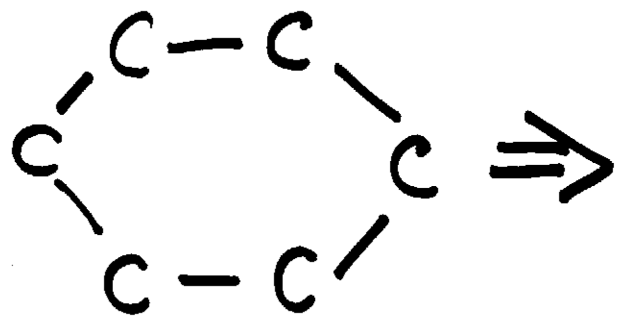
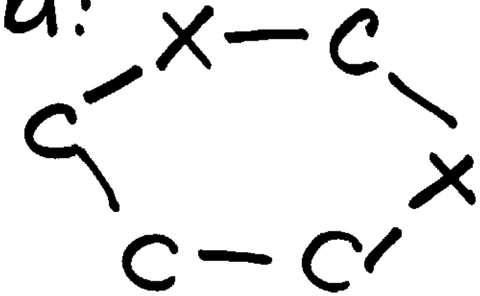
Introduction

Benzene:  New Compound: 

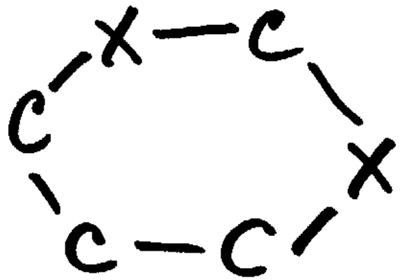
Total Number of possible new compounds: $2^6 = 64$.

Reason: 6 possible spots, each spot has 2 possible elements to choose from.

THIS IS WRONG!!! Why?

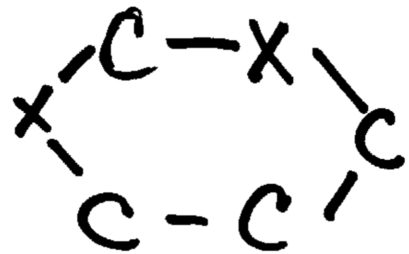
You forgot to account for rotational symmetry.

<u>Introduction</u> on back board near window



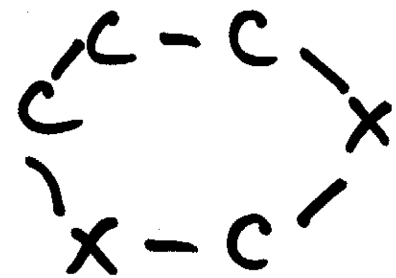
~

60° CCW



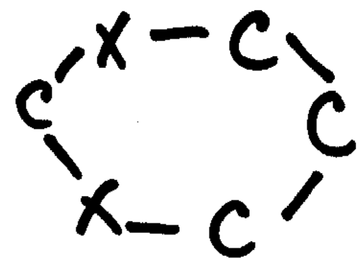
~

240° CCW

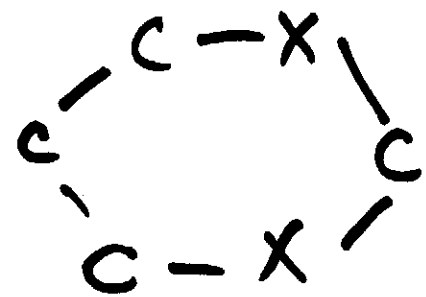


~

120° CCW

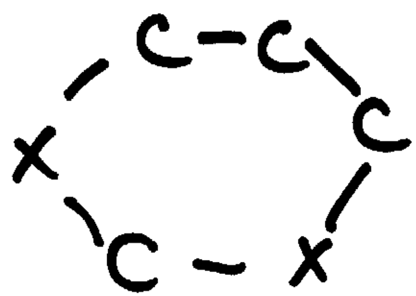


300° CCW



~

180° CCW



* not distinct when rotations are allowed.

Introduction

Note:

1. Some of the $2^6 = 64$ formations you counted are equivalent $\Rightarrow$ you've double counted.

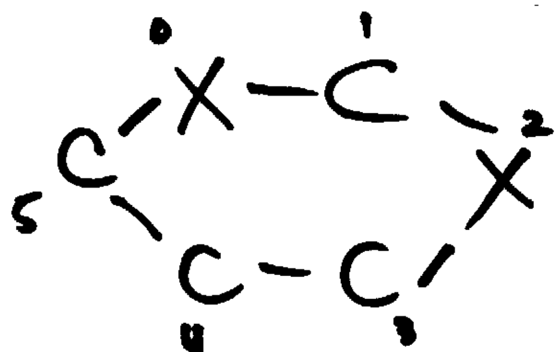
2. Instead of counting total # of formations, why not count the # of groups, each group containing equivalent compounds?

Problem: how many distinct compounds can you make, allowing for rotation?

already written ④

Formalization

1. model benzene rings as length 6 binary strings:



$\Longrightarrow$ 101000
0 1 2 3 4 5

2. Model rotations as permutations.

60° CCW ~ read from index 1	010001
120° CCW ~ read from index 2	100010
180° CCW ~ index 3	000101
240° CCW ~ index 4	001010
300° CCW ~ index 5	010100
360° CCW ~ index 0	101000

Formalization

$S = \{0,1\}^6$, set of linear length 6 binary strings

Each $s \in S$ can be written as $s_0 s_1 s_2 s_3 s_4 s_5$, s.t. $s_i \in \{0,1\}$ for $i \in \{0, \dots, 5\}$.

1. $|S| = 2^6 = 64$
2. example: 000000, 101000, ...

$G = \{g_0, \dots, g_5\}$, each g_i for $i \in \{0, \dots, 5\}$ is a permutation indicating the index position i at which to start reading a linear string $s \in S$. Permutation group G acts on set S. A mapping.

Formalization

Example:

$$s = \underset{0}{1}\underset{1}{0}\underset{2}{1}\underset{3}{0}\underset{4}{0}\underset{5}{0} \implies gs = \underset{2}{1}\underset{3}{0}\underset{4}{0}\underset{5}{0}\underset{0}{1}\underset{1}{0}$$

$$g = g_2$$

An element $g \in G$ acts on an element $s \in S$ is written as gs. Due to properties of groups, one of following happens:

1. $gs = s$, $g \in G$ and $s \in S$.
2. $gs = t$, $t \neq s$, $g \in G$ and $s, t \in S$.

Formalization

1: Example: $s = \underset{012345}{101010}$, $g = g_2$ $\Longrightarrow gs = \underset{234501}{101010}$

* g fixes or stabilizes s.

→ Define: $\mathrm{Stab}_s = \{g : gs = s \text{ for } g \in G\}$, the stabilizer of s is the the set of permutations $g \in G$ s.t. g acting on s maps s to itself. Ex on handout

→ Define: $\mathrm{Fix}_g = \{s : gs = s,\ s \in \mathcal{S}\}$, the set of elements of $\mathcal{S}$ fixed by g. Ex on handout

2: Example: $s = \underset{012345}{101010}$, $g = g_1$ $\Longrightarrow gs = \underset{123450}{010101}$

* g maps s to an element in its orbit.

→ Define: $\mathrm{Orb}_s = \{gs \in \mathcal{S} : g \in G\}$, the orbit of s is all elements that s can be mapped to in $\mathcal{S}$ by applying a permutation $g \in G$. Ex on handout.

Solution

Problem: # of distinct length 6 binary strings when allowing rotation.

Claim: This is the number of orbits that are distinct in S.

Why: By definition, each orbit contains an element $s \in S$ and all possible rotations/permutations reachable from s by applying $g \in G$. Orbits group rotationally equivalent strings.

Solution

8 4 -2

Solution : Burnside's lemma : The number of distinct orbits of S is equal to the average number of elements of S fixed by each $g \in G$.

$$|S/G| = \frac{1}{|G|} \sum_{g \in G} |Fix_g|$$

Where $|S/G|$ = number of distinct orbits of S.

already written ⑨ -1

Solution

We know $|G|=6$, need $|\mathrm{Fix}_g|$ for $g \in G$.

$|\mathrm{Fix}_{g_0}|$: number of $s \in S$ fixed by g_0

$$s_0 s_1 s_2 s_3 s_4 s_5 \xrightarrow{g_0} s_0 s_1 s_2 s_3 s_4 s_5$$

requires: $s_0 = s_0$, $s_1 = s_1$, ... $s_5 = s_5$ $\Longrightarrow$ all $s \in S$ work! $= 64$.

$|\mathrm{Fix}_{g_1}|$: number of $s \in S$ fixed by g_1

$$s_0 s_1 s_2 s_3 s_4 s_5 \xrightarrow{g_1} s_1 s_2 s_3 s_4 s_5 s_0$$

requires: $s_0 = s_1 = s_2 = s_3 = s_4 = s_5$ $\Longrightarrow |\{000000, 111111\}| = 2$.

$|\mathrm{Fix}_{g_2}|$: number of $s \in S$ fixed by g_2

$$s_0 s_1 s_2 s_3 s_4 s_5 \xrightarrow{g_2} s_2 s_3 s_4 s_5 s_0 s_1$$

requires: $s_0 = s_2 = s_4$, $s_1 = s_3 = s_5$ $\Longrightarrow 2^2 = 4$.

$|\mathrm{Fix}_{g_3}|$: number of $s \in S$ fixed by g_3

$$s_0 s_1 s_2 s_3 s_4 s_5 \xrightarrow{g_3} s_3 s_4 s_5 s_0 s_1 s_2$$

requires: $s_0 = s_3$, $s_1 = s_4$, $s_2 = s_5$ $\Longrightarrow 2^3 = 8$

opt. $|\mathrm{Fix}_{g_4}|$: number of $s \in S$ fixed by g_4

$$s_0 s_1 s_2 s_3 s_4 s_5 \xrightarrow{g_4} s_4 s_5 s_0 s_1 s_2 s_3$$

requires: $s_0 = s_4 = s_2$, $s_1 = s_5 = s_3$ $\Longrightarrow 2^2 = 4$

$|Fix_{g_5}|$: number of $s \in S$ fixed by g_5 (9)

$s_0 s_1 s_2 s_3 s_4 s_5$ requires : $s_0 = s_5 = s_4 = s_3 = s_2 = s_1$ -2

$s_5 s_0 s_1 s_2 s_3 s_4$ $\Longrightarrow 2$

Solution : $|S/G| = \frac{1}{|G|} \sum_{g \in G} |Fix_g|$

$= \frac{1}{6}(64 + 2 + 4 + 8 + 4 + 2) = 14.$

board 4

Intuition

define: multiorbit is multiset $M_s = \{gs : g \in G\}$. A multiset allows repetition. Ex on handout.

claim: $|M_s| = |G| \ \forall s \in S$. Trivial.

define: union of multisets A, B as: For each distinct element in A, B, take maximum amount of that element.

ex: $\{2,2,3\} \cup \{1,2,2,2,3\} = \{1,2,2,2,3\}$

define: union of multiorbits: $M = \bigcup_{s \in S} M_s$

claim: $\boxed{|M| = |M_s| \cdot |S/G| = |G| \, |S/G|}$

why: each orbit would have $|M_s|$ elements if repetition was allowed. The reason some have $< |G|$ elements is because orbits are sets, nonrepeating.

<u>Intuition</u>

<u>define</u> : $\text{Fix}_s = \{g : gs = s,\ g \in G\}$, set of elements of G s.t. g fixes s.

<u>claim</u> : $\boxed{\sum_{s \in S} |\text{Fix}_s| = \sum_{g \in G} |\text{Fix}_g|}$ because both sums enumerate pairs (g, s) s.t. $gs = s$.

<u>define</u> : multiplicity of s in M is the number of times s is repeated.

<u>claim</u> : multiplicity of $s \in S$ in M is $|\text{Fix}_s|$.

<u>why</u> : trivial by definition of Fix_s.

<u>claim</u> : $\boxed{|M| = \sum_{s \in S} |\text{Fix}_s|}$ because size of multiset is sum of multiplicity of distinct elements.

Intuition

recap: $|M| = \underline{|G| \cdot |S/G|}$

$$|M| = \sum_{s \in S} |Fix_s|$$

$$\sum_{s \in S} |Fix_s| = \underline{\sum_{g \in G} |Fix_g|}$$

$$\Longrightarrow \sum_{g \in G} |Fix_g| = |G| \cdot |S/G|$$

Burnside's Lemma.