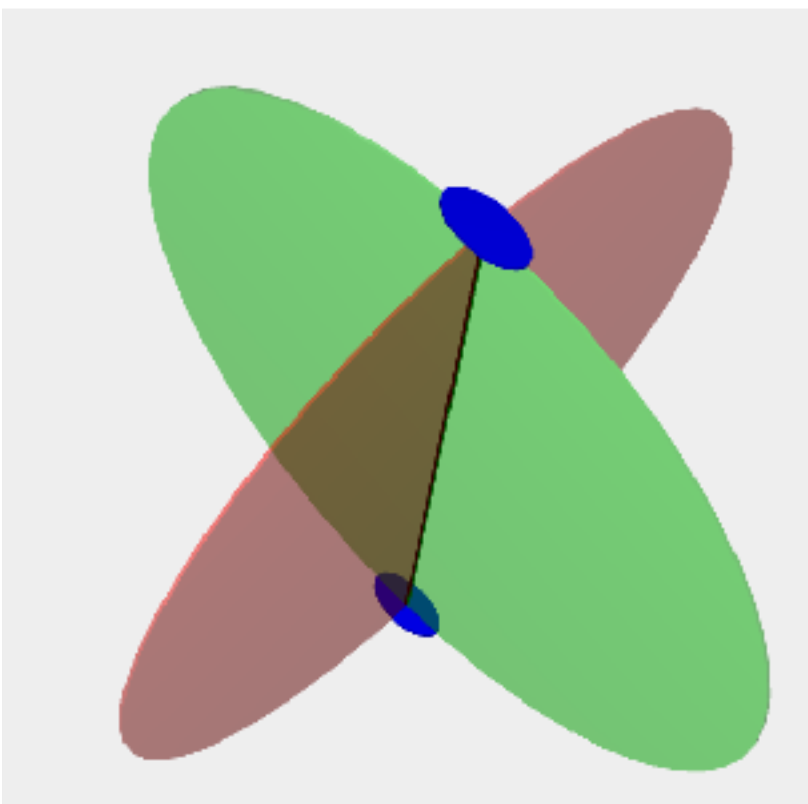
Crystallographic Point Groups

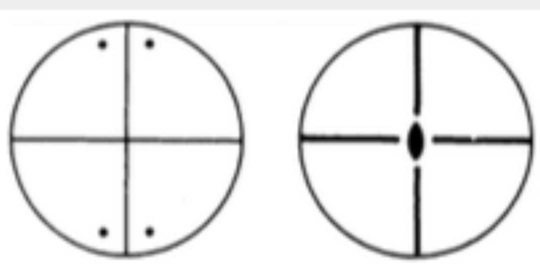
G	$G+\bar{1}G$	G(G')	$G'+\bar{1}(G-G')$
222 (D_2)	$222+\bar{1}.222=2/m2/m2/m$ mmm (D_{2h})	222(2)	2mm (C_{2v})
32 (D_3)	$32+\bar{1}.32=\bar{3}2/m$ $\bar{3}m(D_{3d})$	32(3)	3m (C_{3v})
422 (D_4)	$422+\bar{1}.422=4/m2/m2/m$ $4/mmm(D_{4h})$	422(4) 422(222)	4mm (C_{4v}) $\bar{4}2m$ (D_{2d})
622 (D_6)	$622+\bar{1}.622=6/m2/m2/m$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

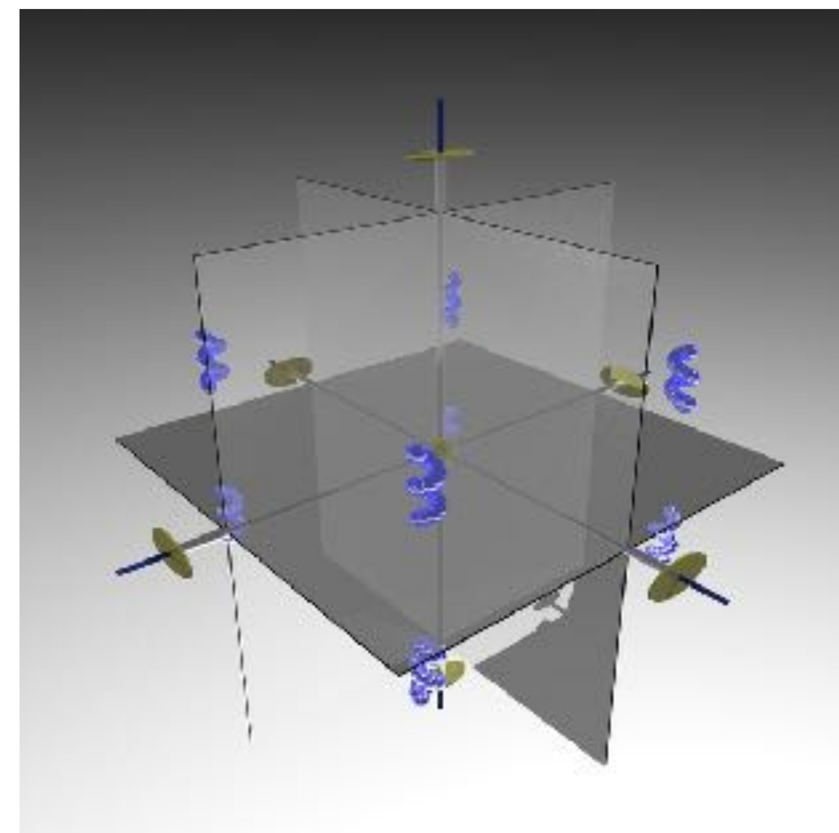


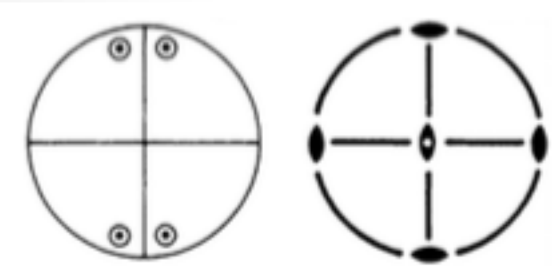






222(2)   2mm (C_{2v})





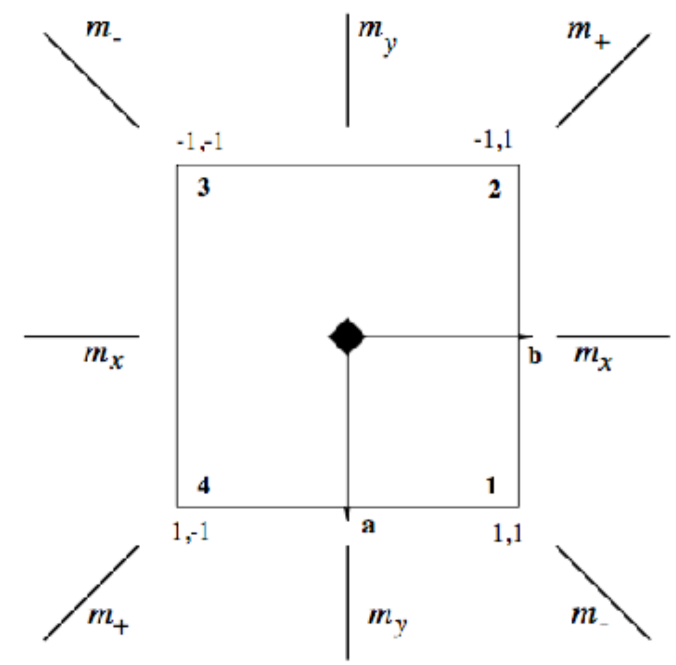
$222+\bar{1}.222=2/m2/m2/m$

mmm (D_{2h})

Crystallographic Point Groups

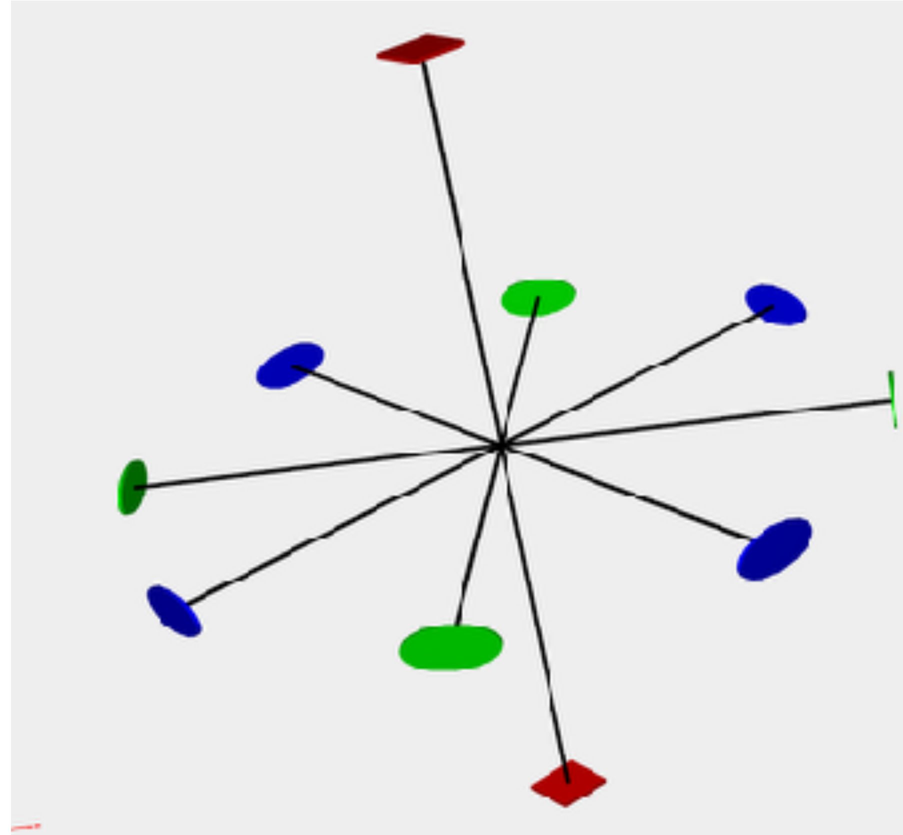
Groups isomorphic to 422

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	$m_x\ m_y$	$2_+ 2_-$

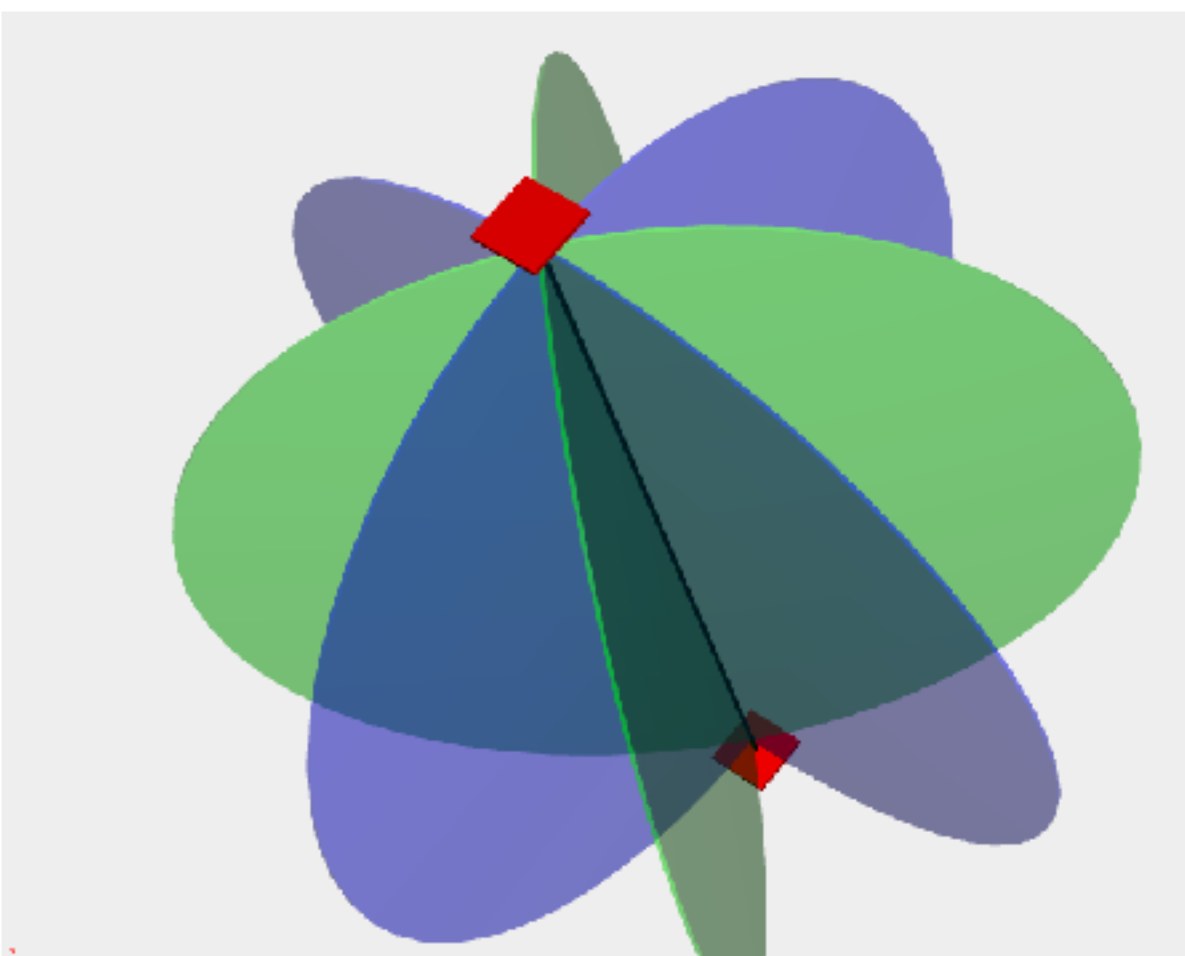


Groups isomorphic to 622

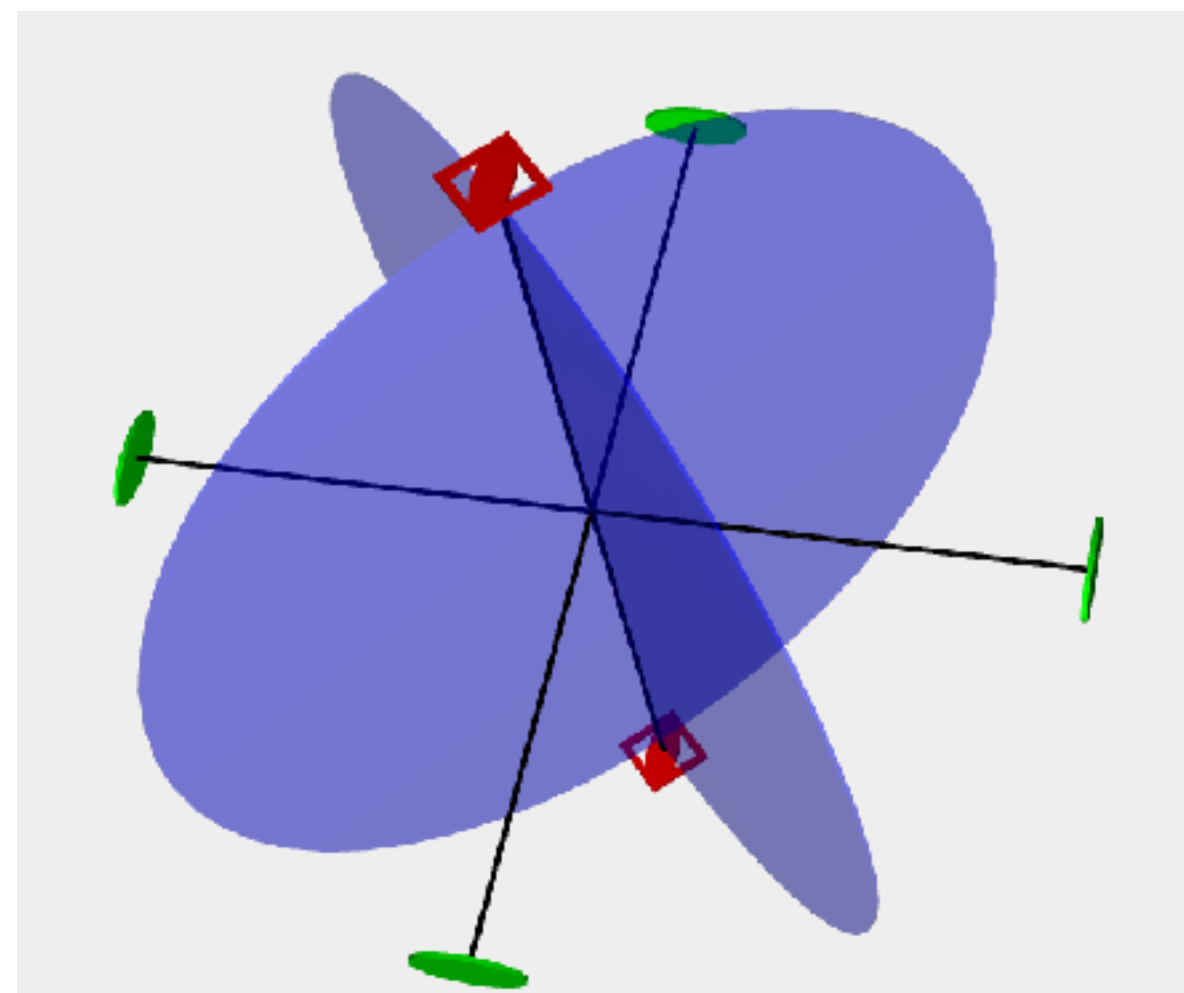
622	e	$6_z 6_z^{-}$	$3_z 3_z^{-}$	2_z	$2_1 2_2 2_3$	$2'_1 2'_2 2'_3$
6mm	e	$6_z 6_z^{-}$	$3_z 3_z^{-}$	2_z	$m_1 m_2 m_3$	$m'_1 m'_2 m'_3$
$\bar{6}2m$	e	$\bar{6}_z \bar{6}_z^{-}$	$3_z 3_z^{-}$	m_z	$2_1 2_2 2_3$	$m'_1 m'_2 m'_3$
$\bar{6}m2$	e	$\bar{6}_z \bar{6}_z^{-}$	$3_z 3_z^{-}$	m_z	$m_1 m_2 m_3$	$2'_1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



422 (D_4)



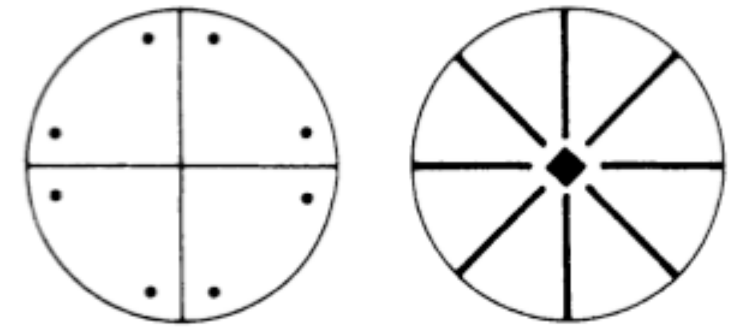
422(4) 4mm (C_{4v})



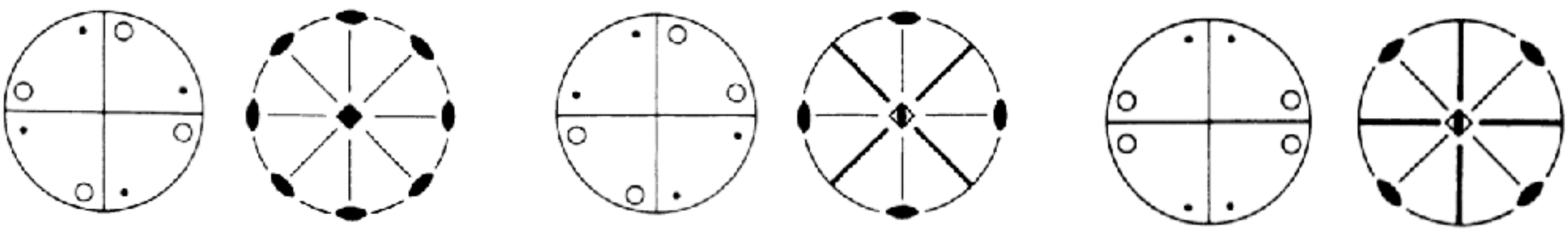
422(222) $\bar{4}2m$ (D_{2d})

Problem 1.7

_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***.

DOUBLE GROUPS

Homomorphism SU(2) —> SO(3)

rotation in $\mathbb{R}^3$ specified by Euler angles (α, β, γ)

$$\left.\begin{array}{l} 0 \le \alpha \le 2\pi \\ 0 \le \beta \le 2\pi \\ 0 \le \gamma \le 2\pi \end{array}\right\}$$ special orthogonal group SO(3)

$$\mathbf{R}(\alpha,\beta,\gamma) = \begin{pmatrix} cos\alpha\ cos\beta\ cos\gamma - sin\alpha\ sin\gamma & -sin\alpha\ cos\beta\ cos\gamma - cos\alpha\ sin\gamma & sin\beta\ cos\gamma \\ cos\alpha\ cos\beta\ sin\gamma + sin\alpha\ cos\gamma & -sin\alpha\ cos\beta\ sin\gamma + cos\alpha\ cos\gamma & sin\beta\ sin\gamma \\ -cos\alpha\ sin\beta & sin\alpha\ sin\beta & cos\beta \end{pmatrix}$$

transformation of a two-component spinor

$$D^{\frac{1}{2}}(\alpha,\beta,\gamma) = \begin{pmatrix} e^{i(\alpha+\gamma)/2}\ cos(\beta/2) & e^{-i(\alpha-\gamma)/2}\ sin(\beta/2) \\ -e^{i(\alpha-\gamma)/2}\ sin(\beta/2) & e^{-i(\alpha+\gamma)/2}\ cos(\beta/2) \end{pmatrix}$$

special unitary (unimodular) group SU(2)

homomorphism

SU(2)

SO(3)

rotation (α) rotation (α+2π)

rotation (α)

$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ kernel $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Double Groups

Bete (1929)
Opechowski (1940)

Definition (Opechowski, 1940):

The double group ${}^{d}\mathbf{G}$ of a group $\mathbf{G}$ of order $|\mathbf{G}|$ (which is a subgroup of the 3-dim rotational group $\mathbf{O}(3)$), is an abstract group of order $2|\mathbf{G}|$ having the same group-multiplication table as the $2|\mathbf{G}|$ matrices of $\mathbf{SU}(2)$ which correspond to the elements of $\mathbf{G}$.

$${}^{d}\mathbf{G} = \mathbf{G} + \bar{E}\mathbf{G} = \{R\} + \{\bar{R}\}$$

$\mathbf{G} = \{R\} < O(3)$

$\bar{E}$ rotation of 2π $\quad \bar{E}R = \bar{R}$

Combinations of symmetry operations

rotation of 2π: $R\bar{E} = \bar{E}R = \bar{R} \quad R \in \mathbf{G}$

rotation C_n: $(C_n)^n = \bar{E} \quad (C_n)^{2n} = E \quad (C_n)^{-1} = (C_n)^{2n-1} = \bar{E}(C_n)^{n-1}$

$n=2$: $(C_2)^{-1} = (C_2)^3 = \bar{E}C_2 = \bar{C}_2$

inversion $\bar{1}$: $(\bar{1})^2 = E \quad \bar{1}\bar{E} = \bar{E}\bar{1}$

reflection m: $(m)^2 = \bar{E} \quad (m)^4 = E \quad (m)^{-1} = (m)^3 = \bar{E}m = \bar{m}$

Example

$$\{e, g_1, g_2, ...\} = \ G \in SO(3)$$

$$\{e, g_1, g_2, ...; \bar{E}, \bar{E}g_1, \bar{E}g_2, ...\} \cong \ {}^dG \in SU(2)$$

Note: $G \not< {}^dG$ the operations of ${}^dG$ that correspond to G do not form a closed set

cyclic group of order n: $G = \{e, C_n, C_n^2, ..., C_n^{n-1}\}$

cyclic group of order 2n: ${}^dG = \{e, C_n, C_n^2, ..., C_n^{n-1}, C_n^n, C_n^{n+1}, ..., C_n^{2n-1}\}$

$$\bar{E} = C_{2\pi} = C_n^n$$

the subset of ${}^dG$ that corresponds to G **does not** form a closed set $\{e, C_n, C_n^2, ..., C_n^{n-1}\} \ntriangleleft \ {}^dG$

Classes of conjugate elements

Double Groups

To each class of G → one or two classes of ^{d}G

OPECHOWSKI RULES

$$\{E\},\ \{\bar{E}\},\ \{\bar{1}\}, \{\bar{1}\bar{E}\}$$
$$\{C_n\},\ \{\bar{C}_n\}\ \text{iff},\ n \neq 2$$
$$\{C_2(n),\ \bar{C}_2(n)\}\ \text{iff}\ \exists\ C_2(n')\ \text{or}\ m(n')\ \text{with}\ n \perp n'$$
$$\{m(n),\ \bar{m}(n)\}\ \text{iff}\ \exists\ C_2(n')\ \text{or}\ m(n')\ \text{with}\ n \perp n'$$
$$\{\bar{C}_n^k,\ \bar{C}_n^{k-1}\}\ \text{iff}\ \{C_n^k,\ C_n^{k-1})\},\ n > 2$$

Examples

$$222 = \{e, 2_{100}, 2_{010}, 2_{001}\}$$

$$^{d}222 = \{e, 2_{100}, 2_{010}, 2_{001}, \bar{E}, \bar{E}2_{100}, \bar{E}2_{010}, \bar{E}2_{001}\}$$

abelian group

classes of conjugate operations

non-abelian group

$$\boxed{\{e\}, \{2_{100}\}, \{2_{010}\}, \{2_{001}\}}$$

$$\boxed{\{e\}, \{\bar{E}\}, \{2_{100}, \bar{E}2_{100}\}, \{2_{010}, \bar{E}2_{010}\}, \{2_{001}, \bar{E}2_{001}\}}$$

$$2_{100}^{-1}2_{001}2_{100} = (\bar{E}2_{100})2_{001}2_{100} = \bar{E}2_{001}$$

Problem 1.8

Construct the double group ${}^{d}mm2$ and distribute its symmetry operations into classes of conjugate operations.

Construct the double group ${}^{d}4mm$ and distribute its symmetry operations into classes of conjugate operations.

What about the classes of conjugate symmetry operations of the double groups ${}^{d}422$ and ${}^{d}\bar{4}m2$?