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KEKÜLE INDEX AND BOUNDS OF ENERGY FOR NANOSTAR DENDRIMERS

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In this paper the Kekülе index of four classes of dendrimer nanostars are computed. Then we apply these quantities to bound the energy of theses nanostars.

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1. Introduction

A dendrimer is a synthetic 3-dimentional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. The topological study of these macromolecules is the aim of this article, see papers[1-6] for details.

An eigenvector of a matrix is a non-zero vector that is either left unaffected or simply multiplied by a scale factor after the matrix. The eigenvalue of a non-zero eigenvector is the scale factor by which it has been multiplied. A real number λ is an eigenvalue of a matrix M if there is a non-zero vector X such that MX = λX.

Suppose G is a molecular graph. Then the eigenvalues of its adjacency matrix are called the eigenvalues of G. The energy of G is defined as the sum of the absolute values of all eigenvalues of G. This quantity has a long known chemical application, for details see surveys [7]. Recently much work on graph energy appeared also in the mathematical literature.[8-13] For the sake of completeness, we mention below some well-known results in this topic which is crucial in our study. We encourage to interested readers to consult mentioned papers and their references.

Theorem 1. The main properties of the energy are as follows:

1. $E(G) \geq 0$, equality is attained if and only if $m = 0$.
2. If the graph G consists of (disconnected) components G_1 and G_2, then $E(G) = E(G_1) + E(G_2)$.
3. If one component of the graph G is G_1 and all other components are isolated vertices, then $E(G) = E(G_1)$.

Theorem 2 ([11]). $E(G) \leq \sqrt{2mn}$ with equality holding if and only if G is regular of degree 0 or 1.

Theorem 3. Suppose G is a (n, m) graph, then

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

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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 both having absolute value $\sqrt{\left[2m-(2m/n)^2\right]/(n-1)}$.

Theorem 4. Suppose G is a (n,m) graph then $2\sqrt{m} \le E(G) \le 2m$. If G has no isolated vertices, then the equality $E(G) = 2\sqrt{m}$ holds if and only if G is a complete bipartite graph. If G has no isolated vertices, then the equality $E(G) = 2m$ holds if and only if G is regular of degree 1.

Theorem 5 ([9]). Let G be graph with n vertices and m edges then

$$\sqrt{2m + n(n-1)\left|\det A\right|^{\frac{2}{n}}} \le E(G) \le \sqrt{2mn} .$$

Theorem 6. Leg G be a graph with n vertices and k Kekule structures. If A is adjacency matrix of G then $(-1)^n \det A = k^2$.

From these results, one can prove $\sqrt{2m + n(n-1)k^{4/n}} \le E_n(G) \le \sqrt{2mn}$.

2. Main Results and discussion

In this section the Keküle index of four classes of dendrimer nanostars are computed. To explain, we assume that G is a molecular graph. A matching for G is a set of edges without common vertex. A perfect matching or Keküle structure is a matching which covers the vertex set of G. We now present four classes $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ of nanostar dendrimers, Figures 1-4.

Fig. 1. The Molecular Graph of $NS_1[n]$.

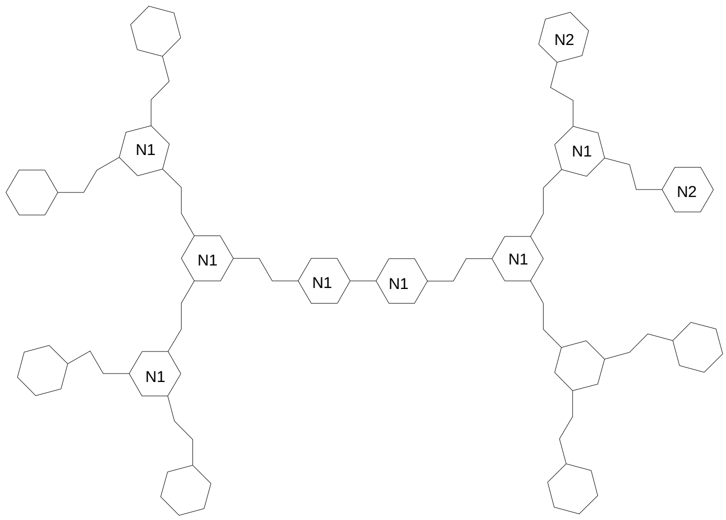

Fig. 2. The Molecular Graph of $NS_2[n]$.

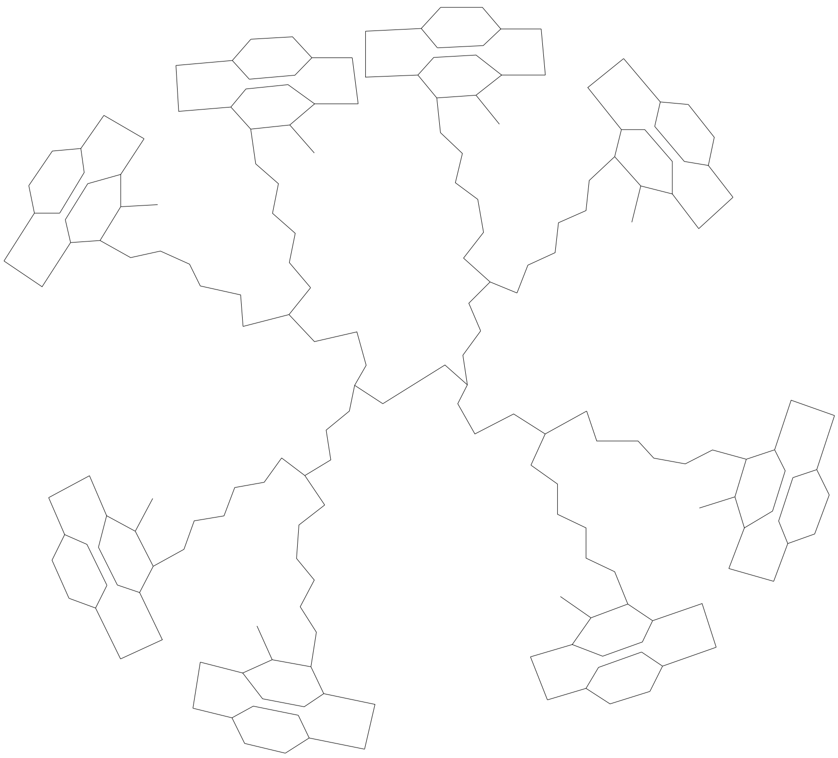

Fig. 3. The Molecular Graph of $\mathrm{NS}_3[\mathrm{n}]$.

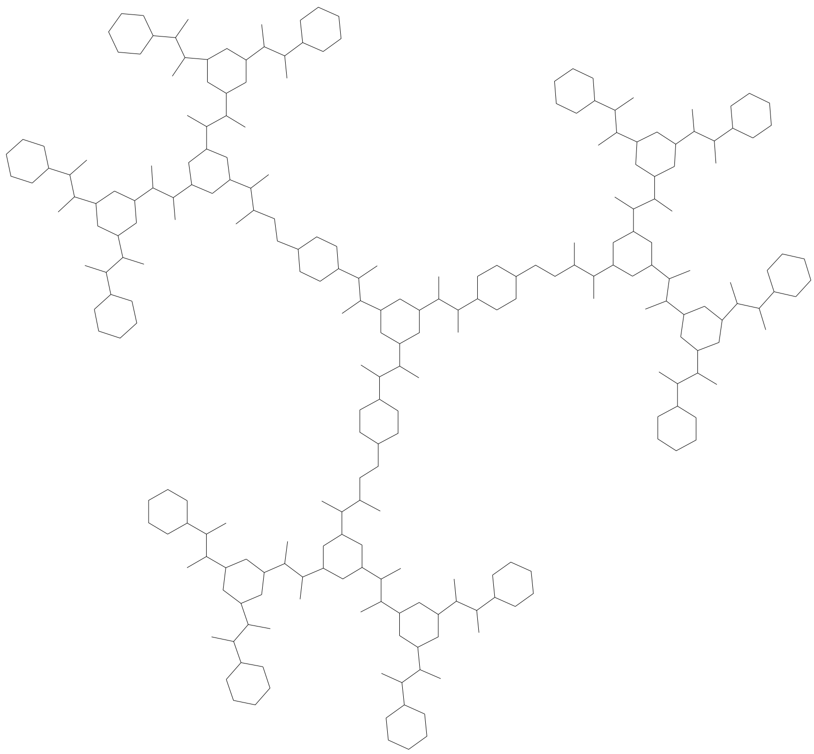

Fig. 4. The Molecular Graph of $\mathrm{NS_4[n]}$.

Using a simple calculation, one can show that $\left|V(NS_1[n])\right| = 24\cdot 2^n - 4$ and $\left|E(NS_1[n])\right| = 27\cdot 2^n - 5$. From Figure 5, one can prove the number of Kekūle structures in core of dendrimer $NS_1[n]$ is equal to 2^6. By using an inductive argument the number of edges in Kekūle structure and in step n is $\left|E_k(NS_1[n])\right| = 12\cdot 2^n - 2$. Therefore,

$$k(NS_1[n]) = 2^6\cdot 2^{3\cdot 2}\cdot 2^{3.2.2}\cdot 2^{3.2.2.2}\cdot \ldots \cdot 2^{3.2^{n-1}} = 2^6\prod_{i=1}^{n-1} 2^{3\cdot 2^i} = 64^{2^{n-1}}.$$

Theorem 7. $\alpha_1 \le E(NS_1[n]) \le \beta_1$ such that α_1 and β_1 are defined as follows:

$$\alpha_1 = \sqrt{2m + n(n-1)K^{4/n}} = \sqrt{54.2^n - 10 + 576.(8^{(2^n)})^{\frac{4}{n}}.4^n - 216.(8^{(2^n)})^{\frac{4}{n}}.2^n + 20.(8^{(2^n)})^{\frac{4}{n}}}$$

$$\beta_1 = \sqrt{2mn} = 2\sqrt{324\cdot 4^n - 114\cdot 2^n + 10}.$$

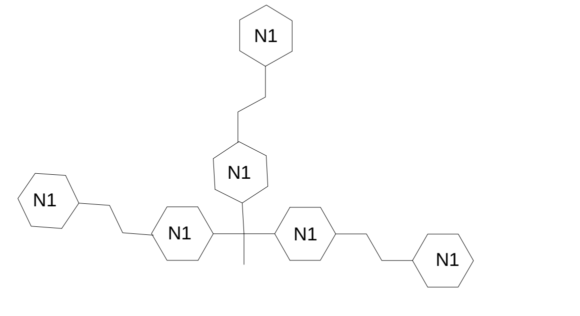	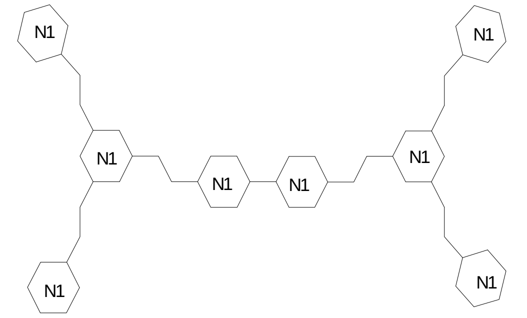
Fig. 5. The core of $\mathrm{NS_1[n]}$.	*Fig. 6. The Core of* $\mathrm{NS_2[n]}$.

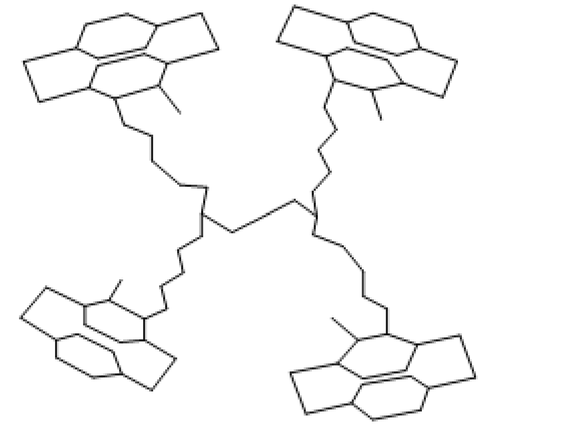

Fig. 7. The Core of $NS_3[n]$.

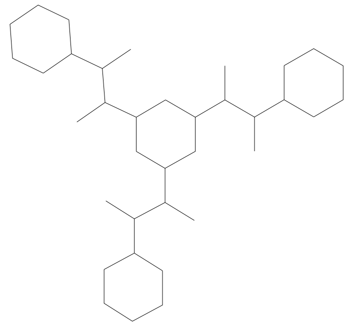

Fig. 8. The Core of $NS_4[n]$.

We now consider the second type nanostar dendrimer $NS_2[n]$. Using a simple calculation as above, one can show that $|V(NS_2[n])| = 60 + 8\sum_{i=2}^{n} 2^{i+1} = 16\cdot 2^{(n+1)} - 4$ and $|E(NS_2[n])| = 67 + 9\sum_{i=2}^{n} 2^{i+1} = 18\cdot 2^{(n+1)} - 5$. On the other hand, the number of Kekūle structures in the core of dendrimer, Figure 6, is equal to 2^8. Therefore, by an inductive argument $|E_k(NS_2[n])| = 30 + 4\sum_{i=2}^{n} 2^{i+1} = 8\cdot 2^{(n+1)} - 2$. This implies that $|k(NS_2[n])| = 2^{2^{n+2}}$.

Theorem 8. Consider the dendrimer nanostar $NS_2[n]$. Then $\alpha_2 \le E(NS_2[n]) \le \beta_2$ such that α_2 and β_2 are defined as follows:

$$\alpha_2 = \sqrt{2m + n(n-1)K^{4/n}} = \sqrt{72\cdot 2^n - 10 + 1024\cdot (16^{2^n})^{\frac{4}{n}}\cdot 4^n - 288\cdot (16^{2^n})^{\frac{4}{n}}\cdot 2^n + 20\cdot (16^{2^n})^{\frac{4}{n}}}$$

$$\beta_2 = \sqrt{2mn} = 2\sqrt{576\cdot 4^n - 152\cdot 2^n + 10}.$$

Consider the dendrimer nanostar $NS_3[n]$, Figure 3. The core of this nanostar is shown in Figure 7. Using a simple calculation, one can show that $|V(NS_3[n])| = 52.2^n - 12$ and $|E(NS_3[n])| = 58.2^n - 13$. The number of Kekule structures in yjr core of this nanostar dendrimer is equal to 3^4. Using inductive argument, one can show that the number of Kekūle structures is in step k is $|E_k(NS_3[n])| = 24.2^n - 2$. Therefore, $|K(NS_3[n])| = 9^{2^n}$.

Theorem 9. Let G be the molecular graph of dendrimer nanostar $NS_3[n]$. Then $\alpha_3 \le E(NS_3[n]) \le \beta_3$, where

$$\alpha_3 = \sqrt{2m + n(n-1)K^{4/n}} = \sqrt{116.2^n - 26 + 2704.(9^{(2^n)})^{4/n}.4^n - 1300.(9^{(2^n)})^{4/n}.2^n + 156.(9^{(2^n)})^{4/n}}$$

$$\beta_3 = \sqrt{2mn} = 2\sqrt{1508\cdot 4^n - 686\cdot 2^n + 78}.$$

In Figure 8, the core of dendrimer nanostar $NS_4[n]$ is depicted. From Figures 4 and 8, one can see that $|V(NS_4[n])| = 96.2^{n-1} - 60$ and $|E(NS_4[n])| = 105.2^{n-1} - 66$. To compute the number of Kekule structures, we have to count the number of hexagons in $NS_4[n]$, which is equal to $9.2^{n-1} - 5$. From Figure 8, it is easy to prove the number of Kekule structures in the core of dendrimer is equal to 3^4. So, a similar argument as above shows that $|E_k(NS_4[n])| = 3.(9.2^{n-1} - 5) + 2.(9.2^{n-1} - 4) = 45.2^{n-1} - 23$. Therefore, $|k(NS_4[n])| = 2^{(9.2^{n-1}-5)}$ and we have:

Theorem 10. $\alpha_4 \leq E(NS_4[n]) \leq \beta_4$, where

$$\alpha_4 = \sqrt{2m + n(n-1)K^{4/n}}$$

$$= \sqrt{105.2^n - 132 + 2304.1048576^{(-1/n)}.(512^{2^{n-1}})^{4/n}.4^n - 5808.1048576^{(-1/n)}.(512^{2^{n-1}})^{4/n}.2^n + 3660.1048576^{(-1/n)}.(512^{2^{n-1}})^{4/n}}$$

$$\beta_4 = \sqrt{2mn} = 3\sqrt{560 \cdot 4^n - 1404 \cdot 2^n + 880}.$$

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