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THE RANDIĆ INDEX OF SOME DENDRIMER NANOSTARS†

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ABSTRACT. Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application, Randić index is one of them. The dendrimer nanostars is a synthesized molecule built up from branched unit called monomers. In this article, we compute the Randić index of two types of polymer dendrimers and a fullerene dendrimer.

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1. Introduction

Let G be a simple graph and consider the m-connectivity index

$$^m\chi(G) = \sum_{i_1 - i_2 - \cdots - i_{m+1}} 1/\sqrt{d_{i_1} d_{i_2} \cdots d_{i_m}} \tag{1}$$

where $i_1 - i_2 - \cdots - i_{m+1}$ runs over all paths of length m in G and d_i denotes the degree of the vertex i. Randić introduced the Randić index as

$$^1\chi(G) = \sum_{i-j} 1/\sqrt{d_i d_j} \tag{2}$$

where $i - j$ ranging over all pairs of adjacent vertices of G. This index has been successfully correlated with physico-chemical properties of organic molecules. Indeed if G is the molecular graph of a saturated hydrocarbon then there is a strong correlation between $^1\chi(G)$ and the boiling point of the substance. [8-12]

There is no universal valance Randić index that would apply to all properties of dendrimers nanostars, but general topological indices are considered in our present work.

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2. Introduction and Preliminaries

Consider a graph G on n vertices, where $n \geq 2$. The maximum possible vertex degree in such graph is $n-1$. Suppose x_{ij} denotes the number of edges of G connecting vertices of degrees i and j. Clearly, $x_{ij} = x_{ji}$. Then Randić index can be written as

$$\chi(G) = \sum_{1 \leq i \leq j \leq n} \frac{1}{\sqrt{d_i d_j}}. \tag{3}$$

Therefore, if the graph G consists of components $G_1, G_2, \cdots, G_p$ then [12-13]

$$\chi(G) = \chi(G_1) + \cdots + \chi(G_p). \tag{4}$$

We now consider three infinite classes $NS_1[n], NS_2[n]$ and $NS_3[n]$ of dendrimer nanostars, Figures 1-3.

3. Main results

The aim of this section is to compute the Randić index of these dendrimer nanostars.

3.1. The Randić Index of the First Class of Dendrimer Nanostars. Consider the molecular graph $G(n) = NS_1[n]$, where n is steps of growth in this type of dendrimer nanostars, see Figure 1.

Define, x_{23} to be the number of edges connecting the vertex of degree 2 with a vertex of degree 3, x_{13} to be the number of edges connecting a vertex of degree 1 with a vertex of degree 3, x_{22} to be the number of edges connecting two vertices of degree 2 and x_{33} to be the number of edges connecting two vertices of degree 3. The molecular graph of $NS_1[n]$, has three similar branches with the same number x'_{23} of edges connecting a vertex of degree 2 with a vertex of degree 3. It is obvious that $x_{23} = 3x'_{23} + 48$.

On the other hand, a simple calculation shows that $x'_{23} = 9(2^{n+1}-2) - 2^{n+1}$. Therefore, $x_{23} = 3 \cdot 9(2^{n+1}-2) - 2^{n+1} + 48 = 6(2^{n+3}-1)$.

Using a similar argument, one can see that, $x_{22} = 2^{n+1} - 2$ and so, $x_{22} = 3x'_{22} + 12 = 6(2^n + 1)$.

A similar calculation as above shows that, $x_{33} = 24, x'_{13} = 2^{n+1}$ so, $x_{13} = 3x'_{13} + 3 = 3(2^{n+1}+1)$.

Theorem 1. *The Randić index of $G(n) = NS_1[n]$ is*

$$\chi(G) = (8\sqrt{6} + 2\sqrt{3} + 3)2^n + (11 + \sqrt{3} - \sqrt{6}).$$

Proof. Since $NS_1[n]$ has three similar branches, therefore by formula (3) one can write

$$\begin{aligned}\chi(G(n)) &= \frac{6(2^{n+3}-1)}{\sqrt{2\cdot 3}} + \frac{6(2^n+1)}{\sqrt{2\cdot 2}} + \frac{24}{\sqrt{3\cdot 3}} + \frac{3(2^{n+1}+1)}{\sqrt{1\cdot 3}} \\ &= \frac{6(2^{n+3}-1)}{\sqrt{6}} + 3(2^n+1) + 8 + \sqrt{3}(2^{n+1}+1)\end{aligned}$$

$$= (8\sqrt{6} + 2\sqrt{3} + 3)2^n + (11 + \sqrt{3} - \sqrt{6})$$

□

3.2. The Randić Index of the Second Class of Dendrimer Nanostars. We now consider the second class $H(n) = NS_2[n]$, where n is steps of growth in this type of dendrimer nanostar, Figure 2. Suppose y_{23} is the number of edges of $H(n)$ connecting a vertex of degree 2 with a vertex degree 3, y_{22} the number of edges of $H(n)$ connecting two vertices degrees 2, y_{33} the number of edges connecting two vertices degrees 3 and y_{12} to be the number of edges connecting a vertex of degree 1 with a vertex of degree 2. By a routine calculation, one can prove $y_{23} = 66(2^{n-1} - 1) + 48$ and so $y_{22} = 54 \cdot 2^{n-1} - 24$ and $y_{33} = 3 \cdot 2^{n+1}$ and finally $y_{12} = 3 \cdot 2^n$.

Theorem 2. *The Randić index of $H(n) = NS_2[n]$ is*

$$\chi(H(n)) = 2^{n-1}(11\sqrt{6} + 4\sqrt{3} + 3\sqrt{2}) - (3\sqrt{6} + 12)$$

Proof. Since $NS_2[n]$ has three similar branches therefore,

$$\chi(H(n)) = \frac{66(2^{n-1} - 1) + 48}{\sqrt{2 \cdot 3}} + \frac{3(2^{n+1})}{\sqrt{3 \cdot 3}} + \frac{54 \cdot 2^{n-1} - 24}{\sqrt{2 \cdot 2}} + \frac{3(2^n)}{\sqrt{2 \cdot 1}}$$
$$= \frac{(66(2^{n-1} - 1) + 48)\sqrt{6}}{6} + 3(2^n + 1) + 8 + 2^{n+1}\sqrt{3}$$

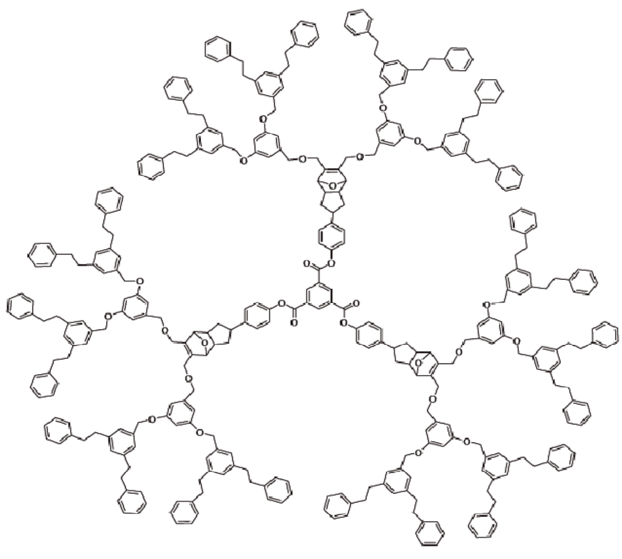

FIGURE 1. Polymer Dendrimer

$$
\begin{aligned}
&+ 27 \cdot 2^{n-1} - 12 + \frac{3\sqrt{2}}{2} \cdot 2^{n} \\
&= 8\sqrt{6} + 11\sqrt{6} \cdot 2^{n-1} - 11\sqrt{6} + 4\sqrt{3} \cdot 2^{n-1} \\
&+ 27 \cdot 2^{n-1} - 12 + 3\sqrt{2} \cdot 2^{n-1} \\
&= 2^{n-1}(11\sqrt{6} + 4\sqrt{3} + 3\sqrt{2}) - (3\sqrt{6} + 12)
\end{aligned}
$$

□

3.3. The Randić Index of the Third Class of Dendrimer Nanostars. At the end of this paper, we consider the molecular graph $K(n) = NS_3[n]$, Figure 3, where n is steps of growth. Define, t_{23} to be the number of edges connecting a vertex of degree 2 with a vertex of degree 3, t_{22} to be the number of edges connecting two vertices of degree 2, t_{13} to be the number of edges connecting a vertex of degree 1 with a vertex of degree 3, t_{33} to be the number of edges connecting two vertices of degree 3, t_{34} to be the number of edges connecting a vertex of degree 3 with a vertex of degree 4 and finally, t_{44} is the number of edges connecting two vertices of degree 4. A similar calculation as above shows t_{33} is all the edges of fullerene except 4 so $t_{33} + 90 - 4 = 36$ and $t_{34} = 6$ and finally $t_{44} = 3$. The molecular graph $NS_3[n]$ has two similar branches and so it is enough to compute the t_{23}, t_{22}. We have, $t_{23} = 32 \cdot 2^{n-1} - 8$ and finally $t_{22} = 2^{n+1} + 2$.

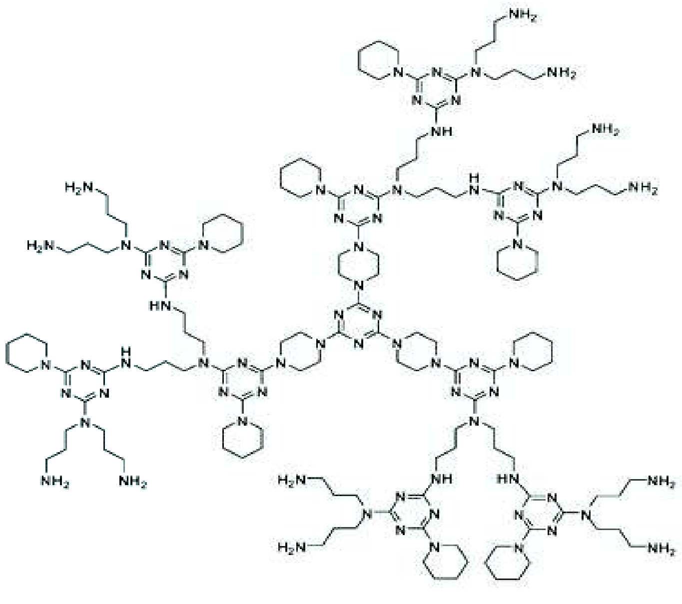

FIGURE 2. Polymer Dendrimer

Theorem 3. *The Randić index of $K(n) = NS_3[n]$ is*

$$\chi(K(n)) = 2^n\left(\frac{32\sqrt{6}+2\sqrt{3}+3}{3}\right)+\left(\frac{365-16\sqrt{6}+12\sqrt{3}}{12}\right).$$

Proof. Since $NS_3[n]$ has two similar branches therefore,

$$\begin{aligned}\chi(K(n)) &= \frac{2^{n+1}}{\sqrt{1\cdot 3}}+\frac{32\cdot 2^{n-1}-8}{\sqrt{3\cdot 2}}+\frac{2^{n+1}+2}{\sqrt{2\cdot 2}}+\frac{86}{\sqrt{3\cdot 3}}+\frac{6}{\sqrt{3\cdot 4}}+\frac{3}{\sqrt{4\cdot 4}}\\ &= \frac{\sqrt{3}2^{n+1}}{3}+\frac{\sqrt{6}(32\cdot 2^{n-1}-8)}{6}+\frac{2^{n+1}+2}{2}+\frac{86}{3}+\frac{6}{2\sqrt{3}}+\frac{3}{4}\\ &= 2^n 2^n\left(\frac{32\sqrt{6}+2\sqrt{3}+3}{3}\right)+\left(\frac{365-16\sqrt{6}+12\sqrt{3}}{12}\right).\end{aligned}$$

□

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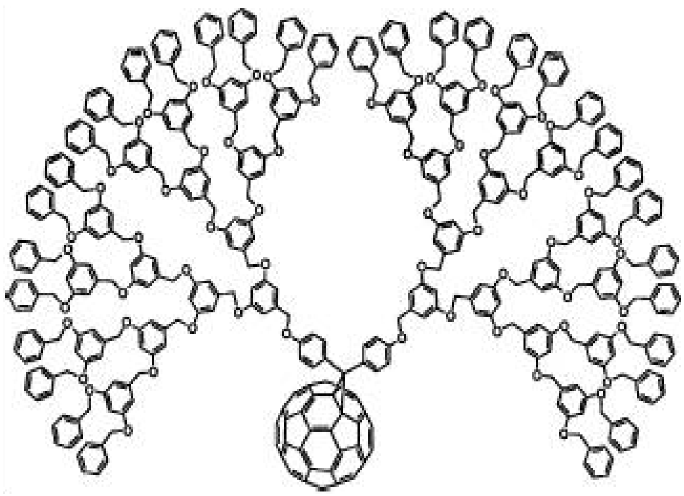

FIGURE 3. Fullerene Dendrimer

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