ON DEGREE SEQUENCES OF LINEAR BENZENOID GRAPH

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Abstract. Graph Theory plays very important role in many fields. In Structural Models, Graph theoretical concepts are mainly used. A degree sequence of the graph is a non-increasing sequence of each degree of all vertices in a graph. This paper obtains that the degree sequence of the molecular graph of Linear Benzenoid Compounds is graphic using Havel-Hakimi algorithm and gives a generalization theorem.

Keywords: Molecular Graph, Sequence, Degree sequence.

1. INTRODUCTION

Chemical Graph theory is the study of graphical representation of Chemical Compound's molecular structures. In a molecular graph, atoms and bonds are considered as vertices and edges respectively [5, 6, and 7]. A Sequence is a computed collection of items in which repetitions are allowed in particular order. The number of terms is called the length of the sequence. A sequence is a list of items with some order. The terms of the Sequences are linked by the previous elements using recursion rela tion. The Degree Sequence is the non-increasing sequence of degree of the vertices of undirected graph [1-4].The Havel–Hakimi algorithm is an algorithm to solve the graph realization problem of degree sequence in graph theory. This is based on a recursive algorithm [3]. The Havel–Hakimi theorem obtains an efficient method to check whether a given sequence is graphical by the following procedure: S = $(d_1, d_2, \dots \dots \dots, d_n)$.

Step.1 Sort the sequence in non-increasing order.

Step.2 Removing first term t = $d_1$and subtracting 1 from the first t terms.

Step.3 If a negative number is obtained, stop. If all $d_i = 0$, then the process ends. Otherwise, go to step 1.

2. GRAPHIC SEQUENCE OF THE MOLECULAR GRAPH OF LINEAR BENZENOID COMPOUNDS

In this paper, it deals with the degree sequence of the molecular graph of Linear Benzenoid Compounds and proves the graphic sequence conditions using Havel-Hakimi algorithm.

2.1 Degree sequence of the molecular graph of Benzene

For Benzene's graph, The number of Hexagons = 1, The number of Vertices = 6 and Degree Sequence = (2,2,2,2,2,2)

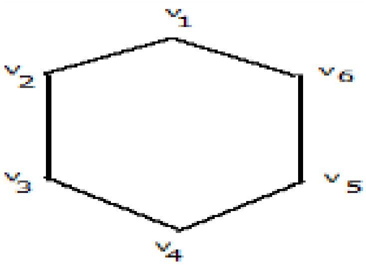

Figure1. Benzene

Using Havel-Hakimi algorithm, It is enough to check whether the degree sequence of Benzene graph is graphic or not.

Step1. Input sequence is (2,2,2,2,2,2)

Deleting first element, we get (2,2,2,2,2)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,2,2,2).

Step2. Rearranged sequence is (2,2,2,1,1)

Deleting first element, we get (2,2,1,1)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,1,1).

Step3. Rearranged sequence is (1,1,1,1)

Deleting first element, we get (1,1,1)

Subtracted 1 from the first 1 elements, resultant sequence is (0,1,1).

*Step4.*Rearranged sequence is (1,1,0)

Deleting first element, we get (1,0).

Subtracted 1 from the first 1 elements, resultant sequence is (0,0).

The rest of the sequence (0,0) contains only zero values.

Hence this degree sequence is graphic.

2.2 Degree sequence of the molecular graph of Naphthalene

For Naphthalene's graph, The number of Hexagons = 2, The number of Vertices = 10 and Degree Sequence = (3,3,2,2,2,2,2,2,2,2).

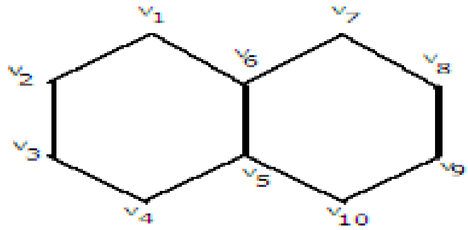

Figure2. Naphthalene

Using Havel-Hakimi algorithm, It is enough to check whether the degree sequence of Naphthalene's graph is graphic or not.

Step1. Input sequence is (3,3,2,2,2,2,2,2,2,2)

Deleting first element, we get (3,2,2,2,2,2,2,2,2)

Subtracted 1 from the first 3 elements, resultant sequence is (2,1,1,2,2,2,2,2,2).

Step2. Rearranged sequence is (2,2,2,2,2,2,2,1,1)

Deleting first element, we get (2,2,2,2,2,2,1,1)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,2,2,2,2,1,1).

Step3. Rearranged sequence is (2,2,2,2,1,1,1,1)

Deleting first element, we get (2,2,2,1,1,1,1)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,2,1,1,1,1)

*Step4.*Rearranged sequence is (2,1,1,1,1,1,1)

Deleting first element, we get (1,1,1,1,1,1)

Subtracted 1 from the first 2 elements, resultant sequence is (0,0,1,1,1,1).

*Step5.*Rearranged sequence is (1,1,1,1,0,0).

Deleting first element, we get (1,1,1,0,0).

Subtracted 1 from the first 1 elements, resultant sequence is (0,1,1,0,0).

*Step6.*Rearranged sequence is (1,1,0,0,0)

Deleting first element, we get (1,0,0,0)

Subtracted 1 from the first 1 elements, resultant sequence is (0,0,0,0).

The rest of the sequence (0,0,0,0) contains only zero values.

Hence this degree sequence is graphic.

2.3 Degree sequence of the molecular graph of Anthracene

For Anthracene's graph, The number of Hexagons = 3, The number of Vertices = 14 and Degree Sequence =(3,3,3,3,2,2,2,2,2,2,2,2,2,2)

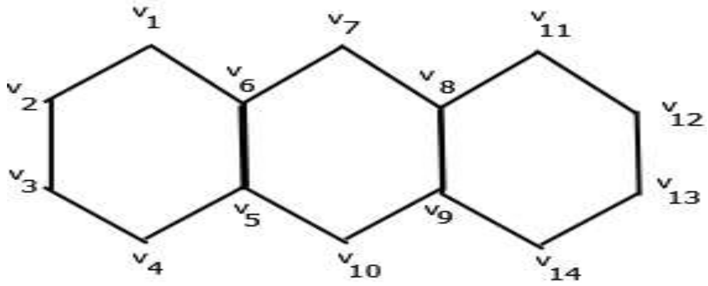

Figure3. Anthracene

Using Havel-Hakimi algorithm, It is enough to check whether the degree sequence of Anthracene's graph is graphic or not.

Step1. Input sequence is (3,3,3,3,2,2,2,2,2,2,2,2,2,2)

Deleting first element, we get (3,3,3,2,2,2,2,2,2,2,2,2,2)

Subtracted 1 from the first 3 elements, resultant sequence is (2,2,2,2,2,2,2,2,2,2,2,2,2).

Step2. Rearranged sequence is (2,2,2,2,2,2,2,2,2,2,2,2,2)

Deleting first element, we get (2,2,2,2,2,2,2,2,2,2,2,2)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,2,2,2,2,2,2,2,2,2,2).

Step3. Rearranged sequence is (2,2,2,2,2,2,2,2,2,2,1,1)

Deleting first element, we get (2,2,2,2,2,2,2,2,2,1,1)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,2,2,2,2,2,2,2,1,1)

Step4. Rearranged sequence is (2,2,2,2,2,2,2,1,1,1,1)

Deleting first element, we get (2,2,2,2,2,2,1,1,1,1)

Subtracted 1 from the first 2 elements, resultant sequence is (1,1,2,1,1,1,1,1,1).

Step5. Rearranged sequence is (2,2,2,2,1,1,1,1,1,1)

Deleting first element, we get (2,2,2,1,1,1,1,1,1).

Subtracted 1 from the first 1 elements, resultant sequence is (1,1,2,1,1,1,1,1,1).

Step6. Rearranged sequence is (2,1,1,1,1,1,1,1,1).

Deleting first element, we get (1,1,1,1,1,1,1,1).

Subtracted 1 from the first 2 elements, resultant sequence is (0,0,1,1,1,1,1,1).

Step7. Rearranged sequence is (1,1,1,1,1,1,0,0).

Deleting first element, we get (1,1,1,1,1,0,0).

Subtracted 1 from the first 1 elements, resultant sequence is (0,1,1,1,1,0,0).

Step8. Rearranged sequence is (1,1,1,1,0,0,0).

Deleting first element, we get (1,1,1,0,0,0).

Subtracted 1 from the first 1 elements, resultant sequence is (0,1,1,0,0,0).

Step9. Rearranged sequence is (1,1,0,0,0,0)

Deleting first element, we get (1,0,0,0,0)

Subtracted 1 from the first 1 elements, resultant sequence is (0,0,0,0,0).

The rest of the sequence (0,0,0,0,0) contains only zero values.

Hence this degree sequence is graphic.

2.4 Degree sequence of the molecular graph of Linear Benzenoid Compounds

Linear Benzenoid Compounds *L (n)* has *4 n + 2* vertices.

Consider X = $\{x_1, x_2, x_3, \ldots\ldots, x_{2n+1}\}$ and Y = $\{y_1, y_2, y_3, \ldots\ldots, y_{2n+1}\}$.

The number of Hexagons = n ,The number of Vertices = 4 n + 2.

Degree Sequence =(3,3,3,3,.......3,3,2,2,2.........2,2).In this sequence, degree 3 and degree 2 occur 2(n-1) times and 2(n+2) times respectively.

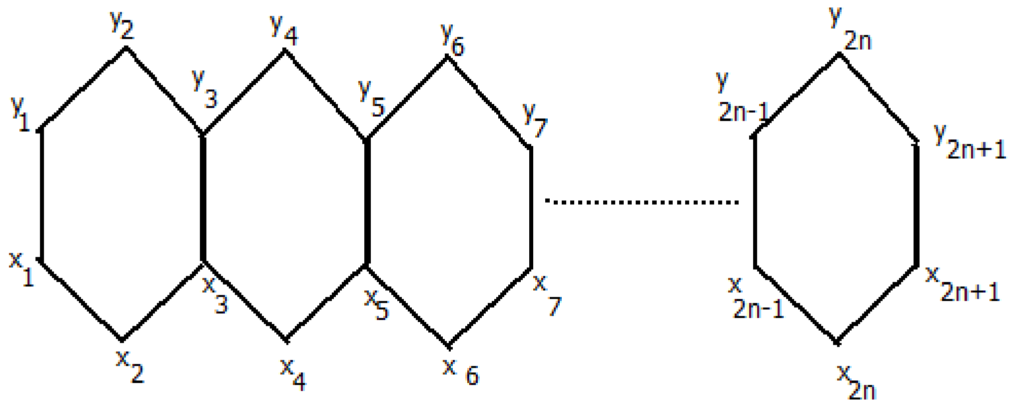

Figure4. Linear Benzenoid Compounds*L (h)*

2.4.1. Proposition

The molecular graph of Linear Benzenoid Compounds L (n) where n is the number of hexagons, is a graphic sequence.

Proof: We prove this statement by Induction method.

Put *n=1* in the molecular graph of Linear Benzenoid Compounds *L(n)*, then we get the molecular graph of Benzene . By (2.1),we can conclude that its degree sequence is graphic.

Put *n=2* in the molecular graph of Linear Benzenoid Compounds *L(n)*, then we get the molecular graph of Naphthalene . By (2.2), we can conclude that its degree sequence is graphic.

Put *n=3* in the molecular graph of Linear Benzenoid Compounds *L(n)*, then we get the molecular graph of Anthracene . By (2.3), we can conclude that its degree sequence is graphic.

In the degree sequence of Linear Benzenoid Compounds,

Take *n=k* in the molecular graph of Linear Benzenoid Compounds *L(n).*

Assume that the molecular graph of Linear Benzenoid Compounds *L(n=k)* is a graphic sequence which contains that the number of *degree 3* vertices is *2(n-1)* and *degree 2* vertices is *2(n+2)*.

We have to show that the molecular graph of Linear Benzenoid Compounds *L (n=k+1)* is a graphic sequence.

The molecular graph of Linear Benzenoid Compounds *L(n= 1)* has 6 vertices. Its degree sequence is (2,2,2,2,2,2).This means that it has no degree 3 vertices and six degree 2 vertices.

For k+1 hexagons, combining k hexagons and 1 hexagon. There are two common vertices with same edge. So only four vertices can be included.

From this, It gets totally 4n+6 vertices with *2n times degree 3* vertices and *2(n+3)* times *degree 2* vertices. Its degree sum is even and each degree $\leq n$.It can be concluded that this degree sequence is a graphic sequence.

Hence the molecular graph of Linear Benzenoid Compounds L (n) where n is the number of hexagons, is a graphic sequence by induction.

3. Conclusion

The main aim of this paper is to present degree sequence concepts in Molecular Graph. Graph Computation Methods are used to identify chemical identification. It gives the degree sequence of Molecular Graph of Linear Benzenoid Compounds is a graphic sequence and a generalization theorem by Induction Method.

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