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EXISTENCE OF GRAPH THEORY IN CHEMICAL SCIENCES

Mathematics

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ABSTRACT

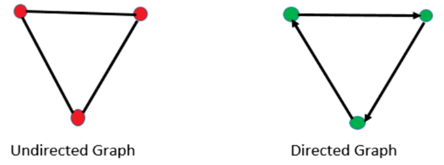
Graph Theory is the stdy of the graph. A graph $G=(V(G),E(G))$ consists of two finite sets $V(G)=\{v_1,v_2,\dots\}$, the vertex set of the graph, which is a non empty set of the elements called vertices, and $E(G)=\{e_1,e_2,\dots\}$, the edge set of the graph , such that each edge e_n is identified with an unordered pair (v_i,v_j) of vertices. The vertices (v_i,v_j) associated with edge e_n are called the end vertices of e_nGraph is represented by diagram, in which the vertices are represented as points and each edge as a line segment joining its end vertices [5]. The paper written by Leonhard Euler on seven bridges of Konigsberg and published in 1736 is regarded as the first paper in the history of graph theory. The term graph was introduced by Sylvester in a paper published in 1878 in Nature, where he draws an analogy between quantic invariants and co-variants of algebra and molecular diagrams.The applications of the graph are not only in Mathematics but also in other fields such as Computer Science, Physics and Chemistry, Biology, etc. In real-life also the best example of graph structure is GPS, where you can track the path or know the direction of the road.

KEYWORDS

Connected, graph, trees, planar, Valence, directed, undirected

INTRODUCTION-

The graphs are basically of two types, directed and undirected.



There are certain terms which are used in graph representation such as Degree, Trees, Cycle etc. .

Degree- A degree in a graph is mentioned to be the number of edges connected to a vertex. It is denoted deg(v), where v is a vertex of the graph.

Regular Graph- If for some positive integer k, deg $(v)= k$ for every vertex v of the graph g, then G is called k-regular. A regular graph is one that is k-regular for some k.

Cycle- A cycle is a closed path in a graph which forms a loop. When the starting and ending point is the same in a graph that contains a set of vertices, then the cycle of the graph is formed. When there is no repetition of the vertex in a closed circuit, then the cycle is a simple cycle. A cycle which has an even number of edges or vertices is called Even Cycle. A cycle which has an odd number of edges or vertices is called Odd Cycle.

Connected Graph- A graph G is called connected if every two of its vertices are connected.

Planer Graph-.A plane graph is a graph drawn in a plane in such a way that any pair of edges meet only at their end vertices. A planar graph is a graph which is isomorphic to a plane graph, i.e. it can be redrawn as a plane graph.

Hamiltonian Graph- A Hamiltonian path in a graph G s a path which contains every vertex of G.A Hamiltonian cycle or Hamiltonian circuit in a graph G is a cycle which contains every vertex of G. A graph is called Hamiltonian if it has a Hamiltonian cycle.

Graph Isomorphism- A graph $G_1=(V_1,E_1)$ is said to be isomorphic to the graph $G_2=(V_2,E_2)$ there is a one to one correspondence between the vertex sets v_2 and v_2 and a one-one correspondence between the edge sets $E_1$and E_2 a way that if ein such$_1$ is an edge with end vertices $u_1$and v_1 in G_1 ,then the corresponding edge e_2 in G_2has its end points the vertices $u_2$and $v_2$in G_2 which correspond to $u_1$and $v_1$respectively. Such a pair of correspondences is called graph isomorphism. Clearly two graphs are isomorphic then they must have same number of vertices and the same number of edges.

Trees-A tree in a graph is the connection between undirected networks which are having only one path between any two vertices. It was introduced by British mathematician Arthur Cayley in 1857. The graph trees have only straight lines between the nodes in any specific direction but do not have any cycles or loops. Therefore trees are the directed graph.

Graph Theory in Chemistry- Graphs naturally model molecules and this modeling provides rules that predict chemical properties, easy classification of compounds, computer simulations and computer-assisted design of new compounds. Given a chemical substance and some of its properties, the chemist would like to find out if this substance is a known compound. Chemists manipulate graphs on a daily basis. If he is able to identify this compound, he may like to know some additional properties of the compound. If compound is new, he would like to know its structure and then include it in dictionary of known compounds. So there is a need of standard representation for a compound.

Given the chemical formula of a new substance and the valence rules, one can generate the list of all distinct chemical structures possible, using graph enumeration techniques. Computer programs have been written to perform this operation. This method of producing an exhaustive list of all possible isomers gets out of hand as the number of atoms in the molecule increases. It is therefore necessary to provide addition chemical information to keep the list to a manageable size. As a part of continuing effort towards a system of automated identification of chemical compounds, a computer language called DENDRAL has been developed at Stanford university [3,4]. One of the programmers in DENDRAL generates the list of all tree type potential isomers from an input of molecular formula and mass spectrum.

In 1857, Arthur Cayley used trees to represent the structures of organic molecules. Recently graph theoretic techniques are coming into use for characterization and identification of chemical compounds. This is due to the advent of the electronic computer with its ability to handle graphs, and the ever-intensifying need of the chemist to have a mechanized information retrieval system capable of dealing with the millions of organic compounds known today. Many notions and theorems from graph theory are used in chemistry with a different name.

SOME EXAMPLES-

1. **Hydrocarbons-** Hydrocarbon Consist of hydrogen (H) and carbon (C) only and is very suitable for modeling as a graphs. Trivially, every hydrocarbon has a graph representation.

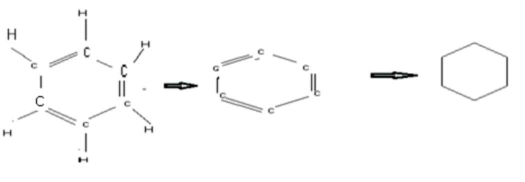


Fig 1

Now question arises-when does a graph represent a real hydrocarbon, what properties of the compound can be inferred from its graph?

Each chemical element is composed of a nucleus and electrons. Carbon has 6 electrons and hydrogen has only 1 electron. Valence electrons of an element are its electrons that participate in chemical bonds.

For now, we can assume that these are electrons in the outer shell. Carbon has 4 valence electrons, hydrogen has 1. Atoms are most stable when their outer shell of electrons is complete". For carbon "complete" means 8 electrons and for hydrogen 2 electrons. Elements share electrons in order to complete their outer shell of electrons, thus forming covalent chemical bonds.

Benzenoids- The graphs of benzenoids consist of hexagons arranged in the plane, such that any two hexagons are either point-disjoint or possess exactly one common line.

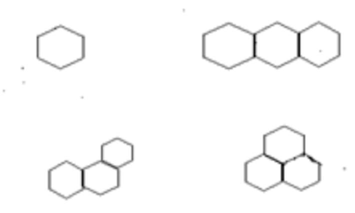


Fig 2

From the graph of a benzenoid we see the bonds of 3 valence electrons of each carbon. To get a stable compound the 4th electron needs to participate in a double bond (C=C). Therefore the compound is stable (has a valid Kekule structure) iff a perfect matching exists in the graph.

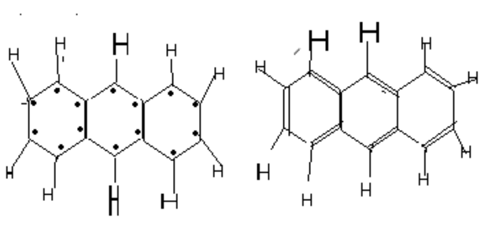


Fig 3

3.Structural graph of amino acetone $C_3 H_7 NO$,with its H atom stripped off, valence for carbon C is 4, for nitrogen N is 3, and for oxygen O , it is 2.

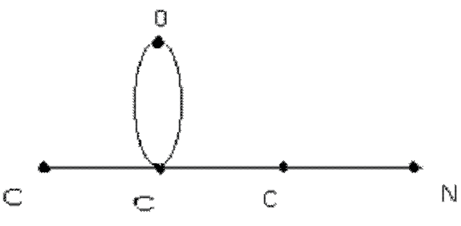


Fig 4

Arthur Cayley shown, how a chemical compound can be represented by means of a connected graph, with the atoms as the vertices and the bonds between them as edges. For compactness the hydrogen atoms are omitted from the representation as they are implied by every unused valence of the other atoms. Cayley discovered trees while he was trying to count the number of structural isomers of the saturated hydrocarbons or paraffin series $C_n H_{2n+2.}$ He used a connected graph to represent the $C_n H_{2n+2.}$ molecule. Carbon atom was represented by a vertex of degree four and hydrogen atom by a vertex of degree one. The total number of vertices in such a graph is v=3n+2 And the total number of edges is $e = \frac{(sum\ of\ degrees)}{2} = \frac{1}{2}(4n + 2n + 2) = 3n + 1$

Since number of edges is one less than the number of vertices and Graph is connected, it is a tree. For this reason problem of counting structural isomers of a given hydrocarbon becomes the problem of counting trees [6].

A graph, in which every vertex is assigned a unique name or label, is called a labeled graph. Cayley and Moon proves that the number of labeled trees with n vertices (n is greater than or equal to 2) is n^{n-2} In the actual counting of isomers of C_nH2_{n+2}, this result is not enough.

Here two observations are made: First the vertices representing hydrogen are pendant, they go with carbon atoms only one way, and hence make no contribution to isomerism. Second the tree representing C_nH2_{n+2} reduces to one with k vertices, each representing a carbon atom. In this tree no distinction can be made between vertices, so it is unlabeled. For butane C_4H_{10} , there are two distinct trees. As every chemist knows, there are exactly two different types of butanes: n-butane and isobutane.

A standard representation of chemical compound structures is necessary for computerized information retrieval system. Chemical compound can be divided into two classes: the aliphatic compounds and the ring compounds. The structural graph of an aliphatic compound has no circuit except circuits of length two, which are represented by parallel edges. Graph of a ring compound contains at least one circuit of length three or more. Graph of an aliphatic chemical compound is a tree; it can easily be given a canonical representation. Every tree has a unique centroid or a pair of centroids (parallel edges are considered as single edges for purposes of locating the centroid). The centroid can be used as the root of the tree and each sub tree attached to the root is a radiacal. The sub trees can be ordered by the number of vertices they contain in a non decreasing order. Each radical is further subdivided into sub radicals, which are ordered in the same manner. Thus produces a unique linear code for each tree-a string .For example, the code for the tree in fig 4 is C(C)(=O)(C(N)) [2].

The structural graph of almost every ring compound is (1) planer (2) a regular graph of degree three and contains a Hamiltonian circuit. So it is not very difficult to find a unique linear code for such a graph.

The problem of determining whether or not two chemical compounds having same chemical formula are identical is the same as the graph isomorphism problem. Two graphs would be isomorphic if and only if their codes were the same. For chemical structures it is generally easer to perform a direct vertex by vertex matching than to first find a unique code for each graph.

We can say that structural graph of a chemical compound contains much more information than molecular formula. But a structural graph does not contain all the information contained in the three dimensional model of the chemical compound. The structural graph does not specify the bond distances or bond angles of the molecule. A slightly more serious shortcoming of a graph is its inability to distinguish between stereo isomers [1]. Thus except for stereochemistry process the structural graph gives a reasonably adequate description of a chemical compound.

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