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MOLECULAR GRAPH OF LINEAR BENZENOID COMPOUNDS AS FRACTALS

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Abstract: This paper obtains that Molecular Graph of Linear Benzenoid Compounds is a fractal which satisfies Self-similarity property proved by Iteration Process of its degree sequence and contains similar shape in its Structure.

Keywords: Molecular Graph, Degree sequence, Self-similarity, Fractals.

I. INTRODUCTION

Chemical Graph theory is the study of molecular structures represents graphs in Graph Theory. In an undirected graph, the degree sequence is a monotonic non-increasing sequence of the degrees of its vertices [1-4]. Graph invariants are most ordinarily mentioned as topological indices and are often defined using degrees of vertices, distances between vertices, Eigen values, symmetries, and lots of other properties of graphs. A molecular formula of an organic compound is often represented by a molecular graph, its vertices be atoms and edges like covalent bonds. The partitions of the degree sequence are self similar. Also, the partitions of *n+1* are similar to the partitions of *n*. It is a property of recursively defined functions. Self-similarity is a pictorial representation of recursion. These details can be found in [5-8].

Benzene structure in organic compounds plays a vital role in Chemical Industries. All over the world, Benzene is demanded for the growing plastics necessitated the production of benzene from petroleum. Benzene is used to produce drugs, plastics, petrol, oil and rubber [9].

When one part of a structure can be expanded (or diminished) to look like the whole structure, it is self-similar. One of the basic properties of fractal geometry is self-similarity. Self-similarity can be classified into three ways. The powerful type of self-similarity is *Exact self-similarity* .This is encountered only in theoretical fractals. These fractals contain exact copies of them selfsame through all scales. Fractal Dimension is a measure of self-similar object. The exactly self-similar method is used to find the Fractal Dimension mathematically generated repeating patterns [10, 11, 12].

II. STRUCTURAL ANALYSIS OF BENZENE

The molecular geometry of a molecule defines its three dimensional structure in terms of its bond angles, bond lengths and dihedral angles. The crystal structure of benzene is one of the most basic and most actively investigated structures. In the molecular graph of Linear Benzenoid Compounds, Its structure forms a perfectly regular hexagon which has exactly the same lengths between all carbon-carbon bonds. In the interior of Linear Benzenoid Compounds, two or more benzene rings fused together.

2.1 MOLECULAR GRAPH OF LINEAR BENZENOID COMPOUNDS [5]

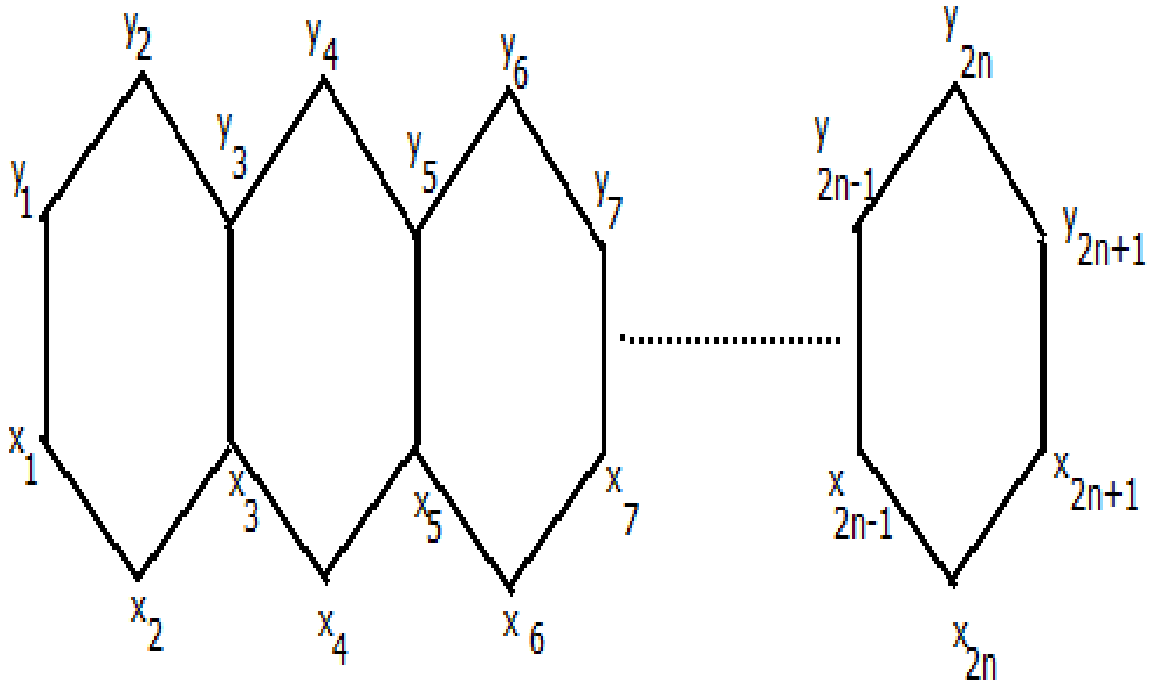


Figure.1. Linear Benzenoid Compounds *L (h)*

Naming vertices of the following as *L (h)* :

Let $X = \{x_1, x_2, x_3, \ldots\ldots\ldots, x_{2n+1}\}$ ..... (1)

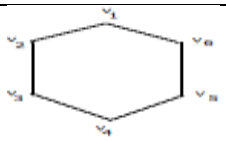
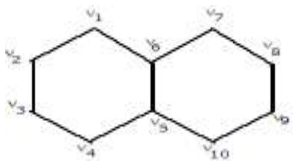
and $Y = \{y_1, y_2, y_3, \ldots\ldots\ldots, y_{2n+1}\}$ ..... (2)

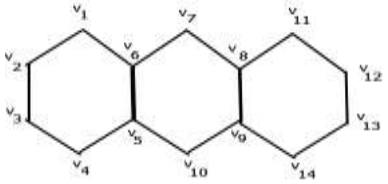
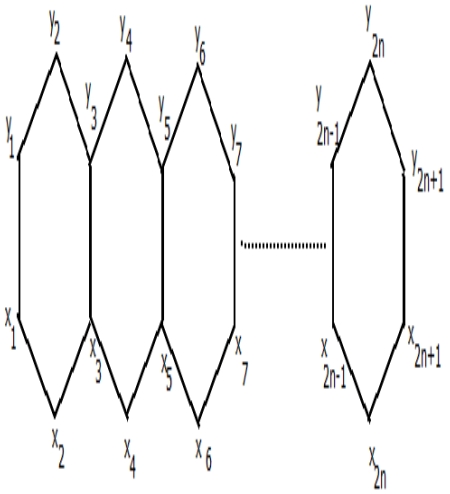
We have G = X ∪ Y which has *(2n+1)* vertices in X and *(2n+1)* vertices in Y.

Totally, G has *4 n + 2* vertices.

The following table explains about Degree Sequence of the molecular graph of Linear Benzenoid Compounds.

Table.1.Computation Table

No. Of Hexagons	Molecular Graph of Linear Benzenoid Compounds	No. Of Vertices	Degree Sequence of the molecular graph with respect to its corresponding number of Hexagons
h =1		6	(2,2,2,2,2,2)
h =2		10	(3,3,2,2,2,2,2,2,2,2)

h =3		14	(3,3,3,3,2,2,2,2,2,2,2,2,2,2)
.....		.....	.....
h = n		4n+2	$(\underbrace{3,3,3,3,3\ldots\ldots\ldots,3,3}_{2(n-1)times},\underbrace{2,2,2,2,2,2,2,2,2,\ldots\ldots\ldots.2,2,2,2}_{2(n+2)times})$

Proposition 2.2

If the degree sequence of the molecular graph of Linear Benzenoid Compounds L(h) has 4h + 2 partitions where h is the number of hexagons, Then the number of degree 3 vertices is 2(h-1) and the number of degree 2 vertices is 2(h+2) at the molecular graph of Linear Benzenoid Compounds L (h).

Proof

Case (i)

If *h=1* in the molecular graph of Linear Benzenoid Compounds *L(h)*, then we get the Structure of Benzene . It has six vertices. The number of *degree 2* vertices is six.

Case (ii)

If *h=2* in the molecular graph of Linear Benzenoid Compounds *L(h)*, then we get the Structure of Naphthalene. It has ten vertices. The number of *degree 2* vertices is eight and the number of *degree 3* vertices is two.

Case (iii)

If *h=3* in the molecular graph of Linear Benzenoid Compounds *L(h)*, then we get the Structure of Anthracene. It has fourteen vertices. The number of *degree 2* vertices is ten vertices and the number of *degree 3* vertices is four.

Continuing this Iteration Process, we get the molecular graph of Linear Benzenoid Compounds *L (h)* which contains that the number of *degree 3* vertices is *2(n-1)* and The number of *degree 2* vertices is *2(n+2)* when *h = n*.

III. SELF-SIMILARITY IN BENZENOID STRUCTURE

The molecular graph of Linear Benzenoid Compounds contains hexagons which all are similar to each other. From *Table.1*, the degree sequence starts from the molecular graph of Benzene and finitely many similar copies inside the extended case. By *Proposition 2.2*, each and every degree sequence of the molecular graph of Linear Benzenoid Compounds always gets a self–similar sequence with respect to the similarity starts with *(2 n -1) degree 3* vertices and *2 (n + 2) degree 2* vertices in its graph. That is, the

extended sequence is, $(\underbrace{3,3,3,3,3\ldots\ldots\ldots,3,3}_{(2n-1)times},\underbrace{2,2,2,2,2,2,2,2,\ldots\ldots\ldots 2,2,2,2}_{(2n+4)times})$ .Benzenoid structure resembles of exactly self -similar shapes. Its molecular graph is a connected and closed. Its outer measure is covered. Hence *Hausdroff Dimension* can be calculated for that structure will be pre-determined.

IV. APPLICATION OF BENZENE STRUCTURE

The known hair dye molecule is p-Phenylenediamine (PPD) which is an organic compound mainly used as an ingredient in hair dyes. Its formula is $C_6H_8N_2$. Its preferable IUPAC name is Benzene-1,4–diamine.The organic compound of p-Phenylenediamine preserves Benzene structure in its molecular structure.

V. CONCLUSION

In the summary of this paper, the degree sequence of Molecular Graph of Linear Benzenoid Compounds gives Self-similarity by using Iteration Process and contains same shape with similar Benzene ring structure. It shows that the degree sequence of Molecular Graph of Linear Benzenoid Compounds satisfies Self-similarity property in its degree sequence as well as its shape. It can be concluded that the Molecular Graph of Linear Benzenoid Compounds is a fractal and also Hausdroff dimension will be calculated. In the future work, these Self-similarity concepts can be satisfied in the molecular graph of some other organic compounds.

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