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Topology in Chemistry

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Abstract

In this article we discuss the importance of topological and combinatorial concepts to count the number of isomers of a chemical compound. We have considered molecules of the kind $(CH)_{2n}$ in this article but the same game can be played with any other chemical compound.

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Introduction

The concept of isomerism was a significant advancement in chemistry; especially in the development of organic chemistry. As the number of isolated organic compounds increased during the early 1800s, the identification of different substances having the same molecular composition was inevitable. Isomerism was first noticed in 1827 by Friedrich Wöhler [1]. He noticed that chemical compounds with same molecular formulas might be different if their atoms are bonded differently (i.e. they have different structural formulas). In mathematical chemistry major areas of research include mathematical study of isomerism, chemical aspects of group theory, stereochemistry, quantum chemistry and topological aspects of chemistry. The basic models for mathematical chemistry are *molecular graph* and *topological index.* In this article we give theoretically possible isomers of Benzene under the assumption that in each isomer every carbon atom is associated with exactly one hydrogen atom.

Definitions and Results

Graph ([2], [3]): In the most common language a graph is an ordered pair G = (V, E) comprising of a set V of vertices together with a set E of edges, which are 2-element

subsets of V. Geometrically vertices are represented by points and edges by line segments (may not be straight) with end points as two element subsets of V which are in E. A graph will be called a multi graph if either there are more than one edges between two vertices or an edge has both the end vertices same (such an edge is called a loop). The sets V and E are usually finite, therefore degree of a vertex may be defined as the number of edges incident at this vertex (a loop is counted twice).

Isomorphic Graphs: Two graphs G and H are called isomorphic graphs if there is a bijection f: G $\rightarrow$ H between the vertex sets of G and H such that any two vertices u and v of G are adjacent in G if and only if f(u) and f(v) are adjacent in H.

Molecular Graph [4]: A molecular graph or a chemical graph is a representation of the structural formula of a chemical compound in terms of a graph. The vertices of this graph correspond to the atoms of the molecule and edges correspond to the chemical bonds. The presence of a double or triple bond makes it a multi-graph.

Topological Index: A topological index is a kind of a molecular descriptor that is based on the molecular graph of a chemical compound. These indices are numerical parameters of the graph which characterize its topology and are usually graph invariants.

Structural Isomers: These are the molecules having same molecular formula but are represented by different molecular graphs e.g. in Figure 1 below two different molecular graphs of the Benzene molecule are shown.

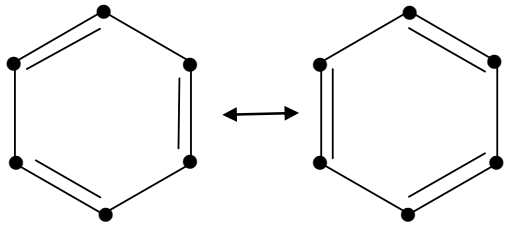

Figure 1: Molecular bond graphs for the Benzene molecule.

These are mirror images of each other and notice that one can not be superimposed onto the other. In above graphs each black dot represents a pair ‘C-H’. Topologically these two molecular graphs are same i.e. they are isomorphic. Our interest in this article is to give non-isomorphic isomers of Benzene.

To be more precise, we shall give *topologically distinct* isomers of $(CH)_6$. Notice that we have used the notation $(CH)_6$ instead of C_6H_6 because in constructing isomers we shall assume that each carbon atom is sharing exactly one of its valence electrons with a hydrogen atom. Moreover while drawing the molecular graphs of $(CH)_6$ we assume C-H as a single vertex (see figure 1). We shall also discuss about *topologically distinct* isomers of the molecule $(CH)_{2n}$. Note that two isomers can be topologically distinct in two ways (1) their molecular graphs are non isomorphic (2)

their molecular graphs are isomorphic but they are embedded differently in the space such that one graph is not deformable onto other continuously e.g. a circle and a trefoil knot are isomorphic as graphs but one cannot be deformed onto the other continuously. This situation cannot occur in the molecule $(CH)_{2n}$ for small values of n.

It is a natural to ask, "How many *topologically distinct* isomers of $(CH)_{2n}$ are there?" This question is really hard if one tries to do it for an arbitrary molecule. That is why I had started with $(CH)_{2n}$ and noticed that even for this very case it is not a trivial problem. It is already known from Polya's work (see [3], [5]) that it is difficult to count k-regular graphs up to isomorphism. However we feel that a computer algorithm together with the knowledge of *incidence matrices,* of the non-isomorphic graphs, may be useful to solve this problem.

Notice that a molecular graph of $(CH)_{2n}$ will be a cubic graph (i.e. each vertex will have degree 3) on 2n vertices and 3n edges. It is so, because a carbon atom has valency 4 and one valency is reserve for a hydrogen atom by our assumption, so each carbon atom in $(CH)_{2n}$ has three valance electrons to share with other valance electrons of the other carbon atoms. Further note that this molecular cubic graph can be a multi graph due the presence of double bonds (we do not consider triple bonds here because in that case we shall have only one possibility i.e n molecules of the type $HC \equiv CH$).

Theorem 1. If 'k' is an odd number then $(CH)_k$ cannot exist.

Proof. Let G be a cubic graph with 'k' vertices and 'm' edges. As each vertex in a cubic graph has degree 3, so sum of the degrees of all of its vertices will be 3k. Also note that in any graph sum of the degrees of vertices is equal to twice the number of edges, so $3k = 2m$. This implies that k must be an even number.

Theorem 2. Prove that there are only two topologically different isomers of $(CH)_4$ and six topologically different isomers of the $(CH)_6$ molecule.

Proof. Suppose that the cubic graph G corresponding to the molecule $(CH)_4$ is connected. So at least one of the following graphs will be a sub-graph of G depending upon whether $(CH)_4$ has no double bond, one double bond or two double bonds.

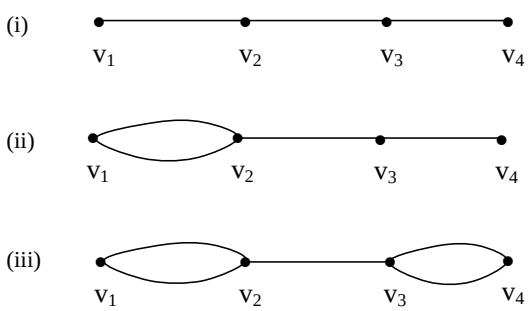

Figure 2

Since G has four vertices and by Theorem 1 there will be six edges in G. In order to complete the cubic graph G, we are to add three edges in (i), two edges in (ii) and only one edge to (iii). It is not hard to see that graph (ii) can not be completed to G without adding one more double bond, so from (i) and (iii) the only two possible isomers of $(CH)_4$ are shown in Figure 3 below.

Figure 3

Topologically different isomers of $(CH)_6$.
Let K be a cubic graph corresponding to the molecule $(CH)_6$. It will have six vertices and nine edges. Since it is connected so at least one of the following graphs will be a sub-graph of K depending upon whether it has no double bond, one double bond, two double bonds or three double bonds.

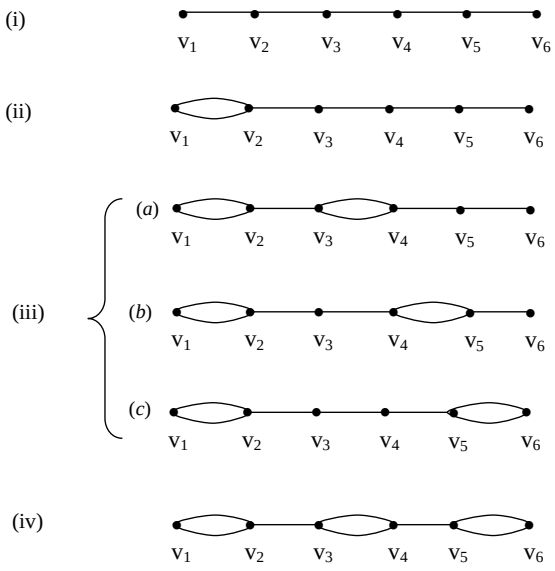

Figure 4

Now we shall construct the required graph K by using the above options. From option (iv) there is only one way to get K (i.e. join v_1 with v_6), which is benzene. From option (iii *c*) there are exactly two ways to get K; one way is to join v_1 with v_4 and v_3 with v_6 the second way is to join v_1 with v_3 and v_4 with v_6. From option (iii *b*) there is again only one way to get K (i.e. join v_6 with v_3 and v_1). From option (iii *a*) there is no way to get K without adding one more double bond. In option (ii) if we

join v_4 with v_1 then v_5 must be joined with v_3 and v_6 will be left with degree 1, so join v_4 with v_6. By further exploring similar kinds of possibilities it can be easily seen that there is only one way to get K from (ii). In order to get K from (i) we consider the incidence matrix of the expected molecular graph. The incidence matrix will be of the following form

$$\begin{array}{c} \\ V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \end{array} \begin{array}{c} \begin{array}{cccccc} V_1 & V_2 & V_3 & V_4 & V_5 & V_6 \end{array} \\ \begin{bmatrix} 0 & 1 & a & b & c & d \\ 1 & 0 & 1 & e & f & g \\ a & 1 & 0 & 1 & h & i \\ b & e & 1 & 0 & 1 & j \\ c & f & h & 1 & 0 & 1 \\ d & g & i & j & 1 & 0 \end{bmatrix} \end{array}$$

Where $a, b, c, d\ e, f, g, h, i, j \in \{0, 1\}$ and sum of the entries of each row and each column is 3. Under these conditions we see that there are only two incidence matrices with different ranks (isomorphic graphs will have the incidence matrices of same rank). So we get two non-isomorphic molecular graphs from (i). Hence there are total six ways to construct non-isomorphic cubic graphs K and therefore there are six possible isomers of the molecule $(CH)_6$ which are shown in Figure 5.

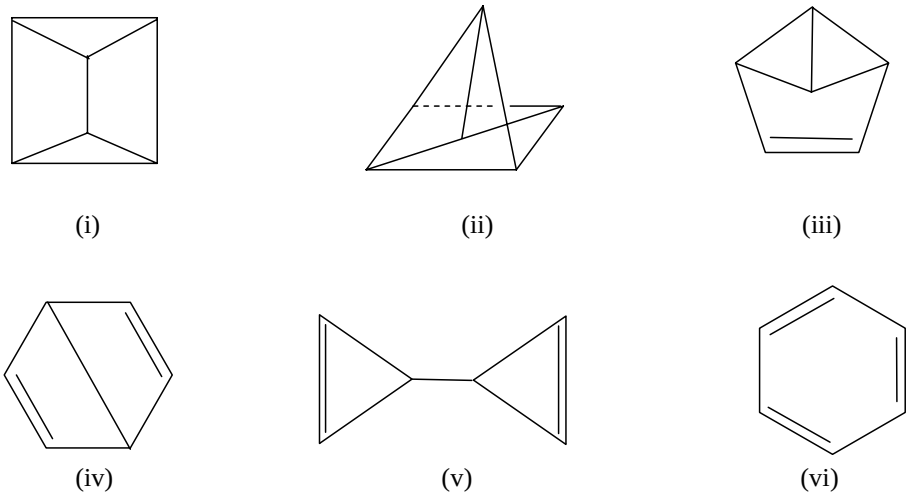

Figure 5

All these isomers are topologically distinct. The first one Prismane was proposed by Ladenburg in 1869, third is Benzvalene (it is not only the most extensively studied

valence isomer of benzene but also one of the most easily synthesized bicycle [1, 1, 0] butane derivatives), fourth is Dewar benzene proposed by Stadeler (1868) and Wichelhaus (1869) independently and the sixth one is benzene. Though Dewar benzene and the Prismane were considered as alternative structures for benzene then but now it is known that each of them is an isomer of benzene and is an independent molecule in its own right.

Not much is known about the existence of (ii) and (v). Notice that except (ii) all other are planar molecular graphs. We hope that non-isomorphic isomers of $(CH)_{2n}$ can be counted by using incidence matrices but as n increases the size of the incidence matrix will also increase so a computer program is required to find all possible incidence matrices. Moreover as n will increase we shall find some isomorphic graphs with topologically different embeddings, so that the level of difficulty of counting the topologically distinct isomers will raise moderately.

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