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Balanced Graph of the Chemical Compound

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ABSTRACT:
A signed graph based on F is an ordinary graph F with each edge marked as positive or negative. Such a graph is called balanced if each of its cycles includes an even number of negative edges. It is easy to show that a signed graph is balanced if and only if the set of its vertices may be partitioned into two disjoint classes in such a way that an edge is negative if and only if its two endpoints belong to distinct classes . In this article we applied the concept of balanced graph into the chemical compound like benzene, ethane and acetylene. Basically all chemical compound have balanced structure. These structure converted into graphical structure and we shows it satisfy the property of balanced graph.

Keywords: Signed graph, Balanced graph, Marked graph, Chemical compound

I. INTRODUCTION:

Spectral graph theory play important role for the chemical structure theory. This is mainly due to the fact that most of the chemical information is associated with the structural formulas. Chemical applications of graph theory proposed the interactions between Chemistry and Discrete Mathematics. A chemical graph is a model of a chemical system, used to characterize the interactions among its components: atoms, bonds, groups of atoms or molecules. A structural formula of a chemical compound can be represented by a molecular graph, its vertices being atoms and edges corresponding to covalent bonds. Weighted graphs for which the weight matrix is a symmetric matrix in which negative and positive entries are called signed graphs. The problem of clustering the nodes of a signed graph was a generalization of the clustering problem for graph. A Signed graph G based on ordinary graph G with each edge marked as positive or negative. A Signed graph G which contains even number of negative edges is called balanced signed graph. Harary and Kabell(1980,1981) described an algorithm for signed graph is balanced. Alexandru T. Balaban is a chemist who significantly contributed to the fields of Organic Chemistry, Theoretical Chemistry, Mathematical Chemistry and Chemical graph theory. A Marked graphs a graph where every vertex has a sign _+‘ or _-_. A Marked graph is called Consistent if every cycle has an even number of negative signs. Consistent marked graph were introduced by Beineke and Harary in 1978. The Energy of the graph is defined by Ivan Gutman in 1978. Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. Some physical properties, such as the boiling point, are related to the geometric structure of the compound. For example, the chemical compound Dimethylnaphthalenis a polycyclic aromatic hydrocarbon. It is one of the ten dimethylnaphthalene isomers, which are derived from naphthalene by the addition of two methyl groups, the structure of Dimethylnaphthalen exists the property of balanced structure compound.

Definition: 1
A **marked graph** is a simple graph where every vertex has a sign + or _.

Definition: 2
A marked graph is called **consistent** if every cycle has an even number of _signs.

Definition: 3
Let G be a graph with order n and size m. The **Laplacian matrix**of the graph G is denoted by $L = (L_{ij})$ is a square matrix and it is defined by

$$L_{ij} = \begin{cases} -1 \text{ if } v_i \text{ is adjacent to } v_j \\ 0 \text{ if } v_i \text{ is not adjacent to } v_j \\ d_i \text{ if } v_i = v_j \end{cases}$$

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Where d_i is the degree of the vertex v_i .

Definition: 4

Let $\mu_1, \mu_2, \ldots\ldots \mu_n$ be the eigenvalues of LE (G), which are called Laplacian eigenvalues of G. The **Laplacian energy** LE(G) of G is defined LE(G)= $\sum_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right|$, where $\frac{2m}{n}$ is the average degree of the graph G.

Definition: 5

If (V,W) is a signed graph where W is a (mxm) symmetric matrix with zero diagonal entries and with the other entries $w_{ij} \varepsilon R$ be arbitrary. The degree of any vertex v_i is defined as $d_i = d(v_i) = \sum_{i=0}^{n} W_{ij}$ and $\bar{D}$ is the **signed degree matrix**where $\bar{D}$ = diag ((v_1),(v_2), ... (v_m)).

Definition: 6

The **Signed Laplacianmatrix** $\bar{L}$ is defined by $\bar{L} = \bar{D} - W$, where $\bar{D}$ is the signed degree matrix. The signed Laplacian matrix is a symmetric positive semi-definite.

Definition: 7

Let G = (V,W) be a signed graph whose underlying graph is connected. Then G is balanced if there is a partition of its vertex set V into two clusters V_1 and V_2 such that all the positive edges connect vertices with V_1 or V_2 and all the negative edges connect vertices between V_1 and V_2. If the signed graph has an even number of negative edges then it is called a **balanced signed graph.**

Harary's Balance Theorem

A signed graph Σ is balanced if and only if there is a bipartition of its vertex set, V=X∪Y, such that every positive edge is induced by X or Y while every negative edge has one endpoint in X and one in Y. Also, if and only if for any two vertices v,w, every path between them has the same sign.

A bipartition of a set V is any pair {X,Y} of complementary subsets, including the possibility that one subset is empty (in which case the bipartition is not, technically, a partition). I call a bipartition of V as in the Balance Theorem a Harary bipartition of V, or of Σ. The Harary bipartition is unique if and only if Σ is connected; if Σ is also all positive (all edges are positive), then X or Y is empty.

Harary later defined Σ to be antibalanced if every even circle is positive and every odd circle is negative; equivalently, $-\Sigma$ is balanced . (The negative of Σ, $-\Sigma$, has signature $-\sigma$.) A basic question about a signed graph is whether it is balanced; in terms of our theme, whether there exists a negative circle. If $\Sigma$is unbalanced, any negative circle provides a simple verification that it is unbalanced, since computing the sign of a circle is easy. The Balance Theorem tells us how to provide a certificate that Σ is balanced, if in fact it is; namely, one presents the bipartition {X,Y},

Chemical graph:

In a graph representing a chemical structure, the vertices and edges represent atoms and bonds, respectively. The bond order corresponds to the edgemultiplicity, and as a result,chemical graphsarevertex and edge-labelled graphs. A vertex and edge-labelled graph is described as a chemical graph where is the set of vertices. . A molecule is saturated if all its atoms are saturated.

BALANCED LAPLACIAN MATRIX OF ACTEYLENE, ETHENE, DIMETHYLHALENE

(i) STRUCTURE OF ACTYLENE

Acetylene is the chemical compound with the formula C_2H_2 and structure H−C≡C−H. Acetylene is an unsaturated hydrocarbon have double or triple covelent bonds between carbon atoms. The functional group of Acetylene is alleyne, which consists of two carbons held together by a ttriple bond. The triple bond which linles the two cabon atom is called a Covalent bond. A covalent bond is created between two atoms by sharing one or more pairs of electronIt is a hydrocarbon and the simplest alkyne. The carbon atom has +ve ion and hydrogen has –ve ion. In the structure of acetylene we represent carbon and hydrogen atom as vertices and joining between two vertices by edges and marked the sign of carbon as +ve sign and hydrogen as –ve sign**.**

H(-) ..... C(+) = C (+) ..... H(-)

The above diagram is balanced structure of acetylene which contains even number of negative edges. So it exists the property of balanced graph

Balanced Laplacian Matrix of Acetylene

In the mathematical field of graph theory, the laplacian matrix also called the graph laplacian. The difference between diagonal matrix and

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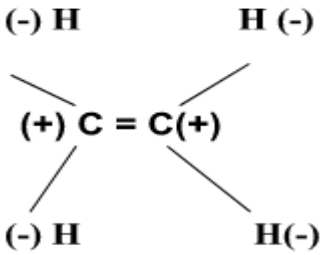
adjacency matrix. The balanced laplacian matrix of actelyene is

$$L(A) = \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & 1 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

(ii) STRUCTURE OF BENZENE

$C_2H_4$is the simplest allene with the chemical name ethyene it is also called ethene or polyethylene (or) etileno ethylene is a hydrocarbon which has the formula C2H4 or $H_2C = CH_2$. It is thesimplestallene ethylene is widely used in the chemical industry, and its worldwide production exceeds that of any other organic compound. It contains two carbon atoms that are double bonded to each other, with each of these atoms also bonded to two Hydrogen atoms.

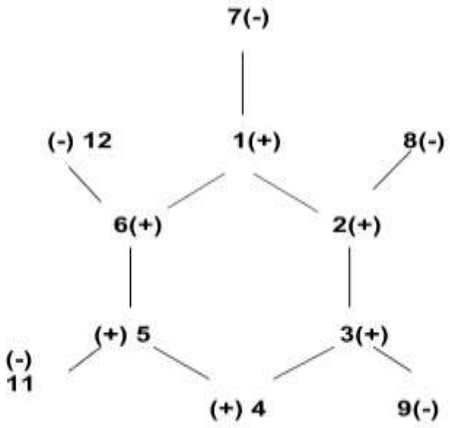


Balanced Laplacian Matrix of Acetylene

$$L(B) = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}$$

(iii)STRUCTURE OF DIMETHYLNAPTHALENE

An organic, arometric molecule that is compased of two conjuoined 6- carbon rings (benzenes). The structure is held together by a series of alter nating single and double bonds, resulting three distinct resounane structures. Balanced graph structure of Dimethylnapthalene is as follow



Laplacian matrix of Dimethylnapthalene

$$L = \begin{pmatrix} 3 & -1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & -1 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Similarly we can able to find balanced laplacian matrix of other chemical compound

II. CONCLUSION

Chemical graph theory is a branch of mathematics combining graph theory and

chemistry. The field was used due to the necessity of mathematical modelling. Molecular structures are represented as graphs and their mathematical analysis is performed based on the graph theorems. One of the key implementations of chemical graphs is the structure elucidation. For the identification of molecular structures, chemists need to build the structures with respect to its spectral data. The methods for the elucidation process are part of chemical graph theory. In this review, we applied the concept of signed graph into chemical compound like Actylene, Benzene and Dimethylnapthalene have balanced structure and also found the laplacian matrix of these compound.

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