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Energy of Smith graphs

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Abstract. In this manuscript, we have evaluated the energies of Smith graphs. In the course of the investigation, we found that only one Smith graph is hypo-energetic. Moreover, we have also established the energy bounds for Smith graphs.

1. Introduction

For all standard terminology and notations in graph theory and those in the theory of spectra of graphs, we refer the reader to Harary [4] and Cvetkovic et. al. [2], respectively. Particularly, all graphs considered in this paper are finite, simple, connected and undirected.

One of the current interests in mathematical chemistry, pharmacology, toxicology and biomedicinal chemistry is the *prediction* of pharmacological and biodynamic properties of molecules from their structure. The tacit assumption underlying this trend of research is that *the structure of a molecule determines its behavior*. To identify the certain classes of chemical compounds, one involves quite sophisticated mathematical techniques, where Graph Theory has come to play a major role. However, there are specific classes of graphs, which are isomorphic to unsaturated conjugate hydrocarbon compounds; for example, the Smith graphs (i.e., a graph whose at least one eigenvalue is 2) W_m and C_m are isomorphic to unsaturated conjugate hydrocarbon compounds (for detail details see [1]). From

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the survey of the literature, we found the there are six kinds of Smith graphs, viz., W_m ($m \geqslant 6$), C_m ($m \geqslant 3$), $K_{1,4}$, H_7, H_8, and H_9.

Let $G = (V, E)$ be a simple graph with vertex set $V = \{v_1, v_2, \ldots, v_m\}$ and edge set $E = \{e_1, e_2, \ldots, e_n\}$. Let $A(G)$ be the adjacency matrix of G. The energy $E(G)$ of graph G is the sum of the absolute values of eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_m$ of its adjacency matrix $A(G)$. A graph G is said to be hypoenergetic if $E(G) < m$, otherwise G is non-hypoenergetic. Two non-isomorphic graphs G_1 and G_2 are said to be equienergetic graphs if $E(G_1) = E(G_2)$ and if they have identical spectra, then the graph is co-spectral equienergetic graphs, otherwise non co-spectral equienergetic graphs. Throughout the paper by S_m, we mean a Smith graph on m vertices and n edges. Except $K_{1,4}$, other Smith graphs are the extended form of Dynkin graphs [3].

Motivated by the earlier study done in [5] on the energy of a graph, in this paper, we have focused on the energy of Smith graphs. Moreover, we have characterized the Smith graphs for which the energy bounds are attained in the inequality $(m-1) \leqslant E(S_m) \leqslant m + \lceil \frac{n}{3} \rceil$.

2. Main results

In this section, we begin with the following existing results reported in [3], and will be found useful to derive new results. Later, we will establish the results on energy bonds of Smith graphs.

Lemma 1. *Let G be a graph and $S(G)$ be the spectrum of G. Then*

(i) $S(W_m) = \{2\cos\frac{r\pi}{m-4} \mid r = 1, 2, \ldots, m-5\} \cup \{-2, 0, 0, 2\}$.
(ii) $S(C_m) = \{2\cos\frac{2r\pi}{m} \mid r = 0, 1, 2, \ldots, m-1\}$.
(iii) $S(H_7) = \{0, \pm 1, \pm 1, \pm 2\}$.
(iv) $S(H_8) = \{2\cos\frac{r\pi}{30} \mid r = 1, 7, 11, 13, 17, 19, 23, 29\}$.
(v) $S(H_9) = \{2\cos\frac{r\pi}{5} \mid r = 1, 2, 3, 4\} \cup \{0, \pm 1, \pm 2\}$.
(vi) $S(K_{1,4}) = \{\pm 2, 0, 0, 0\}$.

In view of Lemma 1, the spectra of Smith graph can be at most $\{0, 0, 0, \ldots, 2, -2, \lambda_1, \lambda_2, \ldots, \lambda_i\}$. In general, the energy bounds on Smith graphs is given by the following result:

Theorem 1. *Let S_m be Smith graph and $E(S_m)$ be its energy. Then*

$$(m-1) \leqslant E(S_m) \leqslant m + \lceil \frac{n}{3} \rceil. \tag{1}$$

Proof. Consider S_m be isomorphic to $K_{1,4}$, whose spectrum is $\{-2, 0, 0, 2\}$. Clearly, $E(K_{1,4})$ is equal to 4, which is also equal to $(m-1)$.

Now we consider S_m to be W_m $(m \geqslant 6)$. In view of Lemma 1, the spectrum of W_m is

$$\left\{2\cos\frac{r\pi}{m-4} \mid r = 1, 2, \ldots, m-5\right\} \cup \{-2, 0, 0, 2\}.$$

Thus, the energy of W_m is strictly greater than $(m-1)$ and strictly less than to $m + \lceil\frac{n}{3}\rceil$.

For the next case, if we consider S_m to be H_7, then $(m-1) < E(H_7) = (m+1) < m + \lceil\frac{n}{3}\rceil$ Let S_m to be H_8. In view of Lemma 1, we get $(m-1) < E(H_8) < m + \lceil\frac{n}{3}\rceil$. If we take S_m to be H_9, then again we get $(m-1) < E(H_9) < m + \lceil\frac{n}{3}\rceil$. Finally, we take S_m to be C_m $(m \geqslant 3)$, for $m = 6$, $E(C_m)$ attains the upper bound $m + \lceil\frac{n}{3}\rceil$ and for other remaining values of m $(m \neq 6)$, the energy of C_m lies between $(m-1)$ and $m + \lceil\frac{n}{3}\rceil$.

From the above analysis, we conclude that

$$(m-1) \leqslant E(S_m) \leqslant m + \lceil\frac{n}{3}\rceil. \qquad \square$$

At this stage we have the following problem:

Problem 1. Characterize the Smith graphs for which the bounds are attained in the Inequality (1).

We answer to the above problem in the following theorems:

Theorem 2. *Let S_m be Smith graph and $E(S_m)$ be its energy. Then $E(S_m) = (m-1)$ if and only if S_m is isomorphic to $K_{1,4}$.*

Proof. Necessity: Let us take $E(S_m) = (m-1)$ and we have to show that the only Smith graph will be $K_{1,4}$. We shall prove it by contradiction. Let us suppose that S_m is not isomorphic to $K_{1,4}$. It means that it is isomorphic to either W_m $(m \geqslant 7)$ or C_m $(m \geqslant 3)$ or H_7 or H_8 or H_9. However none of the listed graphs have energy equal to $(m-1)$. So, our assumption is wrong. Hence, $E(S_m) = (m-1)$.

Sufficiency: Let S_m be isomorphic to $K_{1,4}$. Clearly $K_{1,4}$ have 5 vertices and

$$E(K_{1,4}) = 4 = (m-1).$$

Thus, the result follows. $\square$

Theorem 3. *Let S_m be Smith graph and $E(S_m)$ be its energy. Then $E(S_m) = m + \lceil \frac{n}{3} \rceil$ if and only if S_m is isomorphic to C_6.*

Proof. For the necessity part, let us take $E(S_m) = m + \lceil \frac{n}{3} \rceil$ and we have to show that the only Smith graph will be C_6. We shall prove it by contradiction. Let us suppose that S_m is not isomorphic to C_6. It means that it is isomorphic to other Smith graphs. However, none of the Smith graph except C_6 have energy equal to $m + \lceil \frac{n}{3} \rceil$. So, our assumption is wrong. Hence, $E(S_m) = m + \lceil \frac{n}{3} \rceil$.

For the sufficiency part, let S_m be isomorphic to C_6. C_6 has the spectrum $\{-2, -1, -1, 1, 1, 2\}$, and hence $E(C_6) = 8$, which is equal to $m + \lceil \frac{n}{3} \rceil$. □

Theorem 4. *Let S_m be Smith graph and $E(S_m)$ be its energy. Then $E(S_m) = m$ if and only if S_m is isomorphic to either C_4 or W_6.*

Proof. Necessity: Let us take $E(S_m) = m$ and we shall show that the only Smith graph is C_4 or W_6. Suppose to contrary that S_m is neither isomorphic to C_4 nor W_6, it means S_m can be isomorphic to other Smith graphs. But, the energy of any of the Smith graphs is not equal to m. So, our assumption is wrong. Hence, S_m must be isomorphic to either C_4 or W_6.

Sufficiency: Let us assume that S_m be isomorphic to C_4. Clearly, C_4 have 4 vertices and whose spectrum is $\{-2, 0, 0, 2\}$. Therefore, $E(C_4) = 4$. Now suppose that S_m is isomorphic to W_6 with 6 vertices and the spectrum is $\{-2, -1, 0, 0, 1, 2\}$. Thus, $E(W_6) = 6$. Hence, the result follows. □

Theorem 5. *Let S_m be Smith graph and $E(S_m)$ be its energy. Then $E(S_m) = (m + 1)$ if and only if S_m is isomorphic to either C_3 or H_7.*

Proof. The necessity part of the proof can be given by the same argument as given in proof of Theorem 4.

For the sufficiency part, let us assume that S_m is isomorphic to C_3. Clearly, C_3 have 3 vertices and its spectrum is $\{-1, -1, 2\}$.

Thus, $E(C_3) = 4 = m + 1$. Next let us take S_m to be H_7, which has 7 vertices and spectrum is $\{-1, -1, -2, 0, 1, 1, 2\}$. Therefore, $E(H_7) = 8 = (m + 1)$. Hence, the result. □

Theorem 6. *Let S_1 and S_2 be two Smith graphs having vertices set $V(S_1)$ and $V(S_2)$, respectively such that $|V(S_1)| < |V(S_2)|$. Then, $E(S_1) \leqslant E((S_2)$.*

Proof. In order to show the result, we shall pick up those Smith graphs S_1 and S_2 for which $|V(S_1)| < |V(S_2)|$. First, we consider C_3 whose spectrum is $\{-1, 1, 2\}$. Therefore, $E(C_3) = 4$. We need to tackle the following cases:

Case(i) Let $S_2 \cong C_4$. In light of Lemma 1, $E(C_4) = 4$. Therefore $E(C_3) = E(C_4)$.

Case (ii) Let us take $S_2 \cong K_{1,4}$. Then, clearly $E(K_{1,4}) = 4$. Therefore $E(C_3) = E(K_{1,4})$.

Case (iii) Let $S_2 \cong H_7$ or H_8 or H_9. Then, in view of Lemma 1, we see that energy of each of the listed graphs is greater than $E(C_3)$.

Case (iv) Let us assume $S_2 \cong W_m (m \geqslant 6)$. Due to Lemma 1, we get $E(W_m) > E(C_3)$.

Case (v) When we assume $S_2 \cong C_m$ $(m > 4)$. Clearly, the strict inequality holds between the energy of S_1 and S_2.

Next if we choose S_1 and S_2 to be any of the Smith graph namely $K_{1,4}$ H_7, H_8, H_9, W_m and C_m in such a way that $|V(S_1)| < |V(S_2)|$, then we can easily prove the result for each case by following the same technique. Thus, for any two Smith graph having $|V(S_1)| < |V(S_2)|$, we have $E(S_1) \leqslant E(S_2)$. □

Remark 1. If two Smith graphs have equal number of vertices, then their energies need not be same. As for instance, consider C_5 and $K_{1,4}$. Both the graphs have same number of vertices. However, the energy of C_5 is 6.47 and the energy of $K_{1,4}$ is 4, which are not equal.

Remark 2. The minimum energy of Smith graph is 4. Moreover, the minimum energy is attained by more than one Smith graphs. The graphs C_3, C_4 and $K_{1,4}$ all have the same energy.

Theorem 7. *Among all the Smith graphs $K_{1,4}$ is the only Smith graph which is hypoenergetic.*

Proof. In order to show the result $E(K_{1,4}) < m$ and for all other Smith graph $E(S_m) \geqslant m$.

If we take S_m to be C_6 then by Theorem 3, $E(C_6) = m + \lceil \frac{n}{3} \rceil > m$. Therefore, C_6 is non-hypoenergetic.

Let us assume S_m to be either C_4 or W_6 then by Theorem 4., $E(C_4) = 4$ and $E(W_6) = 6$. Hence C_4 and W_6 are non-hypoenergetic.

Let us take S_m to be either C_3 or H_7 then by Theorem 5. $E(S_m) = (m + 1) > m$. Therefore, C_3 and H_7 are non-hypoenergetic.

If we take S_m be $W_m(m \geqslant 7)$, $C_m(m \neq 3,4,6)$, H_8 and H_9. In view of Theorem 1, $(m-1) < E(S_m) < m + \lceil \frac{n}{3} \rceil$. Thus all listed Smith graph is non-hypoenergetic.

Let we take S_m to be $K_{1,4}$ then by Theorem 2, $E(K_{1,4}) = 4$. Therefore, $E(S_m) = (m-1) < m$. Hence $K_{1,4}$ is a hypoenergetic. From the foregoing analysis, we found that the only hypoenergetic graph is $K_{1,4}$. □

Remark 3. The following are non co-spectral equienergetic graphs

- C_3, C_4 and $K_{1,4}$,
- C_3, C_4 and C_6,
- C_3, C_4 and H_7.

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