Research Article

GRAPH ENERGY

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ABSTRACT.

This is all about the energies of different types of graphs like simple graph, non-simple graph, bipartiate graph, complete bipartiate graph, regular graph. Through the study of the chemical molecular structure, we can construct a graph from the structure and also can find the energies of it. So, from this we can find the energies of molecular structures.

1. INTRODUCTION

In mathematics, the energy of a graph is the sum of the absolute values of the eigenvalues of the adjacency matrix of the graph. This quantity is studied in the context of spectral graph theory.

More precisely, let G be a graph with n vertices. It is assumed that G is simple, that is, it does not contain loops or parallel edges. Let A be the adjacency matrix of G and let $\lambda_i, i = 1,2, \ldots n,$ be the eigenvalues of A. Then the energy of the graph is defined as:

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_p\}$ and size (= number of edges) q.

Lemma 1.

Let G be a graph with an adjacency matrix A and $spec(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_p\}$. Then $\det A = \prod_{i=1}^{p} \lambda_i$. In addition, for any polynomial $P(x)$, $P(\lambda)$ is an eigenvalue of $P(A)$ and hence

$$detP(A) = \prod_{i=1}^{p} p(\lambda_i).$$

Lemma 2.

Let $A = \begin{bmatrix} A_0 & A_1 \\ A_1 & A_0 \end{bmatrix}$be a symmetric 2×2 block matrix. Then the spectrum of A is the union of the spectra of $A_0 + A_1$and $A_0 - A_1$.

Lemma 3 .

Let M, N, P, Q be matrices, and let M be invertible. Let $S = \begin{bmatrix} M & N \\ P & Q \end{bmatrix}$ .Then $det\, S = det\, M.det[Q - PM^{-1}N]$.

If M and P commute, then $detS = det[MQ - PN]$.

Lemma 4 .

Let G be an r −regular connected graph, $r \geq 3$, with $spec(G) = \{r, \lambda_2, \ldots, \lambda_p\}$. Then

$$spec\big(L(G)\big) = \begin{pmatrix} 2r-2 & \lambda_2 + r - 2 & \ldots & \lambda_p + r - 2 & -2 \\ 1 & 1 & \ldots & 1 & p(r-2)/2 \end{pmatrix}.$$

Lemma 5.

Let G be an r −regular connected graph on p vertices with an adjacency matrix A, and let $r, \lambda_2, \ldots, \lambda_m$ be its distinct eigenvalues. Let J be the all-one square matrix of order p. Then there exists a polynomial $P(x)$ such that $P(A) = J$, and

$$P(x) = P\frac{(x-\lambda_2)(x-\lambda_3)\ldots(x-\lambda_{m)}}{(r-\lambda_2)(r-\lambda_3)\ldots(r-\lambda_m)}$$

So that $P(r) = p$ and P(λ_i)=0, $for\ all\ \lambda_i \neq r$.

Lemma 6 .

For every $t \geq 3$, there exists a pair of non-cospectral cubic graphs on $2t$ vertices.

Lemma 7.

Let G be a (p,q)-graph of diameter 2, and let its D-eigenvalues be $\mu_1, \mu_2, \ldots, \mu_p$. Then

$$\sum_{i=1}^{p} \mu_i^2 = 2(2p^2 - 2p - 3q).$$

Theorem 1.1. Let G be an r-regular graph of diameter 2, and let its (ordinary) spectrum be spec(G) = $\{r, \lambda_2, \ldots, \lambda_p\}$. Then the D-spectrum of G is $spec_D(G) = \{2p-r-2, -(\lambda_2 + 2), \ldots, -(\lambda_p + 2)\}$.

Theorem1.2.

Let G be an r-regular graph of diameter 1 or 2 with an adjacency matrix A and spec(G) = $\{\lambda_1,\lambda_2,...,\lambda p\}$. Then H = G×$K_2$ is (r + 1)-regular and of diameter 2 or 3 with

$$spec_D = \begin{pmatrix} 5p-2(r+2) & -2(\lambda_i+2) & -p & 0 \\ 1 & 1 & 1 & p-1 \end{pmatrix}, i = 2,3,\dots,p$$

Theorem 1.3.

The distance energy of the wheel graph is given by $E_D(W_{1,p})=2(p-2+\sqrt{p^2-3p+4})$.

Theorem 1.4.

Let G be a (p,q)-graph of diameter 2 and μ_1 be its greatest D- eigenvalue. Then $\mu_1 \geq (2p^2-2q-2p)/p$. Equality holds if and only if G is a regular graph.

Theorem1.5.

Let G be a (p,q)-graph of diameter 2 and let Δ be the absolute value of the determinant of its distance matrix. Then

$$\sqrt{4p(p-1)-6q+p(p-1)\Delta^{2/p}} \leq E_D(G) \leq \sqrt{2p(2p^2-3q-2p)}.$$

Theorem 1.6.

Let G be an r-regular graph of diameter 2. Then

$$E_D \leq 2p-r-2+\sqrt{p(p-1)[p(r+4)-(r+2)^2]}.$$

Theorem 1.7.

For any graph G of diameter 2, $E_D \leq \frac{1}{p}[2p^2-2q-2p+\sqrt{(p-1)[(2p^2-4q)-4p^2]}$

Theorem 1.8.

Let G be a connected r-regular graph on p vertices with spec(G) = $\{r,\lambda_2,...,\lambda_p\}$. Then

$$spec_D(G\nabla G) = \begin{pmatrix} 3p-r-2 & p-r-2 & -2 & (\lambda_i+2) \\ 1 & 1 & 2 & \end{pmatrix}, i = 2,\dots,p.$$

Theorem 1.9.

For every $p \equiv 0\ (mod\ 6) \geq 18$, there exists a pair of D −equienergetic regular graphs.

Theorem 1.10.

For every $p \equiv 1\ (mod\ 3) \geq 10$, there exists a pair of D −equienergetic graphs.

Lemma 8.

Let G be an r-regular connected graph, with spec(G) ={r,λ_2,...,λ_n}. Then

$$\text{spec}(L^2(G))=\begin{pmatrix} 4r-6\lambda_2+3r-6 & \dots & \lambda_n+3r-6 & 2r-6 & -2 \\ 1 & 1 & \dots\ 1 & \frac{n(n-2)}{2} & \frac{nr(r-2)}{2} \end{pmatrix}$$

Let G be a graph. Then the following construction results in a self-complementary graph $\mathcal{H}$. Recall that a graph $\mathcal{H}$ is said to be self-complementary if $\mathcal{H} \cong \overline{\mathcal{H}}$, where $\overline{\mathcal{H}}$ is the complement of $\mathcal{H}$.

Construction of $\mathcal{H}$:

Replace each of the end vertices of P_4, the path on 4 vertices, by a copy of G and each of the internal vertices by a copy of $\bar{G}$. Join the vertices of these graphs by all possible edges whenever the corresponding vertices of P_4 are adjacent.

Theorem 1.11. Let G be a connected k-regular graph on n vertices, with an adjacency matrix A and spectrum {k,λ_2,...,λ_n}. Then the distance spectrum of $\mathcal{H}$ consists of $-(\lambda_i + 2)$ and $\lambda_i - 1$, i = 2,3,...,n, each with multiplicity 2, together with the numbers

$$\frac{1}{2}\left[7n-3 \pm \sqrt{(2k+1)^2+45n^2-12nk-6n}\right] \text{ and}$$

$$-\frac{1}{2}\left[n+3 \pm \sqrt{(2k+1)^2+5n^2+4nk+2n}\right] \quad .$$

Corollary 1. Let G be a connected k-regular graph on n vertices with an adjacency matrix A and spectrum {k,λ_2,...,λ_n}. Let $\mathcal{H}$ be the self-complementary graph obtained from G by the above-described construction. Then

$$E_D(\mathcal{H}) = 7n - 3 + \sqrt{(2k+1)^2 + 5n^2 + 4nk + 2n} + \sum_{i=2}^{n} |\lambda_i + 2| + \sum_{i=2}^{n} |\lambda_i - 1|$$

Theorem 1.12.

For every n ≥ 8, there exists a pair of 4-regular non-cospectral graphs on n vertices.

Theorem 1.13.

Let G be a connected 4-regular graph on n vertices, with an adjacency matrix A and spectrum $\{4,\lambda_2,...,\lambda_n\}$. Let H = $L^2(G)$ and $\mathcal{H}$ be the P_4 self- complementary graph obtained from H , according to the above described construction. Then

$$E_D(\mathcal{H}) = 3\left[8(3n-1) + \sqrt{20n^2 + 28n + 49}\right].$$

Theorem 1.14.

For every n = 48t and n = 24(2t+1), t≥4, there exists a pair of D-equienergetic self-complementary graph.

D-Energy of Some Self-Complementary Graphs

The D-energy of some self-complementary graphs $\mathcal{H}$ is easily deduced from the adjacency spectra of the respective parent graphs G.

1. If G≅Kn , the complete graph on n vertices, then

$$E_D(\mathcal{H}) = \begin{cases} 4 + 2\sqrt{10} & for\ n = 1 \\ 6 + 3\sqrt{17} + \sqrt{41} & forn = 2 \\ 22 + 2\sqrt{85} & for\ n = 3 \\ 13n - 9 + \sqrt{13n^2 - 6n + 1} & for\ n \geq 4 \end{cases}$$

2. If G≅$K_{p,p}$, the complete bipartite graph on n = 2p vertices, then

$$E_D\,(\mathcal{H}) \;=\; 15n - 17 \;+\sqrt{8n^2 \;+\; 4n \;+\; 1}\,.$$

3. If G≅CP(n), the cocktail party graph on n vertices, then

$$E_D(\mathcal{H}) = 13n - 9 + \sqrt{13n^2 - 18n + 9}.$$

The distance spectrum and energy of the compositions of regular graphs

Let G be a simple graph on n vertices and let $\lambda_1,\ldots,\lambda_n$ be the eigenvalues of its adjacency matrix A. The energy of a graph

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|,$$

.that other energy-type invariants can be defined as the absolute deviation of eigenvalues from their average value for a suitable graph matrix. For example, let D be the distance matrix of G, indexed by the vertices of G, where D_{uv} represents the length of the shortest path between u and v in G.

Definition 1. The distance energy DE(G) of a graph G is the sum of absolute values of the eigenvalues of the distance matrix of G

Several invariants of this type(as well as a few others)were studied by Consonni and Todeschini for possible use in QSPR modelling. Their study showed, among other things, that the distance energy is a useful molecular descriptor, since the values DE(G) orDE(G)/n appear among the best univariate models for the motor octane number of the octane isomers and for the water solubility of polychlorobiphenyls.

Since the distance energy is calculated from the distance spectrum, Graphs with the same distance spectrum trivially have the same distance energy. To avoid trivial cases, we say that the graphs G and H of the same order are DE-equienergetic if DE(G) = DE(H), while they have distinct spectra of distance matrices.

The join G∇H of two vertex-disjoint graphs G and H is the graph obtained from the union G∪H by adding all edges between a vertex of G and a vertex of H. Our main result is the description of the distance spectrum and the distance energy of the join of regular graphs in terms of their adjacency spectrum. This description is then used to show that there exist a number of families of sets of DE-equienergetic graphs, such that for any n∈N, each family contains a set with at least n graphs. The simplest such family consists of sets of complete bipartite graphs.The distance spectrum of the join of a regular graph with the union of two regular graphs of distinct vertex degrees,and provide further families of sets of DE-equienergetic graphs.

Join of regular graphs

Theorem 1.17. For i=1,2,let G_i be an ri-regular graph with n_i vertices and eigen values of the adjacency matrix A_{Gi}, $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,ni}$. The distance spectrum of $G_1 \nabla G_2$ consists of eigenvalues $-\lambda_{i,j} - 2$ for i = 1,2 and j = 2,3,...,n_i and two more eigenvalues of the form

$$n_1 + n_2 - 2 - \frac{r_1 + r_2}{2} \pm \sqrt{\left(n_1 - n_2 - \frac{r_1 - r_2}{2}\right)^2 + n_1 n_2}.$$

Corollary 3. The distance spectrum of the complete bipartite graph $K_{m,n}$ consists of simple eigenvalues $m + n - 2 \pm \sqrt{m^2 - mn + n^2}$ and an eigenvalue

-2 with multiplicity m+n−2.

If m,n≥2,then $m+n-2 \geq \sqrt{m^2 - mn + n^2}$ and we get

Corollary 4. $DE(K_{m,n}) = 4(m+n-2)$ for m,n≥2.

So, any two complete bipartite graphs with the same number of vertices, apart from stars, have the same distance energy. Since the distance eigenvalues different from −2 uniquely determine parameters m and n, different complete bipartite graphs have different distance spectra. Thus, our simplest family of sets of DE-equienergetic graphs is given by

$$\{\{K_{2,n-2}, K_{3,n-3}, \ldots, K_{[n/2],[n/2]}\} : n \geq 4\}.$$

The key to the successful application of Theorem **2** lies in regular graphs for which most (if not all) adjacency eigenvalues are at least−2, and so the corresponding eigenvalue $-\lambda - 2$ of the

distance matrix is always negative. Such graphs are, for example, the empty graph $\overline{K_m}$,the complete graph K_m, the complete bipartite graph $K_{m/2,m/2}$ for even m, the cycle C_m, as well as regular line graphs (which are themselves line graphs of regular or semi-regular graphs). For such graphs, we can use the well-known fact that the sum of all adjacency eigenvalues is zero in order to determine the distance energy of their join.

Theorem 1.18. For i = 1,2, let G_i be an r_i-regular graph with n_i vertices, whose smallest eigenvalue of the adjacency matrix is at least -2 and such that $G_i \ncong K_n$. Then

$$DE(G_1 \nabla G_2) = 4(n_1 + n_2) - 2(r_1 + r_2) - 8.$$

The join of a regular graph with the union of regular graphs

A computer search for pairs of DE-equienergetic graphs revealed that, among others, the wheel $W_9 \cong K_1 \nabla C_8$ and $K_1 \nabla (C_5 \cup K_3)$, which are DE-equienergetic by **Theorem 5**, are also DE-equienergetic to $K_1 \nabla (C_4 \cup K_4)$. However, $C_4 \cup K_4$ is not regular, but rather a union of regular graphs. Motivated by this example, we consider the distance spectrum of the graph $G_0 \nabla (G_1 \cup G_2)$, where G_0,G_1 andG_2 are regular graphs.If G_1 and G_2 have equal vertex degrees,then the distance spectrum of $G_0 \nabla (G_1 \cup G_2)$ is given by **Theorem 2**.Thus,we consider the case when G_1 andG_2 have distinct vertex degrees only.

Theorem 1.19. For i=0,1,2, let G_i be an r_i-regular graph with n_i vertices and eigenvalues $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,n_i}$ of the adjacency matrix A_{Gi}.If $r_1 \not\equiv r_2$, then the distance spectrum of $G_0 \nabla (G_1 \cup G_2)$ consists of eigenvalues $-\lambda_{i,j} - 2$ for i=0,1,2 and j=2,3,...,n_i and three more eigenvalues which are solutions of the cubic equation in ν:

$$(2n_0 - r_0 - 2 - \nu)(\nu + r_1 + 2)(\nu + r_2 + 2) + [2(\nu + r_0 + 2) - 3n_0][n_1(\nu + r_2 + 2) + n_2(\nu + r_1 + 2)] = 0.$$

Corollary7.

Graphs $K_1 \nabla (C_P \cup G)$, $P \in P_n$,form a set of DE-equienergetic graphs.

2. MOLECULAR ENERGIES OF AMMONIA (by graph energy)

In this section we are going to find the energies of ammonium molecule using graph energy. For this we need structure of ammonium molecule, Graph from the structure of ammonia and complement of the graph.

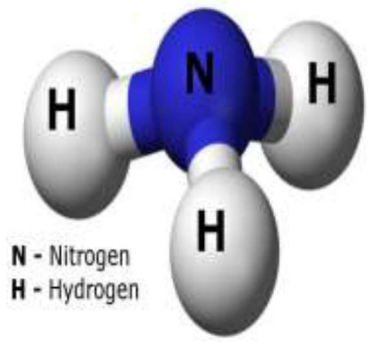
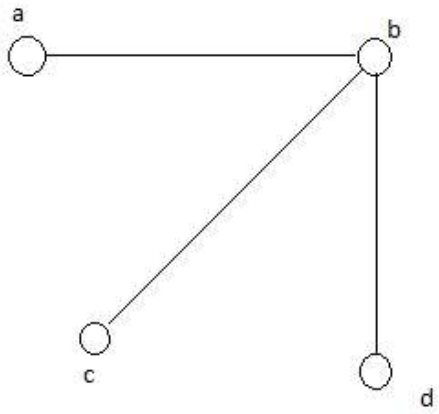
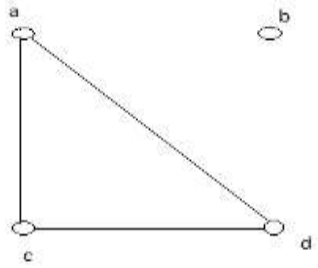


Fig 1—structure of ammonium molecule.



Graph 1 - Graph from the structure of ammonium molecule.

From graph 1 we can construct it's complement.



Graph 2 - Complement graph of graph 1

We have to find the distance energy matrix. The distance energy matrix = $A + 2\bar{A}$

Adjacency matrix A=$\begin{bmatrix}0 & 1 & 0 & 0\\1 & 0 & 1 & 1\\0 & 1 & 0 & 0\\0 & 1 & 0 & 0\end{bmatrix}$

Adjacency matrix $\bar{A} = \begin{bmatrix}0 & 0 & 1 & 1\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\\1 & 0 & 1 & 0\end{bmatrix}$

$\therefore$ Distance energy matrix D = $\begin{bmatrix}0 & 1 & 0 & 0\\1 & 0 & 1 & 1\\0 & 1 & 0 & 0\\0 & 1 & 0 & 0\end{bmatrix} + 2 \times \begin{bmatrix}0 & 0 & 1 & 1\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\\1 & 0 & 1 & 0\end{bmatrix}$

$= \begin{bmatrix}0 & 1 & 2 & 2\\1 & 0 & 1 & 1\\2 & 1 & 0 & 2\\2 & 1 & 2 & 0\end{bmatrix}$

Eigenvalues of adjacency matrix A= $\lambda_1 = -\sqrt{2}, \lambda_2 = \sqrt{2},\ \lambda_3 = 0,\ \lambda_4 = 0$

Spec(G)=$\{-\sqrt{2}, -\sqrt{2}, 0, 0\}$

Eigenvalues of distance matrix $\bar{A} = \mu_1 = -2,\ \mu_2 = -2,\ \mu_3 = 2 - \sqrt{7},\ \mu_4 = 2 + \sqrt{7}$

Energy values of ammonia

Energy from the graph 1,

$E(G) = \sum_{i=1}^{n} |\lambda_i|$.

E(G)=$\sqrt{2} + \sqrt{2} + 0 + 0 = 2.8284$J

Energy from the distance graph is

$E_D(G) = \sum_{i=1}^{p} |\mu_i|$

E_D(G)=2+2+$(2-\sqrt{7}) + (2 + \sqrt{7})$=9.2915J

A graph is define as (p,q) form. we know that p(vertices)=4,

Then from lemma 7,

$\sum_{i=1}^{p} \mu_i^2 = 2(2p^2 - 2p - 3q)$

$(-\sqrt{2})^2+(\sqrt{2})^2+0^2+0^2)=2(32 - 8 - 3q) \Rightarrow -22 = -3q \Rightarrow q = 7.33.$

By using theorem 1.5 we get the bounds for the distance energy

$\sqrt{4p(p-1) - 6q + p(p-1)\Delta^{2/p}} \leq E_D(G) \leq \sqrt{2p(2p^2 - 3q - 2p)}.$

we can find the $\Delta^{2/p}$ value, $\prod_{i \neq j} |\mu_i|^{2/p} = \Delta^{2/p}$ by substituting the values we get $\Delta^{2/p} = 3.4641$

By substituting the values, we get 6.7519J≤9.291J≤ $12J$.

By graph theory energy levels of ammonia varies from 6.7519J to 12J.

3. MOLECULAR ENERGIES: METHANE (by graph energy)

In this section we are going to find the energies of methane molecule using graph energy. For this we need structure of methane molecule, Graph from the structure of methane, and complement of the graph.

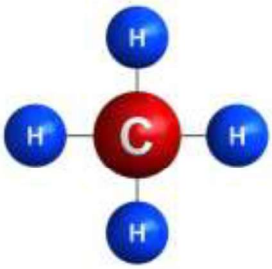
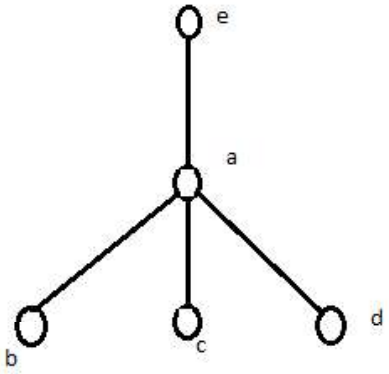
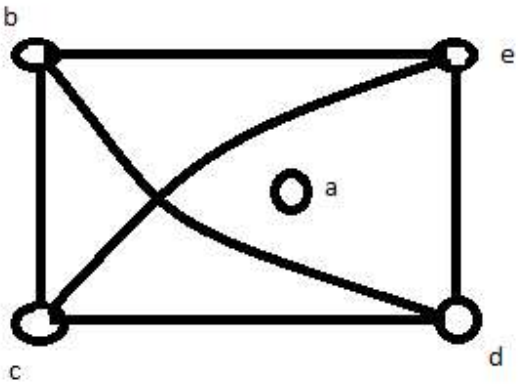


Fig 2 -Structure of methane



Graph 3 - Graph from the structure of methane molecule

From graph 3 we can construct it's complement.



Graph 4 - complement graph of graph 3

We have to find the find the distance energy matrix.

Distance energy matrix=$A + 2\bar{A}$

Adjacency matrix A=$\begin{bmatrix}0&1&1&1&1\\1&0&0&0&0\\1&0&0&0&0\\1&0&0&0&0\\1&0&0&0&0\end{bmatrix}$

Adjacency matrix $\bar{A} = \begin{bmatrix}0&0&0&0&0\\0&0&1&1&1\\0&1&0&1&1\\0&1&1&0&1\\0&1&1&1&0\end{bmatrix}$

∴ Distance energy matrix D=$\begin{bmatrix}0&1&1&1&1\\1&0&0&0&0\\1&0&0&0&0\\1&0&0&0&0\\1&0&0&0&0\end{bmatrix}$+2$\begin{bmatrix}0&0&0&0&0\\0&0&1&1&1\\0&1&0&1&1\\0&1&1&0&1\\0&1&1&1&0\end{bmatrix}$

=$\begin{bmatrix}0&1&1&1&1\\1&0&2&2&2\\1&2&0&2&2\\1&2&2&0&2\\1&2&2&2&0\end{bmatrix}$

Now we can find the eigenvalues of adjacency matrix A=$\begin{bmatrix}0&1&1&1&1\\1&0&0&0&0\\1&0&0&0&0\\1&0&0&0&0\\1&0&0&0&0\end{bmatrix}$

$R_3 \to R_3-R_2$; $R_4 \to R_4-R_2$; $R_5 \to R_5-R_2$

$\sim \begin{bmatrix}0&1&1&1&1\\1&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\end{bmatrix}$ $R_1 \leftrightarrow R_2$

$\sim \begin{bmatrix}1&0&0&0&0\\0&1&1&1&1\\0&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\end{bmatrix}$ is a upper triangular matrix

Eigenvalues are diagonal entries

Eigenvalues =1,1,0,0,0

$$\mu_1 = 1, \mu_2 = 1, \mu_3 = 0, \mu_4 = 0, \mu_5 = 0$$

Eigenvalues of distance matrix $\bar{A}$

$$\lambda_1 = -2, \lambda_2 = -2, \lambda_3 = -2, \lambda_4 = -0.6055, \lambda_5 = 6.6055$$

Energy values of methane

Energy from the graph 3 is $E(G) = \sum_{i=1}^{n} |\lambda_i|$.

E(G)=1+1+0+0+0=2J

Energy from the distance graph is $E_D(G) = \sum_{i=1}^{p} |\mu_i|$

E_D(G)=2+2+2+0.6055+6.6055=13.211

A graph is define as (p,q) form. We know that p(vertices)=5,

Then from lemma 7,

$\sum_{i=1}^{p} \mu_i^2 = 2(2p^2 - 2p - 3q)$

$(1^2+1^2+0+0+0) = 2(2\times 25 - 2 \times 5 - 3q)$

-39=-3q => q=13.

By using theorem 1.5 we get the bounds for the distance energy

$$\sqrt{4p(p-1) - 6q + p(p-1)\Delta^{2/p}} \leq E_D(G) \leq \sqrt{2p(2p^2 - 3q - 2p)}. \quad (1)$$

From the proof of theorem 1.5we can find the $\Delta^{2/p}$ value,

$$\prod_{i \neq j} |\mu_i|^{2/p} = \Delta^{2/p}$$

$(2^{2\backslash 5} \times 2^{2\backslash 5} \times 2^{2\backslash 5} \times 0.6055^{2\backslash 5} \times 6.6055^{2/5})$=3.999

By substituting the values in equation 1 we get $9.044 \leq 13.211$

For methane there doesn't exist an upper bond.

4. CONCLUSION

We have seen that the compositions of regular graphs based on the join of graphs yield a number of families containing large sets of DE-equi-energetic graphs. From this project we can conclude that the eigenvalues of the adjacent matrix of the graph from the selected molecule can construct the distance spectrum. And also, by using the eigenvalues we can find the energy of the selected molecule. Also, distance energy of the molecules can find by the graph energy equations. Lower and upper bounds of the energy variations.

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