1. The elementary properties of groups

1.1 Basic definitions

The mathematical concept of group is due to E. Galois (1823)

Def: BINARY COMPOSITION is a law that associates to two abstract elements of a set g_i and g_k a third element g_K. e.g. The set of square matrices with matrix multiplication. In general the binary composition is called multiplication in group theory. Another example of binary composition is the sum with natural numbers.

Def: GROUP is a set $\mathcal{G}$ of elements and a binary composition $(\cdot)$ with the following 4 properties

1. $A \in \mathcal{G}$ and $B \in \mathcal{G} \Rightarrow A \cdot B \in \mathcal{G}$
2. $\exists\ E \in \mathcal{G}: \quad A \cdot E = E \cdot A = A \quad \forall A \in \mathcal{G}$
3. $\forall\ A, B, C \in \mathcal{G} \quad (A \cdot B) \cdot C = A \cdot (B \cdot C)$
4. $\forall\ A \in \mathcal{G}\ \exists A^{-1} \in \mathcal{G}: \quad A \cdot A^{-1} = A^{-1} \cdot A = E$

In words: 1. $\mathcal{G}$ is closed with respect to $\cdot$; 2. $\mathcal{G}$ contains the identity with respect to $\cdot$; 3. the associative law is valid; 4. Every element of $\mathcal{G}$ has an inverse in $\mathcal{G}$. The number of elements in $\mathcal{G}$ is the order of $\mathcal{G}$.

Notice that $AB = C$ is uniquely defined but in general $AB \neq BA$

If $AB = BA \quad \forall A, B \in \mathcal{G} \Rightarrow$ the group is called Abelian.

Comments on the definition of group.

1. There are several algebraic structures based on "partial" group definitions

- MONOID : closure, associative law, neutral ~~t~~element (identity) $(\mathbb{N}^+, \{0\}, +)$
- SEMIGROUP: closure, associative law $(\mathbb{N}^+, +)$

2. The associative law is taken as elementary. => (feeling...) I do not thing it can be derived from other. Counter example OCTONION.

3. In the case of point groups it is not necessary to prove the associative law due to the homomorphism of the linear point ~~(group)~~ ~~transf~~ symmetry operations with the unitary matrices with line by row product.

$$A \cdot (B \cdot C) = (A \cdot B) \cdot C$$

In fact, by taking the element ij on both sides

$$\sum_k A_{ik} \left(\sum_l B_{kl} C_{lj}\right) \overset{\text{distributive property}}{=} \sum_{kl} A_{ik}\left(B_{kl} C_{lj}\right) \overset{\text{associative in } \mathbb{R}(\mathbb{C})}{=} \sum_{kl} \left(A_{ik} B_{kl}\right) C_{lj}$$

$$\overset{\text{d.p.}}{=} \sum_l \left(\sum_k A_{ik} B_{kl}\right) C_{lj} = \left[(AB) \cdot C\right]_{ij}$$

Def: <u>CONJUGATE ELEMENTS</u> : if $A, B, C \in \mathcal{G}$ and $ABA^{-1} = C \Rightarrow C$ is called the transform of B through A and B and C are conjugate elements

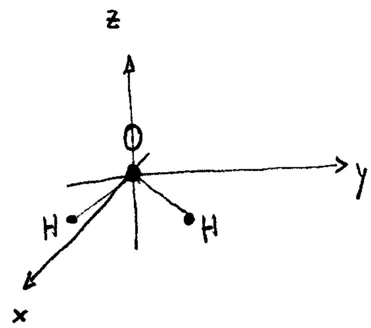
Def: <u>CLASS</u> : a complete set of the elements conjugate to A forms the class $\mathcal{C}_A$. The number of elements in the class is called order of the class.

Def: <u>HOMOMORPHISM</u> : a mapping $f : \mathcal{G} \to \mathcal{G}'$ which respects the multiplication $f(A \cdot B) = f(A) \cdot f(B)$

Def: <u>ISOMORPHISM</u> : a homomorphism between two groups $\mathcal{G}$ and $\mathcal{G}'$ with the same order such that $\forall A' \in \mathcal{G}' \ \exists! A \in \mathcal{G} : A' = f(A)$.

(1.2) The multiplication table and Rearrangement theorem

•	group elements
group elements	results of the multiplication



Example of multiplication table for the group C_{2v} (the symmetry group of water)

	E	C_2	σ_{yz}	σ_{xz}
E	E	C_2	σ_{yz}	σ_{xz}
C_2	C_2	E	σ_{xz}	σ_{yz}
σ_{yz}	σ_{yz}	σ_{xz}	E	C_2
σ_{xz}	σ_{xz}	σ_{yz}	C_2	E

C_2 is the rotation of π around z axis

$\sigma_{yz,xz}$ is a mirror reflection with respect to the plane yz, xz.

The product is "apply the two operations in a row, from right to left".

<u>Theorem</u>: REARRANGEMENT THEOREM, If $E, g_1, \dots, g_h$ are the elements of a group $\mathcal{G}$ and if g_k is an arbitrary group element, then the ensembly of elements

$$g_k E, g_k g_1, \dots, g_k g_h = S$$

contains each element of the group once and only once.

<u>proof</u>

1. we show that every element is contained. g an arbitrary element $\Rightarrow \exists\, g_r : \; g_r = g_k^{-1} g \;\; (g_k^{-1}$ exists, $g_k^{-1} g \in \mathcal{G})$
$\Rightarrow g = g_k g_r$. $\quad \mathcal{G} \subseteq S$
2. $S \subseteq \mathcal{G}$ is trivial since every element of S has the form $g_k g_r$ with $g_k, g_r \in \mathcal{G}$.

$\square$

Because of the rearrangement theorem, every row and column of a multiplication table contains each element once and only once.

Two groups with the same multiplication table are isomorphic and represent the same abstract group.

(1.3) Symmetry operations and point groups

The groups in which we are interested in this context are made of SYMMETRY OPERATIONS.

Def: SYMMETRY OPERATION is an operation that leaves an object in an indistinguishable configuration which is said to be equivalent.

Among other symmetry operations, the ones needed for studying finite size objects (as for example molecules) are POINT symmetry operations that always keep at least one point invariant in the space.

A list:

- E identity (from german Einheit)
- C_n (proper) rotation of $\frac{2\pi}{n}$ radians around a certain axis. The axis with the larger n is called principal axis. If there are twofold axes perpendicular to the principal axis they are called dihedral and denoted C_2' and C_2''.
- S_n Rotation of $\frac{2\pi}{n}$ around a certain axis followed by a reflection with respect to the plane perpendicular to the rotation axis. Also called improper rotation (Rotoreflection)
- i inversion with respect to a point.
- σ mirror operation (from Spiegel = mirror) with respect to a plane

  σ_h perpendicular to the main rotation axis

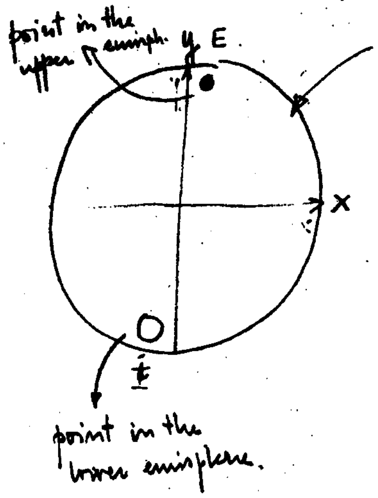
  σ_v containing the main rotation axis

  σ_d special case of σ_v but with the plane bisecting the angle between 2 dihedral axes.

Def: SYMMETRY ELEMENT is a point, a line or plane with respect of which a point symmetry operation is carried out. The notation given above is in reality the Schönflies for symmetry elements.

Def: A <u>POINT GROUP</u> is a group whose elements are POINT symmetry operations.

Projection diagrams are useful representations of point groups



projection of a sphere of unity radius in the xy plane

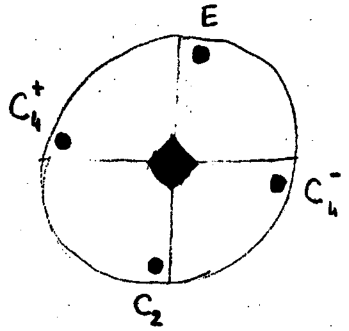
The order of the main rotation axis is given by dark "poligon" in the center

⬮ ▲ ■ ⬟ ⬢ ...

PROPER GROUPS

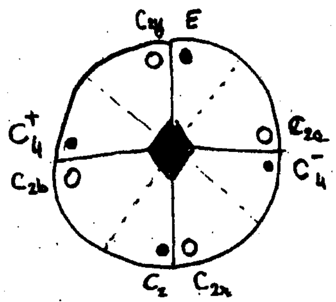
i $\boxed{\text{Cyclic groups}}$ C_n there is only 1 axis of rotation and the group elements are E, $C_{n[z]}^{(\pm k)}$

example C_4



ii $\boxed{\text{Dihedral groups}}$ Proper rotations that transform a regular n-sided prism into itself. The symmetry elements are C_n and $n\,C_2'$. The symbol D_n

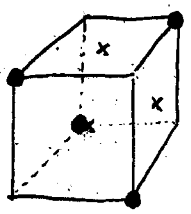
example D_4

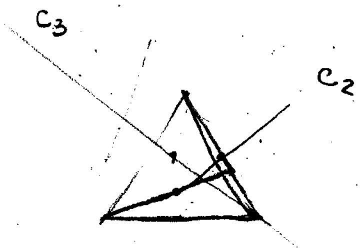


$a = \frac{1}{\sqrt{2}}[1\,1\,0]$

$b = \frac{1}{\sqrt{2}}[\bar{1}\,1\,0]$

iii $\boxed{\text{Tetrahedral group}}$ proper rotations that transform a tetrahedron into itself. Called T. The symmetry elements are $3C_2$ and $4C_3$





iv $\boxed{\text{Octahedral or cubic group}}$ called O. proper rotations that transform a cube or an octahedron into itself.

The symmetry elements $3C_4$ $4C_3$ $6C_2$

v $\boxed{\text{Icosahedral group}}$ called Y. Consists of the proper rotations that transform an icosahedron or pentagonal dodecahedron into itself. The symmetry operations

$$Y = \{E \quad 6C_5^{\pm} \quad 10C_3^{\pm} \quad 15C_2\}$$

the symmetry elements are $6C_5$ $10C_3$ $15C_2$

IMPROPER GROUPS

It is useful for the most compact definition of the improper groups to introduce the definition of outer direct product.

$A = \{a_i\}$ group of order a $\qquad A \otimes B = G = \{g_k\} \quad g_k = (a_i, b_j)$

$B = \{b_j\}$ group of order b

$(a_i, b_j)(a_l, b_m) = (a_i a_l, b_j b_m) = (a_p, b_q)$ due to closure of A and B.

If $(a_i, b_j) = a_i b_j$ (same product definition in A and B

$\Rightarrow$ ① $a_l b_j = b_j a_l \quad \forall\, l, j$

② $A \cap B = E$

i) From C_n — if n is odd $C_n \otimes C_i = S_{2n}$

$C_i = \{E, i\}$

— if n is even $C_n \otimes C_i = C_{nh}$

h stands for horizontal reflection plane which arises since $i C_2 = \sigma_h$

ii) From D_n — if n is odd $D_n \otimes C_i = D_{nd}$

d denotes dihedral planes bisecting the angles between C_2' dihedral axes.

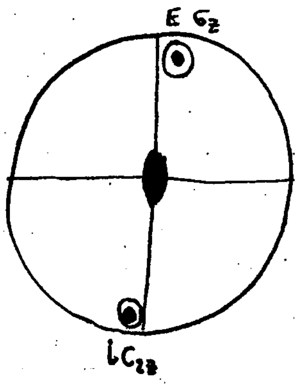
— if n is even $D_n \otimes C_i = D_{nh}$

iii) $T \otimes C_i = T_h$

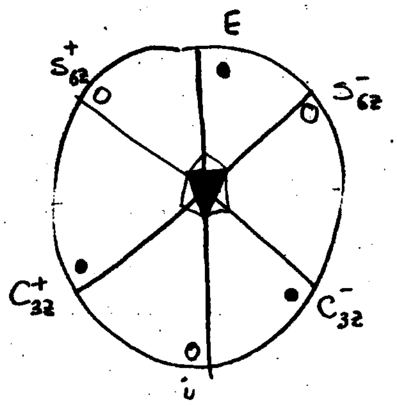
iv) $O \otimes C_i = O_h$

v) $Y \otimes C_i = Y_h$

<u>Example</u>



C_{2h}



S_6

$C_{2h} = C_2 \otimes C_i$ $\qquad$ $S_6 = C_3 \otimes C_i$

IDENTIFICATION OF MOLECULAR POINT GROUPS

Linear molecules

- no σ_h → $C_{\infty v}$ (Hydrogen chloride H - Cl)
- σ_h → $D_{\infty h}$ (Carbon dioxide O = C = O)

Non-linear molecules

- no proper axis of symmetry
  - σ — C_s
  - i — C_i
  - neither σ nor i — C_1
- C_n, $n > 1$
  - $\leqslant 1\, C_3$
    - $n C_2' \perp C_n$
      - σ_h — D_{nh} ⇝ Benzene
      - $n\sigma_d$ — D_{nd}
      - no σ — D_n
    - no $C_2' \perp C_n$
      - σ_h — C_{nh}
      - $n\sigma_v$ — C_{nv}
      - i — S_{2n}
      - no σ, no i — C_n
  - $> 1\, C_3$
    - $10\, C_3$, $6\, C_5$
      - i — I_h
      - no i — I
    - $4\, C_3$
      - $3 S_4$ — T_d ⇝ Methane
      - $3 C_4$
        - i — O_h
        - no i — O
      - $3 C_2$
        - i — T_h
        - no i — T