



Graph Theory in structural studies of Benzene and its derivative compounds

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ABSTRACT

This literature survey aims to discover the relationship between graph theory and chemical molecular structures that can be applied in practice. This is done in order to gain insight into the physical properties of the compound. Various papers based on graph theory have been studied and an overview is discussed in this literature survey.

KEYWORDS: Hexabenzocoronene, polycyclic aromatic hydrocarbon, Molecular connectivity, Graph theory in chemical structures.

INTRODUCTION

Graph theory in chemical molecular structure is an interdisciplinary that involves combining methods and theorem from Mathematics and Chemistry. Chemical structure includes the bond angle, type of bonds, size of the molecule and the interactions between the molecules.

Molecular structure is represented graphically. In the molecular graph, nodes and edges represent atoms and bonds respectively. Vertex degrees and edge multiplicities correspond to the valences of the atom and bond. (Chi Chen, 2019). The distance between two vertices is the number of edges with the shortest path. In a graph, a path means a walk in which a vertex is visited only once. In a connected graph like molecular graph for every vertex pair there must be at least one path.

Alexandru Balaban and Harry Wiener significantly contributed to Chemical graph theory. The first application of Chemical graph was registered in the late eighteenth century.



Various applications include Isomer Enumeration, Chemical Graph Generation, Molecular Fragmentation, Molecular Descriptors and other types of molecular descriptors exist. Among them, chemical indices, topological indices, (Hong Yang, 2019), autocorrelation descriptors, geometrical descriptors and some of the molecular fingerprints used in chemical graphs, representing the hypothetical forces between atoms. Within the molecules, despite the fact, chemical bonds were not yet identified, still various graph theory in molecular structure have been reported. This survey's key take-away is linking polyaromatic hydrocarbons (a molecular structure) with chemical graph theory.

Types of Graphs

Simple Graph: A simple graph with no loops and no parallel edges is called the undirected graph. The degree of every vertex is at most $n-1$ for a simple graph which has n vertices. **Undirected Graph:** The edges are not directed in a graph is called undirected graph. **Directed Graph:** The graph with the edges is directed by arrows is called directed graph. These graphs are called digraphs. **Complete Graph:** A graph in which every pair of vertices is joined by exactly one edge is called complete graph. It contains all possible edges. A complete graph with n vertices contains exactly n_{C_2} edges and is represented by K_n .

Connected Graph: A graph in which we can have adjacency from any one vertex to any other vertex is called connected graph. In this connected graph, at least one edge exists between every pair of vertices. **Regular Graph:** A graph in which degree of all the vertices is equal is called Regular Graph. All the vertices have same degree k , then it is called k -regular graph.

Cyclic Graph: A graph with ' n ' vertices (where, $n \geq 3$) and ' n ' edges forming a cycle of ' n ' with all its edges is known as cycle graph. A graph with at least one cycle is known as a cyclic graph. In the cycle graph, degree of each vertex is 2. The cycle graph which has n vertices is denoted by C_n . **Bipartite Graph:** A bipartite graph is a graph in which the vertex set can be partitioned into two sets such that edges only go between sets, not within them. A graph $G(V, E)$ is called bipartite graph if its vertex-set $V(G)$ can be decomposed into two non-empty disjoint subsets $V_1(G)$ and $V_2(G)$ in such a way that each edge $e \in E(G)$ has its one last joint in $V_1(G)$ and other last point in $V_2(G)$. The partition $V = V_1 \cup V_2$ is known as bipartition of G .

Star Graph: A star graph is a complete bipartite graph in which $n-1$ vertices have degree 1 and a single vertex have degree $(n-1)$. This exactly looks like a star where $(n-1)$ vertices are connected to a single central vertex. A star graph with n vertices is denoted by S_n . **Planar Graph:** A graph with no two edges of it cross each other except at a vertex to which they are meeting.

Recent New Graphs: Fan graph, butterfly, double butterfly graph, Friendship graph, Jelly graph, Honey Comb Network graph and many existing now.

The Domination, Labelling, Coloring are play vital role in Graph theory.

A dominating set for a graph $G = (V, E)$ is a subset D of V such that every vertex not in D is adjacent to at least one member of D . The domination number $\gamma(G)$ is the number of vertices in a smallest dominating set for G . Types of Domination: Factor and Global Domination, Distance Domination, Connected Domination, total domination, Paired domination, k -domination, k -tuple domination so many new domination types are evolved.



Coloring: Graph coloring is an assignment of labels called "colors" to elements of a graph subject to certain conditions.

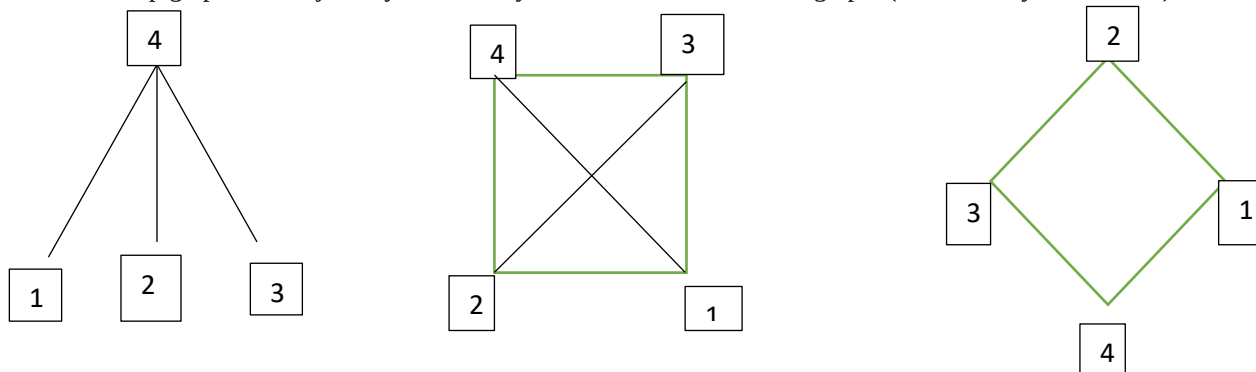
The coloring means the vertices of a graph in such way that no two adjacent vertices are of the same color; this is called a vertex coloring. Similarly, an edge coloring assigns a color to each edge in such way that no two adjacent edges are of the same color, and a face coloring of a planar graph assigns a color to each face or region so that no two faces that share a boundary have the same color.

Labelling: A graph labelling is the assignment of labels, by using integers, to edges and or vertices of a graph. For, given a graph $G = (V, E)$, a vertex labelling is a function of V to a set of labels; a graph with such a function defined is called a vertex-labelled graph. Similarly, an edge labelling is a function of E to a set of labels. In this case, the graph is called an edge-labelled graph. When the edge labels are members of an ordered set (e.g., the real numbers), it may be called a weighted graph. Types of Labelling: Graceful labelling, Edge graceful labelling, Harmonious labelling, Graph colouring, Lucky labelling and some more new Labelling are existing now days.

Recent New Graphs: Fan graph, butterfly, double butterfly graph, Friendship graph, Jelly graph, Honey Comb Network graph and many existing now.

The adjacency and graph isomorphism are the basic link between graph theory and chemical structures

The adjacency matrix is called as connection matrix, matrix with rows and columns labelled by graph vertices, with a 1 or 0 in position (v_i, v_j) according to whether v_i and v_j are adjacent or not. The adjacency matrix must have 0's on the diagonal, for no self-loop graph. The adjacency matrix is symmetric for an undirected graph. (John W. Raymond, 2017)



The adjacency matrices for the above graph are given below:

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

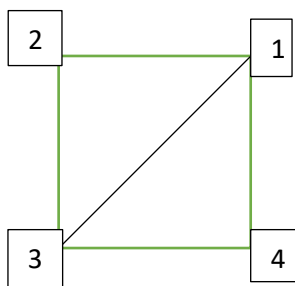
$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

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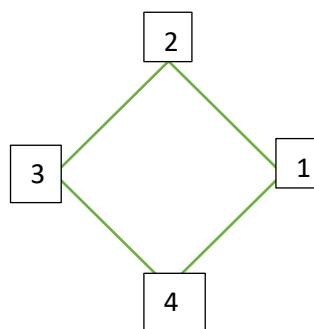


GRAPH ISOMORPHISM

A Graph $G(V, E)$ is a set of vertices and Edges. If there is an Edge between the vertices, it is said to be adjacent of neighbour and if there is a relation between vertices, it is called as adjacency relation. Adjacency matrix is used to represent graph in memory, where 1 represents edge and 0 represents no edge. Graph Isomorphism. If two graphs are looking same, but number of vertices and edges are not same then it is not isomorphic. If there is one to one mapping function between the vertices then it is called as isomorphic. If all properties of graph isomorphism are satisfied then two graphs are said to be isomorphic else not. Properties of graph isomorphism are as follows: 1. Number of vertices should be equal for both the Graphs. 2. Number of Edges should be Equal for both the Graphs. 3. In Degree and Out Degree should be equal. 4. Number of connected components should be same. 5. Number of loops should be same. 6. Number of parallel edges should be same. (John W. Raymond, 2017)



Graph G1



Graph G2

Graph G1 and G2 are Isomorphic graphs. 1. Number of Vertices=4(G1&G2). 2. Number of Edges =5(G1&G2) 3. Number of Degree=2(G1&G2). 4. Connectedness= Fully 5. Pairs of connected vertices= Yes.

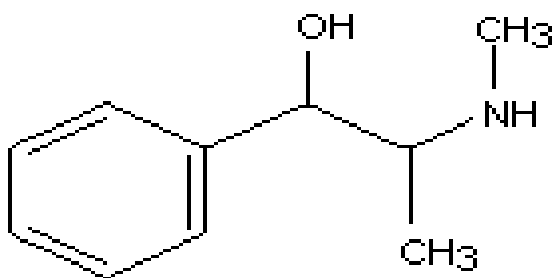
Subgraph Isomorphism algorithm for chemical structures is Maximum Common Subgraph which is used for matching 2D and 3D Structures (John W. Raymond, 2017). Author introduced a subgraph isomorphism algorithm for biochemical data (Vincenzo Bonnici, 2013) This algorithm is not using pruning rules and domain reduction procedure which reduces the search space.

Applications of Benzene in real life

At low exposure levels, benzene is rapidly metabolized and excreted predominantly as conjugated urinary metabolites. At higher exposure levels, metabolic pathways appear to become saturated, and a large portion of an absorbed dose of benzene is excreted as a parent compound in exhaled air. Benzene and benzene-based molecules are part of many medications used to relieve pain, alleviate cold and flu symptoms, and as a weight-loss aid. phenylpropanolamine (PPA), which contains has been used in decongestants. Decongestants cut down on the fluid in the lining of nose. That relieves swollen nasal passages and congestion. Analgesics contain benzene which is produced when one of the hydrogen atoms is replaced by another molecule. Analgesic drugs include the nonsteroidal anti-inflammatory drugs (NSAIDs). NSAIDs such as aspirin, naproxen and acetaminophen.



phenylpropanolamine (PPA)



Manufacture of Tire/Rubber: Various steps in the production of rubber involve the utilization of benzene. Adhesion substance used to attach rubber soles also contains benzene.

Paints/Printing Products: Various products employed in the print industry contain benzene. It is also a constituent of various painting products.

Fuel Oils: Fuel oils like petroleum, gasoline, and kerosene contain benzene. Benzene is also a precursor for the production of asphalt.

Plastics: Benzene is used widely in the plastic industry. The production of products like nylon, styrene, and Styrofoam also require benzene.

Chemicals: Chemicals like insecticides, pesticides, detergents, dyes, and fertilizers require benzene in the production process.

Automobiles: Benzene is used in the repair and maintenance of the automobiles.

Polycyclic Aromatic Hydrocarbons (PAH)

A polycyclic aromatic hydrocarbon is a hydrocarbon—a chemical compound containing only carbon and hydrogen—that is composed of multiple aromatic rings. The group is a major subset of the aromatic hydrocarbons. Many of them are found in coal and in oil deposits, and are also produced by the thermal decomposition of organic matter—for example, in engines and incinerators or when biomass burns in forest fires. These compounds tend to persist in the environment because PAH are insoluble in water. Mammals can absorb PAH by inhalation, dermal contact and ingestion. (Alexandro T, 1985).

Plants can absorb PAH from soil through their roots and translocate them to other plant parts. PAH are moderately persistent in the environment, and can bio-accumulate. PAH have moderate to high acute toxicity to aquatic life and birds. Although the emphasis is on avoiding exposures to PAH, some of these molecules are useful for making medicines, plastics, dyes and pesticides. PAH includes compound like Coronene ($C_{24}H_{12}$), ovalene ($C_{82}H_{14}$),



Perylene($C_{20}H_{12}$) and HEXABENZOCORONENE ($C_{42}H_{18}$) and much more. It consists of a central coronene molecule, with an additional benzene ring fused between each adjacent pair of rings around the periphery. Figure 1 is the structure of benzene. Figure 2 is the structure of hexabenzocoronene and Figure 3 is the structure of hexa-peri-hexabenzocoronene

Result and discussions of benzene and hexabenzocoronene

The molecular graph of the benzene ring embedded in the P-type surface network is depicted in Figure (4). The cardinality of vertices and edges of the given molecular graph are $24mn$ and $32mn - 2m - 2n$, respectively. The vertex set consists of two vertex partitions in the benzene ring embedded in the P-type surface network, as shown in Table 1. Furthermore, the edge set consists of three edge partitions. The first edge partition contains $4m + 4n$ edges uv , where $\deg(u) = \deg(v) = 2$. The second edge partition contains $16mn$ edges uv , where $\deg(u) = 2$ and $\deg(v) = 3$. The third edge partition contains $16mn - 2m - 2n$ edges uv , where $\deg(u) = \deg(v) = 3$. Table 2 shows the edge partition in the benzene ring embedded in the P-type surface network. They compute the M-polynomial of the benzene ring embedded in the P-type surface network. Also, they present the graphical representation of this graph in 2D and 3D by using Maple 13. In the end, they compute and simplify the topological indices by using the M-polynomial of the benzene ring embedded in the P-type surface network. (Hong Yang ,2019)

In particular, topological indices such as Wiener and Szeged indices used to predict the bio-activity of the chemical structures. They compute the Wiener and Szeged indices Hexabenzocoronene (HBC(n)) (Jasinth Quadras,2016)

Table 1: Vertex partition of the benzene ring embedded in the P type surface network based on degrees of each vertex.

d_v	2	3
Frequency	$8mn + 4m + 4n$	$16mn - 4m - 4n$

Table 2: Edge partition of the benzene ring embedded in the P-type surface network based on degrees of end vertices of each edge

(d_u, d_v)	(2,2)	(2,3)	(3,3)
Frequency	$4m + 4n$	$16mn$	$16mn - 6m - 6n$



Figure 1



Figure 2

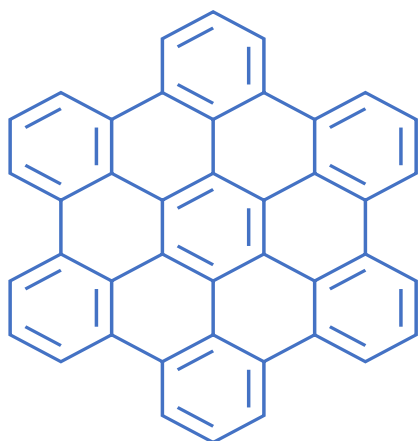


Figure 3

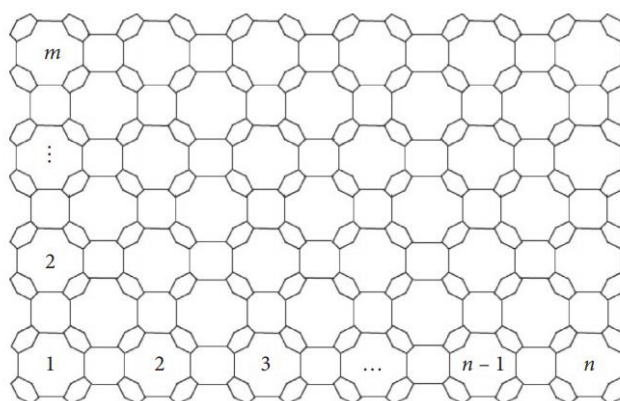


Figure 4

Conclusion:

In this paper, the molecular graph and application of Chemical graph for the compound's benzene and hexabenzocoronene are discussed. It is observed benzene and its derivative like hexa-peri-hexabenzocoronene (Jasinth Quadras, 2016), phenylpropanolamine with the chemical graph theory helps us to fore see the various combinations that are available and plays



an important role in many industries like drugs, plastics and rubber. Chemical Structures: In this structure nodes represents atoms and edges represents covalent bonds. Structural formula shows chemical information and the formula should be uniquely indexed and identified. Molecule structures are studied by graph theory.

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