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Definitions and Cayley Tables

- What is a (sub)group, a group law and the group axioms? Name some examples.

  Solution:

  Definition: A group is a set, G, together with an operation $\cdot$ (called group law of G) that combines any two elements A and B to form another element $C = A \cdot B$. To qualify as a group, the set and operation, $(G, \cdot)$, must satisfy four requirements known as the group axioms:

  (i) **Closure**
  Each "multiplication" of any two elements of the group will also yield an element of this very group.
  $$\forall A, B \in G\ \exists C \in G \colon A \cdot B = C \tag{1}$$

  (ii) **Associativity**
  The order of "multiplication" does not matter as long as the sequence of operands is not changed.
  $$\forall A, B, C \in G \colon (A \cdot B) \cdot C = A \cdot (B \cdot C) \tag{2}$$

  (iii) **Identity element**
  In every group there is an identity element that, after "multiplication" with any other group element, will yield the very same element as result. It can be shown, that the identity is unique.
  $$\exists! E \in G\ \forall A \in G \colon A \cdot E = E \cdot A = A \tag{3}$$

  (iv) **Inverse element**
  Each group element has exactly one inverse which is also part of the group and which has the property to yield identity after multiplying with the original element.
  $$\forall A \in G\ \exists!\, A^{-1} \in G : A \cdot A^{-1} = A^{-1} \cdot A = E \tag{4}$$

  Additional properties:

  Commutativity (only for abelian groups)
  The order of operands is irrelevant, i. e. they commute. A group is then called abelian.
  $$\forall A, B \in G \colon A \cdot B = B \cdot A \tag{5}$$

  Subgroups
  Subsets U of a group $(G, \cdot)$ are called subgroups if they also form a group under the group operation $\cdot$. The trivial subgroup $\{E\}$ consists only of the identity element and is subgroup to every group by virtue of axiom (iii).
  See also `https://en.wikipedia.org/wiki/Subgroup`

  Order
  The order of a (finite) group, a. k. a. cardinality, is the number of its elements.

  Examples

  - $\{1, -1\}$ and $\{1, -1, \mathrm{i}, -\mathrm{i}\}$ with multiplication, $E = 1, 1^{-1} = -1$
  - $\mathbb{R} \setminus \{0\}$ with mutiplication, $E = 1, X^{-1} = 1/X$
  - $\mathbb{R}$ or $\mathbb{Z}$ with addition, $E = 0, X^{-1} = -X$
  - 3x3 orthogonal matrices with matrix multiplication $\rightarrow O(3)$ group, $E = \mathbb{1}, X^{-1} = X^{\intercal}$

- Point symmetry transformations.
  Point group elements (as a subgroup of the orthogonal group O(3)) can be realized as sets of orthogonal matrices M that transform a point x into a point y by virtue of $y = Mx$, where the origin is the fixed point.
- Translations with vector addition (infinite group!)
- Euclidean group $E(3)$ (leave distance between any 2 points in space unchanged) with subgroups i) translation group T, ii) rotation group $O^+(3)$, iii) inversion group C_i.
  Orthogonal group: $O(3) = O^+(3) \times C_i$.

- What is a group multiplication table (a. k. a. Cayley table)? As an example, fill such a table (if possible) for the following groups and name their identity and inverse elements:
  1. $(G_1, \cdot) = (\{1, -1, i, -i\}, \cdot)$,
  2. $(G_2, \cdot) = (\mathbb{R}^x, \cdot)$ with $\mathbb{R}^x \equiv \mathbb{R} \setminus \{0\}$,
  3. $(G_3, \cdot) = (\mathbb{R}, +)$,
  4. $(G_4, \cdot) = (\mathbb{Z}/m\mathbb{Z}, +)$, where $\mathbb{Z}/m\mathbb{Z}$ is the set of all sections modulo m, i. e. all sections of the form $[a]_m = a + m\mathbb{Z} = \{b|b \equiv a \bmod (m)\}$, ($\hat{=}$ m-fold rotations). Show for $m = 4$.
  5. $(G_5, \cdot)$ = point group C_n^k, i. e. rotations about an n-fold symmetry axis $\hat{=}$ rotation by angles $\varphi = k\frac{2\pi}{n}$. Show for $n = 3$.

  Which of them are abelian groups? What subgroups can you identify?
  If the modulo operation and residue classes are new to you, have a look here:
  https://de.wikipedia.org/wiki/Restklasse
  https://groupprops.subwiki.org/wiki/Group_of_integers_modulo_n

  Solution: a)

$\cdot$	1	-1	i	-i
1	1	-1	i	-i
-1	-1	1	-i	i
i	i	-i	-1	1
-i	-i	1	-i	i

d)

$\mathbb{Z}_4, +$	0	1	2	3
0	0	1	2	3
1	1	2	3	0
2	2	3	0	1
3	3	0	1	2

e)

$C_3, +$	E	C_3	C_3^2
E	E	C_3	C_3^2
C_3	C_3	C_3^2	E
C_3^2	C_3^2	E	C_3

  All groups are abelian; $g = \{E\}$ is always a subgroup; Caley table exist only for finite groups.
  1. $E = 1, A^{-1} = 1/A \quad \rightarrow \quad 1^{-1} = 1 \in G_1, \mathrm{i}^{-1} = -\mathrm{i} \in G_1$ ✓
     SG $= \{1, -1\}$, $\quad g = \{\mathrm{i}, -\mathrm{i}\}$ is not a SG, because $\mathrm{i} \cdot \mathrm{i} = -1 \notin g$
  2. Infinite group → no Caley table; $\quad E = 1, A^{-1} = 1/A \in G_2$ ✓
     infinite SGs: $\mathbb{R}^+$ (positive real numbers), $\mathbb{R}^-$ (negative real numbers), and many more, e. g. $\forall b \neq \pm 1 : g = \{b^n\}$ is infinite SG with $E = 1$ and $b^n \cdot b^m = b^{n+m}$ and $(b^n)^{-1} = b^{-n}$;
     finite SG: $\{1, -1\}$ (sign group); $\mathbb{R}^x \cong \mathbb{R}^+ \times \{1, -1\}$
  3. Infinite group → no Caley table; $\quad E = 0, A^{-1} = -A \in G_3$ ✓
     infinite SGs: $\mathbb{Z}$ (integers), $\mathbb{Q}$ (rational numbers), $a\mathbb{Z} = \{na \mid n \in \mathbb{Z}, a \in \mathbb{R}\}$ and more;
     no finite SGs besides $\{0\}$
  4. $(\mathbb{Z}_4, +)$ has $E = 0, A^{-1} = -A \in G_4$ ✓
     $[0]_4 = \{\ldots, -8, -4, 0, 4, 8, \ldots\} \ = \{b|b = 0 + 4n, n \in \mathbb{Z}\}$
     $[1]_4 = \{\ldots, -7, -3, 1, 5, 9, \ldots\} \ = \{b|b = 1 + 4n, n \in \mathbb{Z}\}$
     $[2]_4 = \{\ldots, -6, -2, 2, 6, 10, \ldots\} = \{b|b = 2 + 4n, n \in \mathbb{Z}\}$
     $[3]_4 = \{\ldots, -5, -1, 3, 7, 11, \ldots\} = \{b|b = 3 + 4n, n \in \mathbb{Z}\}$
  5. C_3^k has E = "no rotation" $\hat{=}$ rotations with $\varphi = 2\pi n,\ n \in \mathbb{Z}$ and $A^{-1} = C_3^{-k}$

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- Have a look at the Cayley table for the point group C_{3v}. What can you tell about its properties, i. e. corresponding symmetry elements, number of symmetry transformations, commutativity (abelian group?), possible duplicates?

C_{3v}	E	C_3	C_3^2	σ_{v1}	σ_{v2}	σ_{v3}
E	E	C_3	C_3^2	σ_{v1}	σ_{v2}	σ_{v3}
C_3	C_3	C_3^2	E	σ_{v2}	σ_{v3}	σ_{v1}
C_3^2	C_3^2	E	C_3	σ_{v3}	σ_{v1}	σ_{v2}
σ_{v1}	σ_{v1}	σ_{v3}	σ_{v2}	E	C_3^2	C_3
σ_{v2}	σ_{v2}	σ_{v1}	σ_{v3}	C_3	E	C_3^2
σ_{v3}	σ_{v3}	σ_{v2}	σ_{v1}	C_3^2	C_3	E

Solution:

- Symmetry elements: C_3 and $3 \times \sigma_v$ (for naming scheme details see next exercise sheet)
- Symmetry operations: See e. g. first row or column
- Subgroups besides identity are the point group C_s (reflection through a single plane, which is isomorphic to the cyclic group of order 2, $C_s \cong C_2$), and the group C_3

C_s	E	σ
E	E	σ
σ	σ	E

C_3	E	C_3	C_3^2
E	E	C_3	C_3^2
C_3	C_3	C_3^2	E
C_3^2	C_3^2	E	C_3

(6)

  $\{E, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}\}$ is not a subgroup, b/c most of their products do not belong to the set.
- Non-abelian, because table is not symmetric: $C_3\sigma_{v1} = \sigma_{v2}$ but $\sigma_{v1}C_3 = \sigma_{v3}$
- No element occurs more than once in each row or column. This holds for every Cayley table! In fact, each row/column is "only" a permutation of the set of symmetry operations.
- Search Youtube for step-by-step explanations on how to build the table, there are plenty of resources available.
- Wolfram Demonstration Project (Mathematica): interactive visualization of the C_{3v} group http://demonstrations.wolfram.com/OperationsOfC3vSymmetryGroupAppliedToAmmonia (unfortunately really slow)
- Examples from chemistry: NH_3, trichlormethane, $POCl_3$, 1,3,5-trichlorecyclohexane (all equatorial or all axial conformation)

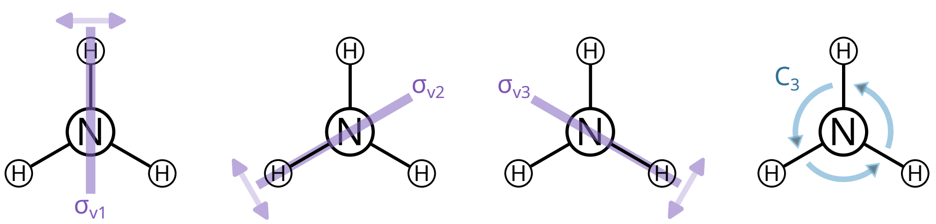

Figure 1: Ammonia as an example for the C_{3v} symmetry group. There are three mirror planes $\sigma_{v1}, \sigma_{v2}, \sigma_{v3}$, each containing the same 3-fold rotation axis C_3.

- Fill the Cayley table for the point group C_{2v} with help of the H_2O or 1,3-Dichlorobenzene molecule as an example.

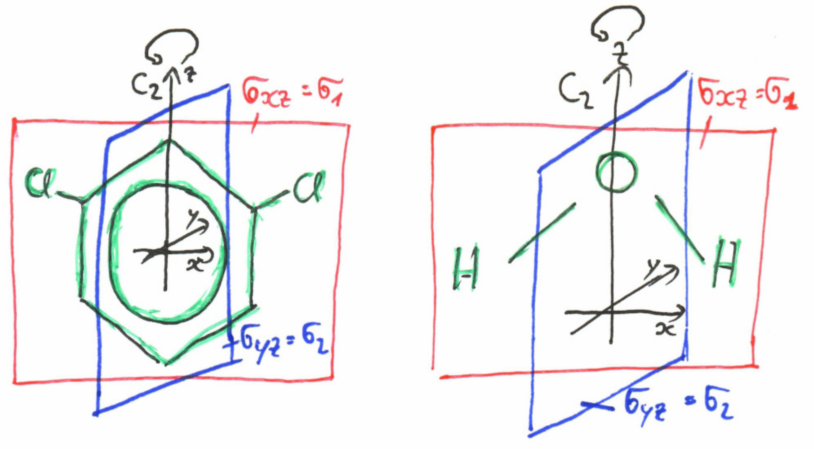

Figure 2: H_2O and 1,3-Dichlorobenzene are molecules illustrating symmetries according to the point group C_{2v}.

Solution:
Steps to reproduce:

1. Fill the row and column for identity.

$$\begin{array}{c|cccc} C_{2v} & E & C_2 & \sigma_{v1} & \sigma_{v2} \\ \hline E & E & C_2 & \sigma_{v1} & \sigma_{v2} \\ C_2 & C_2 & & & \\ \sigma_{v1} & \sigma_{v1} & & & \\ \sigma_{v2} & \sigma_{v2} & & & \end{array} \tag{7}$$

2. Since we can ignore the order (and potential non-commutativity) for the product of an element with itself, $m \cdot m = E$ with $m = C_2, \sigma_{v1}, \sigma_{v2}$, we can easily deduce how the main diagonal is populated.

$$\begin{array}{c|cccc} C_{2v} & E & C_2 & \sigma_{v1} & \sigma_{v2} \\ \hline E & E & C_2 & \sigma_{v1} & \sigma_{v2} \\ C_2 & C_2 & E & & \\ \sigma_{v1} & \sigma_{v1} & & E & \\ \sigma_{v2} & \sigma_{v2} & & & E \end{array} \tag{8}$$

3. Finally, we fill the missing relations

$$C_2 \cdot \sigma_{v1} = \sigma_{v1} \cdot C_2 = \sigma_{v2} \tag{9}$$
$$C_2 \cdot \sigma_{v2} = \sigma_{v2} \cdot C_2 = \sigma_{v1} \tag{10}$$

and can complete the table.

$$\begin{array}{c|cccc} C_{2v} & E & C_2 & \sigma_{v1} & \sigma_{v2} \\ \hline E & E & C_2 & \sigma_{v1} & \sigma_{v2} \\ C_2 & C_2 & E & \sigma_{v2} & \sigma_{v1} \\ \sigma_{v1} & \sigma_{v1} & \sigma_{v2} & E & C_2 \\ \sigma_{v2} & \sigma_{v2} & \sigma_{v1} & C_2 & E \end{array} \tag{11}$$

As subgroups we can again identify C_s for each of the two mirror planes, as well as C_2. Further, the group C_{2v} is obviously abelian.

- What is the symmetric group? Construct the Cayley table for the symmetric group S_3. What is this group's order and degree? How is it connected to the Cayley theorem?

Solution:

The symmetric group S_n, sometimes also called permutation group, is the group of all permutations π of a set M with n elements. The group operation is the composition of permutations, while a permutation can be thought of as bijective function from a set to itself.

The permutations are usually noted in one of the following three forms:

Cauchy's two-line notation

The first line lists the element of a set M, the second line tells you where each element is mapped to.

Example:

$$\pi = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 & x_5 \\ \pi(x_1) & \pi(x_2) & \pi(x_3) & \pi(x_4) & \pi(x_5) \end{pmatrix}, \qquad \pi = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 5 & 4 & 3 & 1 \end{pmatrix} \tag{12}$$

One-line notation

Effectively identical to the first variant except that the first row may be omitted in case there is a natural order of elements in M, e. g. for $M = 1, 2, 3, 4, \ldots, n$ or $M = x_1, x_2, x_3, \ldots, x_n$ and if there are no duplicates or repeated sequences as e. g. in $M = 1, 2, 3, 6, 1, 2, 3, 7$.

Example:

$$\pi = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 5 & 4 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 5 & 4 & 3 & 1 \end{pmatrix} \tag{13}$$

Cyclic notation

Here, the set is decomposed into "disjoint cycles", i. e. in subsets of elements that individually perform a cyclic rotation. Unrotated elements may be ommited. The subsets are found by successively applying the permutation on an arbitary element until the initial value is retained (without listing it twice): $(x, \pi(x), \pi(\pi(x))), \ldots)$.

Example:

$$\pi = \begin{pmatrix} 2 & 5 & 4 & 3 & 1 \end{pmatrix} = (125)(34) = (34)(512) \neq (34)(521) \tag{14}$$

Let's try to construct the Cayley table for such a permutation group. As an example, we will take the symmetric group of all permutations of three elements, S_3, which comprises the following 6 permutations[1] (hence is of order 6):

Element	Operation	Permutations	Cycle decomposition
e	identity	123 → 123	(1)(2)(3)
a	swap 1 and 2	123 → 213 → 123	(12) or (12)(3)
b	swap 2 and 3	123 → 132 → 123	(23) or (1)(23)
c	a • b • a	123 → 321 → 123	(13) or (13)(2)
d	a • b	123 → 231 → 312 → 123	(123)
f	b • a	123 → 312 → 231 → 123	(132)

Table 1: The symmetric group S_3 comprises all possible permutations of the set $M = \{1, 2, 3\}$. Cyclic decompositions are found by repeatedly applying the permutation on a single set element until the starting value is retained.

From here, we can construct the corresponding Cayley table by simply calculating all possible products:

$$\begin{array}{c|cccccc} S_3 & \mathrm{e} & \mathrm{a} & \mathrm{b} & \mathrm{c} & \mathrm{d} & \mathrm{f} \\ \hline \mathrm{e} & \mathrm{e} & \mathrm{a} & \mathrm{b} & \mathrm{c} & \mathrm{d} & \mathrm{f} \\ \mathrm{a} & \mathrm{a} & \mathrm{e} & \mathrm{d} & \mathrm{f} & \mathrm{b} & \mathrm{c} \\ \mathrm{b} & \mathrm{b} & \mathrm{f} & \mathrm{e} & \mathrm{d} & \mathrm{c} & \mathrm{a} \\ \mathrm{c} & \mathrm{c} & \mathrm{d} & \mathrm{f} & \mathrm{e} & \mathrm{a} & \mathrm{b} \\ \mathrm{d} & \mathrm{d} & \mathrm{b} & \mathrm{c} & \mathrm{a} & \mathrm{f} & \mathrm{e} \\ \mathrm{f} & \mathrm{f} & \mathrm{c} & \mathrm{a} & \mathrm{b} & \mathrm{e} & \mathrm{d} \end{array} \tag{15}$$

We notice again, that every row or column is just a permutation of the group elements. Further, the group is non-abelian since the Cayley table is not symmetric to the main diagonal. Last but not least, we can immediately identify the following subgroups:

- Order 1: trivial group $\{e\}$
- Order 2: three, each generated by one of the transpositions: $\{e, a\}$, $\{e, b\}$, $\{e, c\}$
- Order 3: the alternating group A_3 formed by the 3-cycle $\{e, d, f\}$

$$\begin{array}{c|cc} \cdot & e & a \\ \hline e & e & a \\ a & a & e \end{array} \qquad \begin{array}{c|cc} \cdot & e & b \\ \hline e & e & b \\ b & b & e \end{array} \qquad \begin{array}{c|cc} \cdot & e & c \\ \hline e & e & c \\ c & c & e \end{array} \qquad \begin{array}{c|ccc} A_3 & e & d & f \\ \hline e & e & d & f \\ d & d & f & e \\ f & f & e & d \end{array}$$

Apparently, these subgroups are again isomorphic to the cyclic group of order 2 and 3, just like before for the C_{3v} group. Hence, it is not surprising that C_{3v} itself is isomorphic to S_3.

Note: Do not confuse the order of a symmetric group (= number of *group* elements) with its degree (= number of elements in the underlying *set* which is permuted) or with the order of an element g in a group G, which is defined by the smallest positive integer n such that $g^n = e$.

As abstract group, S_3 and C_{3v} are isomorphic to the dihedral group D_3 of degree 3 and order 6, which also happens to be the smallest non-abelian group.

Abelian groups:
Generally, the following statements hold regarding abelian groups:

- Order 1: only the trivial group, obviously abelian.
- Order 2: Any group of order 2 is isomorphic to the cyclic group C_2, which is abelian.
- Order 3: Any group of order 3 is isomorphic to the cyclic group C_3, which is abelian.
- Order 4: Only (i) cyclic group C_4 and (ii) Klein four-group $V_4 = C_2 \times C_2$, both abelian.
- Order 5: Any group of order 5 is isomorphic to the cyclic group C_5, which is abelian.

Hence, the smallest non-abelian group is of order 6 and, as discussed before, isomorphic to S_3.

Cayley's Theorem:
Every group of order n is isomorphic to a subgroup of the symmetric group S_n. It follows, that

i) no element is mapped to itself except if the permutation is identity

ii) in each row or column of a Cayley table, the same element cannot occur more than once

[1] Here, a · b is to be understood as "first do b, then do a".