COMPARISON BETWEEN CONSISTENT MARKED GRAPH AND SOME CHEMICAL COMPOUNDS

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Abstract:

A marked graph is a graph with a + or − sign on each vertex and is called consistent if each cycle has an even number of − signs. This concept is applied with the halide compounds like sodium chloride, potassium chloride, silver chloride etc., and we compared these compounds with the bipartite graphs and also obtained their energy and balanced Laplacian energy.

Keywords:

Bipartite graph, Balanced Laplacian Energy, Consisent marked graph, Halide compounds, Signed graph

SMS Classification: 05C50, 05C69

1.INTRODUCTION:

Consistent marked graphs were introduced by Beineke and Harary. A signed graph is called balanced if every cycle has an even number of − signs[1,2,3]. For example, Sodium chloride is one of the Halide compounds formed when sodium atoms iteract with chlorine atoms. When this occurs, sodium will donate an electron to chlorine. This makes sodium slightly positive and chlorine slightly negative. Harary and Kabell described signed graph as a balanced graph by setting up a correspondence between marked graphs and balanced signed graphs. [13]

Let G be a graph with order n and size m and A be the adjacency matrix of the graph $A = (a_{ij})_{nxn}$ and it is defined as

$$a_{ij} = \begin{cases} \sigma_{ij} \; if \; v_i \; is \; adjacent \; to \; v_j \\ 0 \; otherwise \end{cases}$$

The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A are assumed in the non increasing order of the graph G. The energy E(G) of G is defined as the sum of the absolute values of the eigenvalues of G. i.e., $E(G) = \sum_{i=1}^{n} |\lambda_i|$. [4,5,6,17]

I.Gutman and B.zhou defined the Laplacian energy of a graph G in the year 2006. Let G be a finite , simple and connected graph with order n and size m . The Laplacian matrix of the graph G denoted by L(G) = D(G) - A(G) is a square matrix of order n, where D(G) is the diagonal matrix of vertex degrees of the graph G and A(G) is the adjacency matrix. Let $\mu_1, \mu_2, \ldots, \mu_n$ form the Laplacian spectrum of its Laplacian matrix of G then the Laplacian energy LE(G) of G is defined as $LE(G) = \sum_{i=0}^{n} \left|\mu_i - \frac{2m}{n}\right|$ where $\frac{2m}{n}$ is th average degree of the graph G. [7,8,9,12,15,16,20]

2. Definitions:

Definition: 2.1

A **marked graph** is a simple graph where every vertex has a sign + or −.

Definition: 2.2

A marked graph is called **consistent** if every cycle has an even number of − signs.

Definition: 2.3

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

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

Where d_i is the degree of the vertex v_i .

Definition: 2.4

Let $\mu_1, \mu_2, \ldots, \mu_n$ 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: 2.5

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 ($(v_1), (v_2), \ldots, (v_m)$).

Definition: 2.6

The **Signed Laplacian matrix** $\bar{L}$ 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: 2.7

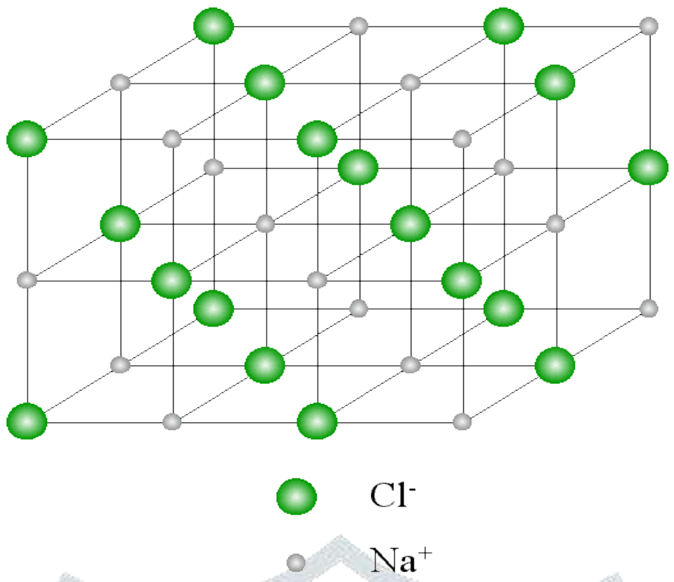
Let G = (V,W) be a signed graph whose underlying graph is connected. Then G is balanced if there is a partition of its vertex set V into two clusters V_1 and V_2 such that all the positive edges connect vertices with V_1 or V_2 and all the negative edges connect vertices between V_1 and V_2. If the signed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

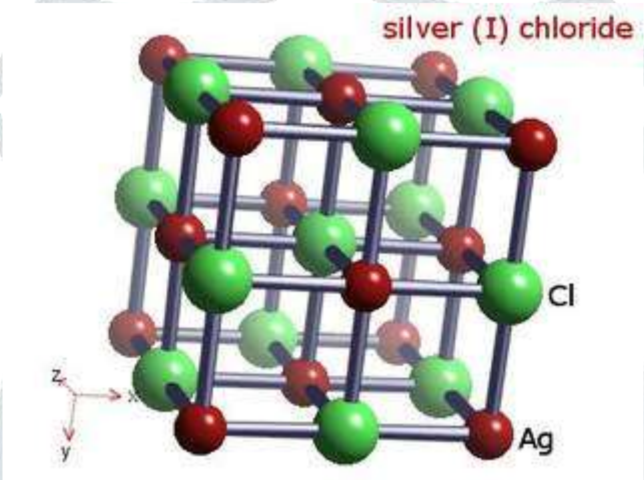
Definition: 2.8

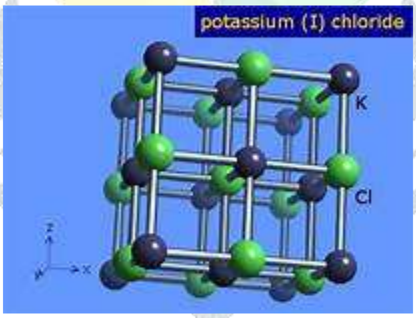
Adding just one edge to a spanning tree will create a cycle, such a cycle is called a **fundamental cycle**. There is a distinct fundamental cycle for each edge. There is a one-to-one correspondence between fundamental cycles and edges not in the spanning tree. For a connected graph G with the vertex set V, any spanning tree will have $|V| - 1$ edges, and thus, a graph of edge set E and one of its spanning trees will have $|E - V + 1|$ fundamental cycles. For any given spanning tree the set of all $|E - V + 1|$ fundamental cycles forms a **cycle basis,** which forms a basis for the **cycle space.**

3.Crystal Structure of Halide compounds:

A halide is a binary phase, in which one part is a halogen atom and other part is an element or radical that is less electronegative (or more electropositive) than the halogen, to make a fluoride, chloride, bromide, iodide, astatide or theoretically tenneside compound. A halide ion is a halogen atom bearing a negative charge. The halide anions are fluoride(F^-), chloride(Cl^-), bromide(Br^-), iodide(I^-) and astatide (At^-). Such ions are present in all ionic halide salts. Halide minerals contain halides. Examples of halide compounds are Sodium chloride(Nacl), Potassium chloride(KCl), Potassium Iodide(PI), Lithium chloride(Licl), Copper (II) chloride ($Cucl_2$), Silver chloride (Agcl), Calcium chloride ($Cacl_2$) and Chlorine Fluoride(ClF). The crystal structure of sodium chloride shows that each atom has six nearest neighbours, with octahedral geometry. Sodium chloride forms crystals with cubic symmetry.







In this larger chloride ions , (shown to the right) as spheres are arranged as a cubic ion in a close –packing, while the smaller sodium ions (shown to the right) as spheres, filled in the octahedral gaps between them. Each ion is surrounded by six ions of other kinds. The above is the basic structure found in many other minerals, and is known as the halite structure. This arrangement is known as cubic closed packed(ccp). It can be represented as two interpenetrating face-centered(fcc) lattices.

4. Relation between Consistent Marked graph, Balanced signed graph, Bipartite graph with the Halide compounds:

Given a marked graph M, it is naturally associated with a signed graph, by taking the sign of each edge to be the product of the signs of its two vertices. We explored the relationship between the marked graph, signed graph and the bipartite graph in the following results. The above halide compounds contain naturally +ve ions and -ve ions. We assumed that the marked graph M and the signed graph S both having the same unmarked unsigned underlying graph G have correspondence with each other if the sign of each edge in S is the product of the signs of its two vertices in M.

4.1 Correspondence Theorem: (13)

Each connected marked graph corresponds to precisely one balanced signed graph. Each connected balanced signed graph corresponds to two (possibly isomorphic) marked graphs. If a marked graph G is consistent and u,v ∈ V(G), then u and v receive the same sign.

Proof:

Let G be a marked graph and x,y ∈ V(G) with the same sign.

Case (i) :

Let the vertices be positive. Then a path joining x and y is said to be coherent if it contains an even number of negative vertices. Otherwise, the path is said to be incoherent.

Case (ii):

Let the vertices be negative. Then a path joining x and y is said to be coherent, if it contains an odd number of negative vertices. Otherwise, the path is said to be incoherent.

A marked graph G is consistent if and only if for any two vertices u and v with the same sign, any two vertex disjoint paths between u and v are either coherent or incoherent. A bipartite graph is a graph where the vertices are decomposed into two vertex subsets such that no two graph vertices within the same set are adjacent. The consistent marked graph and balanced signed graph are applied into the halide compounds and we found that the laplacian energy of the bipartite graph exists.

5. OBSERVATIONS:

In this section, we listed some previously known results that are needed for the subsequent sections.

Lemma 1: A Bipartite graph G = (V,E) is a graph whose vertex set V can be partitioned into two subsets V_1 and V_2 such that every edge of G has one end in V_1 and another end in V_2. If $|V_1| = |V_2|$, then we say that G is balanced. (18,19,21)

Lemma2: A Signed graph is balanced if every cycle has an even number of negative edges. (22)

Lemma 3: An all negative signed graph G is balanced if and only if G is bipartite. (14)

Lemma 4: If marked graph G is consistent, then

(i)G[V −] is bipartite.

(ii) Between each connected component of G[V +] and each set in the bipartition of each component of G[V −], there is atmost one edge. (14)

Lemma 6: A Signing of a graph is an assignment of weight + 1 or -1 to each of its edges . A cycle C of a signed bipartite graph G is balanced if the sum of the weights of the edges in C is congruent to 0 (mod 4). (22)

Lemma 6: Let G be a bipartite graph and T be a spanning tree of G. All cycles in G have length 0 (mod 4) if and only if G satisfies the following two conditions:

(i) Each fundamental cycle corresponds to T has length 0 (mod 4).

(ii) Each cycle which is a symmetric difference of two fundamental cycles also has length 0(mod 4). (23)

6. Main results:

In halide compounds, divide each compound into two clusters in the form of positive ions and negative ions. We consider these ions as two vertex sets V_1 and V_2. If each edge connecting between these two clusters by negative sign then the resulting graph is a bipartite graph containing even number of negative edges. Thus, it is a balanced signed graph. From the crystal structure of halide compounds the corner vertices have three degrees and the remaining vertices have four degrees. First we consider the bipartite graph which has eight vertices (four +ve and four -ve vertices). Then the resulting bipartite graph G is shown in the following figure(i).

Result 6.1:

The bigraph of order 8 possesses signed Laplacian energy.

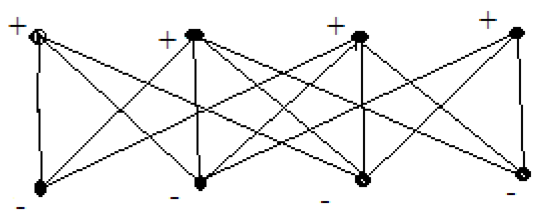


Figure (i) Bipartite graph G

The adjacency matrix of the above graph is as follows

$$A(G) = \begin{pmatrix} 0 & 0 & 0 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 \\ -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}_{(8X8)}$$

The characteristic equation of A(G) is $\mu^8 - 14\,\mu^6 + 17\,\mu^4 - 4\,\mu^2 = 0$.
The eigen values are -3.5616, -1, -0.5616, 0, 0, 0.5616, 1, 3.5616.
Hence the energy of the graph is E(G) = 10.2464 approximately.
The Signed Laplacian matrix of the graph in Figure (i) is

$$\bar{L}\,E(G) = \begin{pmatrix} 3 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 4 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 4 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 3 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 3 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 4 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 4 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 3 \end{pmatrix}_{(8X8)}$$

The characteristic equation is $\mu^8 - 28\,\mu^6 + 328\,\mu^5 - 2088\mu^4 + 7808\mu^3 - 1.7152\mu^2 + 20480\mu - 10240 = 0$.
The eigen values are 0, 2, 2.7639, 4, 4, 4, 4, 7.2361.
Here order is n and size is 2n-2.
Average degree 4(n-1)/n.
Average degree is 3.5.
Hence the balanced laplacian energy of $\bar{L}$ E(G) the graph G is 11.4722 approximately

Result 6.2:

The bipartite graph of order 10 possesses signed Laplacian energy.

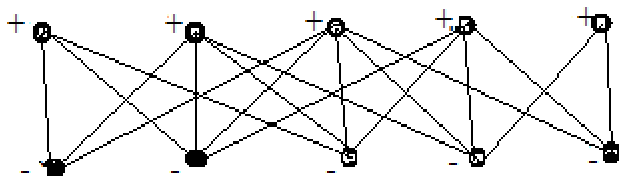


Figure (ii) Bipartite graph G

The adjacency matrix of the graph G is

$$A(G) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 \\ -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_{(10X10)}$$

The characteristic equation is $\mu^{10} - 18\mu^8 + 67\,\mu^6 - 82\mu^4 + 33\,\mu^2 - 4 = 0$.

The eigen values are −3.6691, − 1.6180, −1.1451, −0.6180, −0.4760, 0.4760, 0.6180, 1.1451, 1.6180, 3.6691.

Hence, the energy of the graph E(G) is 15.0524 approximately.

.The balanced Laplacian energy of bipartite graph is

$$\bar{L}\,E(G) = \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 4 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 4 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 4 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 4 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 3 \end{pmatrix} \quad (10X10)$$

The charteristic equation is $\mu^{10}+4\mu^9+56\,\mu^8 - 505\mu^7+2844\,\mu^6 - 10457\,\mu^5 + 2506\mu^4 - 37737\mu^3 + 32321\mu^2 - 11970\mu = 0$.

The eigen values are 0,1.5858, 2.5505, 3, 3, 4, 4.4142, 5, 5,7.4495

Average degree = 3.6

Hence the balanced Laplacian energy $\bar{L}$ E(G) of the graph G is 15.7274 approximately.

Proceeding like this, for the bipartite graph of order n and size m, we found that the Balanced Laplacian energy of graphs of order n follow the formula 2n – 5 approximately.

References:

[1] Ameenal Bibi K,Vijayalakshmi B, Jothilakshmi R, Bounds of Balanced Laplacian Energy of a Complete Bipartite graph, International Journal of Computational Intelligence Research, ISSN: 0973 – 1873, Volume 13 number 5(2017) pp. 1157-1165.

[2] Ameenal Bibi K,Vijayalakshmi B, Jothilakshmi R, Balanced Laplacian Energy of a Friendship graph, International Journal of advanced Research in computer science, volume – 8, No. 6 July 2017 (special issue III) ISSN No. 0976-5697

[3] Ameenal Bibi K,Vijayalakshmi B, Laplacian Energy of a Balanced graph, International Research Journal in advanced Engineering and Technology, ISSN: 2454-4752, p- ISSN: 2454 - 4744, Vol 2 issue 5(2016) pages 1269-1276.

[4] Balakrishnan. R, The energy of a graph, Linear Algebra and its applications(2004) 287-295

[5] Bapat R. B. , Pati S, Energy of a graph is never an odd integer. Bull.Kerala Math. Assoc. 1, 129-132 (2011).

[6] Bo Zhou, Energy of a graph, MATCH commu. Math. Chem. 51(2004), 111-118.

[7] Bo Zhou and Ivan Gutman, On Laplacian energy of a graph, Match commu. Math. Comput. Chem. 57(2007) 211-220.

[8] Bo Zhou, More on Energy and Laplacian Energy Math. Commun. Math. Comput. Chem.64(2010) 75-84.

[9] Bo Zhou and Ivan Gutman, On Laplacian energy of a graph, Linear algebra and its applications, 414(2006) 29-37.

[10] Cvetkovi'c .D, Doob M, Sachs H, Spectra of graphs - Theory and applications, Academic Press, New York 1980.

[11] Cornelis Hoede, A characterization of consistent Marked graphs, University of Tente Enschede, Netherlands.

[12] Fath Tabar G.H, Ashrafi A.R. , I. Gutman, Note on Laplacian Energy of graphs, class Bulletin T(XXXVII de l'Academics Serbe des Sciences et des arts(2008).

[13] Frank Harary and Jerald A. Kabell, Counting balanced signed graphs using marked graphs, Proceedings of the Edinburgh Mathematical Society (1981) 24, 99-104.

[14] Fred. S. Roberts, Shaoji Xu, Charaterizations of consistent Marked graphs, DIMACS Technical Report 99-16, March 1999.

[15] Gholam Hossein, Fath - Tabar and Ali Reza Asharfi, Some remarks on Laplacian eigen values and Laplacian energy of graphs, Math. Commun., vol.15, No.2, pp. 443-451(2010).

[16] Ivan Gutman , Emina Milovanovic, and Igor Milovanovic - Bounds or Laplacian- Type graph energies, vol. 16 (2015), No. 1, pp. 195-203.

[17] Ivan Gutman, The energy of a graph. Ber. Math – statist. Sekt. Forschungsz. Graz 103, 1-22(1978).

[18] Juan Rada, Antonio Tinio, Upper and Lower bounds for the energy of bipartite graph, Journal of Mathematics analysis and application, vol.289, pgs. 446-455(2004).

[19] Kinkar Ch. Das, Seyed Ahamed Mojallal, Ivan Gutman , On energy and Laplacian energy of bipartite graphs, Applied Mathematics and Computation 273(2016) 759-766.
[20] Merris .M, Laplacian matrices of graphs, A survey, Lin. Algeba Appl. 197-198(1994)143-176.
[21] Nathan Reff, New Bounds for the Laplacian Spectral Radius of a Signed graph, arXiv:1103, 4629VI[Math.Co] 23 Mar 2011.
[22] Stanley F. Florkowski III, Spectral Graph theory of the Hypercube (Thesis).
[23] Xiaogen chen, Wanwen xie, Energy of hypercube and its complement, International Journal of Algebra, Vol 6, no.16, 799 - 805(2012).