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Bounds for energy of some nanostar dendrimers

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The energy $E(G)$ of a graph G is the sum of the absolute values of the eigenvalues of G. The nanostar dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. In this paper, using some inequalities, we obtain bounds for energy of some nanostars.

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1. Introduction

A simple graph $G=(V,E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

If A is the adjacency matrix of G, then the eigenvalues of A, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are said to be the eigenvalues of the graph G. The energy of the graph G is defined as $E = E(G) = \sum_{i=1}^{n} |\lambda_i|$. This definition was put forward by I. Gutman [4] and was motivated by earlier results in theoretical chemistry [5].

Recently much work on graph energy appeared also in the mathematical literature [6-9]. For the sake of completeness, we mention below some well-known results in this topic which is crucial in our study. We encourage interested readers to consult mentioned papers and their references.

Theorem 1. ([8]) Let G be a graph of order n and size m. Then,

$$E(G) \leq \sqrt{2mn}$$

with equality holding if and only if G is regular of degree 0 or 1.

Theorem 2. ([6,7]) Let G be a graph of order n and size m. Then,

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2m - \left(\frac{2m}{n}\right)^2\right)}$$

with equality if and only if G is either a regular graph of degree 0, 1 or $n-1$, or a non-complete connected strongly regular graph with two non-trivial eigenvalues.

Theorem 3. ([3]) Let G be a graph of order n and size m. If A is the adjacency matrix of G, then,

$$\sqrt{2m + n(n-1)\,|\det A|^{2/n}} \leq E(G) \leq \sqrt{2mn}$$

A subset M of $E(G)$ is called a matching in G if its elements are not loops and no two of them are adjacent in G; the two ends of an edge in M are said to be matched under M. A matching M *saturates* a vertex v, and v is said to be M-saturated if some edges of M is incident with v.

If every vertex of G is M-saturated, then the matching M is perfect. It is obvious that C_6 has a perfect matching. Graph with kekule structure is a unicyclic graph with perfect matching (see [9]).

The following theorem gives bounds of energy of graphs by the number of kekule structures of graphs.

Theorem 4. ([3]) Let G be a graph of order n, size m and k kekule structures. If A is the adjacency matrix of G, then $(-1)^n \det A = k^2$. Therefore

$$\sqrt{2m + n(n-1)k^{4/n}} \leq E(G) \leq \sqrt{2mn}\,.$$

The nanostar dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. Nanostars have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nano-science are unlimited.

In Section 2, similar to [1], we obtain bounds for energy of some nanostar dendrimers.

2. Bounds of energy of certain nanostars

In this section, we shall find bound for energy of certain nanostars. First we obtain bounds for energy of the nanostars denoted by $NS_1[n]$. Fig. 1 shows the kind of nanostar has grown 3 stages ($NS_1[3]$).

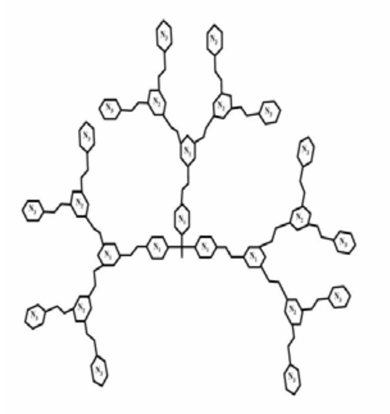

Fig 1. $NS_1[3]$.

Theorem 5. ([2])

(i) The order of $NS_1[n]$ is $|V(NS_1[n])| = 24\times 2^n - 4$.

(ii) The size of $NS_1[n]$ is $|E(NS_1[n])| = 27\times 2^n - 5$.

To compute the number of Kekule structures of $NS_1[3]$, we have to count the number of hexagons in $NS_1[3]$. Using inductive argument, one can show that the number of Keküle structures of $NS_1[3]$ is 3×2^n.

Theorem 6.

(i) The lower bound for energy of $NS_1[3]$ is

$$L_e(S_1) = \sqrt{27\times 2^{n+1} - 10 + (24\times 2^n - 4)(24\times 2^n - 5)(3\times 2^n)^{4/(24\times 2^n - 4)}}$$

(ii) The upper bound for energy of $NS_1[3]$ is

$$U_e(S_1) = \sqrt{(27\times 2^{n+1} - 10)(24\times 2^n - 4)}$$

Proof. It follows from Theorems 4, 5 and the number of kekule structures. ■

Now we shall study the bounds of another kind of nanostars which has grown n steps denoted $NS_2[n]$.

Fig. 2 shows $NS_2[3]$.

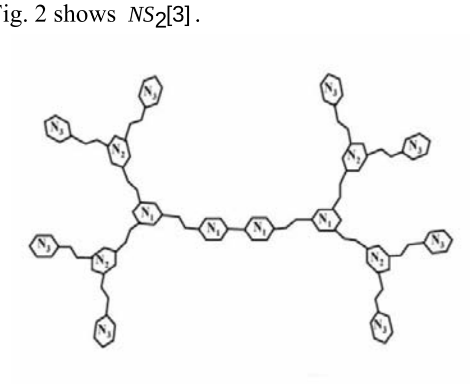

Fig 2. $NS_2[3]$.

Theorem 7. ([2])

(i) The order of $NS_2[n]$ is $|V(NS_2[n])| = 16\times 2^n - 4$.

(ii) The size of $NS_2[n]$ is $|E(NS_2[n])| = 18\times 2^n - 5$.

To compute the number of Kekule structures of $NS_2[n]$, we have to count the number of hexagons in $NS_2[n]$. Using inductive argument, one can show that the number of Keküle structures of $NS_2[n]$ is 2^{n+1}.

Theorem 8.

(i) The lower bound for energy of $NS_2[n]$ is

$$L_e(S_2) = \sqrt{18\times 2^{n+1} - 10 + (2^{n+4} - 4)(2^{n+4} - 5)(2^{n+1})^{1/(2^{n+2} - 1)}}$$

(ii) The upper bound for energy of $NS_2[n]$ is

$$U_e(S_2) = \sqrt{(18\times 2^{n+1} - 10)(2^{n+4} - 4)}$$

Proof. It follows from Theorem 4, 7 and the number of kekule structures. ■

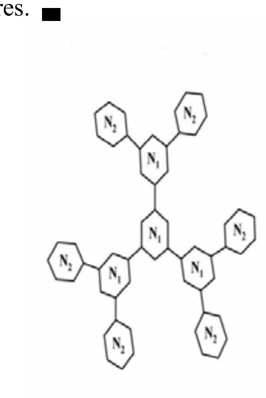

Fig 3. $NS_3[2]$.

Here we find bounds for another kind of nanostars has grown n stages. We denote this graph by $NS_3[n]$. Fig. 3 shows $NS_3[2]$.

We need the following theorem:

Theorem 9. ([2])

1. The order of $NS_3[n]$ is $|V(NS_3[n])| = 18\times 2^n - 12$.
2. The size of $NS_3[n]$ is $|E(NS_3[n])| = 21\times 2^n - 15$.

To compute the number of Kekule structures, we have to count the number of hexagons in $NS_3[n]$. Using inductive argument, one can show that the number of Keküle structures of $NS_3[n]$ is $3\times 2^n - 2$.

Theorem 10.

(i) The lower bound for energy of $NS_3[n]$ is

$$L_e(S3) = \sqrt{21\times 2^{n+1} - 30 + (18\times 2^n - 12)(18\times 2^n - 13)(3\times 2^n - 2)^{1/(9\times 2^{n-1} - 3)}}$$

(ii) The upper bound for energy of $NS_3[n]$ is

$$U_e(S_3) = \sqrt{(21\times 2^{n+1} - 30)(18\times 2^n - 12)}$$

Proof. It follows from Theorem 4, 9 and the number of kekule structures.

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