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THE SECOND-ORDER CONNECTIVITY INDEX OF DENDRIMER NANOSTARS

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A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. In this paper we compute the second-order connectivity indices of PAMAM dendrimer and G_3 dendrimer.[1,2]

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1. Introduction

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. The endgroup (i.e., the groups reaching the outer periphery) can be functionalized, thus modifying their physico-chemical or biological properties. Dendrimers 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. We encourage the reader to consult papers by A. R. Ashrafi et al., M. B. Ahmadi et al. and M. V. Diudea and his coauthors.[6-14]

Dendrimers have been also studied from the topological point of view, including vertex and fragment enumeration and calculation of some topological descriptors, such as topological indices, sequences of numbers or polynomials.

Let G be a simple connected graph of order n. The $m-$connectivity index ${}^m\chi_\alpha(G)$ of an organic molecule whose molecular graph is G, is the sum of weights $(d_{i_1}d_{i_2}\ldots d_{i_{m+1}})^\alpha$, where $i_1-i_2-\ldots-i_{m+1}$ runs over all paths of length m in G and d_i denotes the degree of vertex v_i. The connectivity index of an organic molecule whose molecular graph is G is defined by:

$$^1\chi_\alpha(G)=\sum_{u-v}(d(u)d(v))^\alpha$$

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where $d(u)$ denotes the degree of the vertex u of the molecular graph G, where the summation goes over all pairs of adjacent vertices of G and where $\alpha\,(\alpha \neq 0)$ is a pertinently chosen exponent. In 1975, Randić introduced the respective structure-descriptor for $\alpha \neq -\frac{1}{2}$ (which he called the branching index, and is now also called the Randić index) in his study of alkanes. The Randić index is defined as:

$$\chi = \chi(G) = \sum_{uv \in E(G)} 1/\sqrt{d_u d_v}$$

In particular, 2-connectivity index is defined as follows:

$$^{2}\chi(G) = \sum_{i_1-i_2-i_3} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}}$$

In this article we compute the 2-connectivity index of two classes of nanostars which are known as PAMAM dendrimer and G_3 dendrimer in literatures.[1, 2] See Figures 1 and 2. Poly (amido amido) (PAMAM) dendrimers represent an exciting new class of macromolecular architecture called “dense star’’ Polymers.

2. Main results and discussion

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} denote the number of edges of G connecting vertices of degrees i and j. Clearly, $x_{ij} = x_{ji}$. Then Randic index can be written as $\chi(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{x_{ij}}{\sqrt{ij}}$.

Besides, we have 2-connectivity index as

$$^{2}\chi(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{x_{ijk}}{\sqrt{ijk}},$$

where x_{ijk} is as the number of 2-edges paths with 3 vertices of degree i, j and k respectively. It is clear that $x_{ijk} = x_{kji}$.[3-6]

Here we consider two infinite classes $NS_1[n]$ and $NS_2[n]$ of dendrimer nanostars, Figures 1and 2. The aim of this two subsections is to compute the 2-connectivity indices of these dendrimer nanostars.[7,8]

2.1 *The 2-Connectivity Index of the First Class of Dendrimer Nanostars*

To compute the 2-connectivity index of the molecular graph of $G(n) = NS_1[n]$, first we define x_{322} to be the number of edges connecting the three vertices of degree 3, 2 and 2, x_{221} to be the number of edges connecting the three vertices of degree 2, 2 and 1, x_{222} to be the number of edges connecting three vertices of degree 2, x_{231} to be the number of edges connecting the three vertices of degree 2, 3 and 1. x'_{322} to be the number of edges connecting the three vertices of degree 3, 2 and 2. It is obvious that $x_{322} = 3x'_{322} + 3$. On the other hand, a simple calculation shows that $x'_{322} = 3(2^n - 1) + 5(2^{n-1} - 1) + 1$ so $x_{322} = 9(2^n - 1) + 15(2^{n-1} - 1) + 3 + 3 = 9.2^n + 15.2^{n-1} - 18$. Using a similar argument, one can see that $x'_{221} = 2^{n-1}$ then $x_{221} = 3x'_{221} = 3.2^{n-1}$ and we have $x'_{222} = 2^n - 1$ so $x_{222} = 3x'_{222} = 3(2^n - 1)$. A similar calculation as above shows that $x'_{231} = 2(2^n - 1)$ and so $x_{231} = 3x'_{231} = 6(2^n - 1)$.

Theorem 1. The 2-connectivity index of $G(n) = NS_1[n]$ is computed as follows:

$$ {}^2\chi(G(n)) = 2^n \left(\frac{11\sqrt{3} + 3\sqrt{2} + 4\sqrt{6} + 3}{4}\right) - \left(3\sqrt{3} + \sqrt{6} + \frac{3\sqrt{2}}{4}\right) $$

Proof. From the figure 1 we see that $NS_1[n]$ has three similar branches, therefore we have,

$$ \begin{aligned} {}^2\chi(G(n)) &= \frac{9.2^n + 15.2^{n-1} - 18}{\sqrt{3.2.2}} + \frac{3.2^{n-1}}{\sqrt{2.2.1}} + \frac{3.2^n - 3}{\sqrt{2.2.2}} + \frac{6.2^n - 6}{\sqrt{2.3.1}} \\ &= \frac{9\sqrt{3}}{6}2^n + \frac{15\sqrt{3}}{6}2^{n-1} - \frac{18\sqrt{3}}{6} + \frac{3.2^{n-1}}{2} + \frac{3\sqrt{2}}{4}2^n - \frac{3\sqrt{2}}{4} + \frac{6\sqrt{6}}{6}2^n - \frac{6\sqrt{6}}{6} \\ &= 2^n \left(\frac{11\sqrt{3} + 3\sqrt{2} + 4\sqrt{6} + 3}{4}\right) - \left(3\sqrt{3} + \sqrt{6} + \frac{3\sqrt{2}}{4}\right) \end{aligned} $$

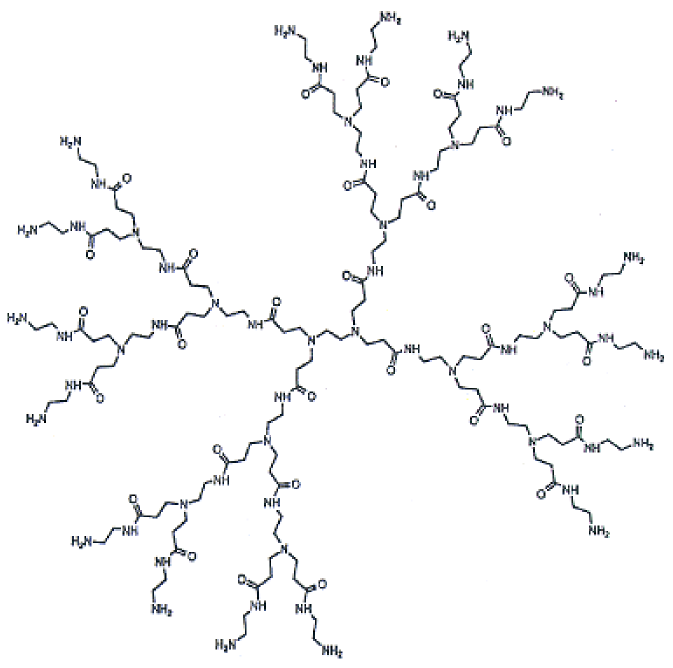

Fig. 1. PAMAM dendrimer

2.2 *The 2-Connectivity Index of the seconed Class of Dendrimer Nanostars*

Here we consider the second class $H(n) = NS_2[n]$, where n is steps of growth in this type of dendrimer nanostar, see Figure 2. Now for computing the 2-connectivity index of the molecular graph of $H(n) = NS_2[n]$ we define y_{422} to be the number of edges connecting the 3 vertex of degree 4, 2 and 2, y_{221} to be the number of edges connecting the 3 vertex of degree 2, 2 and 1, y_{222} to be the number of edges connecting three vertices of degree 2. A similar calculation as above shows that $y_{422} = 20.3^{n-1} - 10,\ y_{222} = 8(3^n - 1),\ y_{221} = 4.3^{n-1}.$

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

$$^2\chi(H(n)) = 3^{n-1}(7 + 6\sqrt{2}) - (2\sqrt{2} + \frac{5}{2})$$

Proof. Since $NS_2[n]$ has four similar branches, as it is easily seen, therefore we can write,

$$\begin{aligned} ^2\chi(H(n)) &= \frac{20.3^{n-1} - 10}{\sqrt{4.2.2}} + \frac{8(3^n - 1)}{\sqrt{2.2.2}} + \frac{4.3^{n-1}}{\sqrt{2.2.1}} \\ &= 5.3^{n-1} - \frac{10}{4} + 2\sqrt{2}.3^n - 2\sqrt{2} + 2.3^{n-1} \\ &= 3^{n-1}(7 + 6\sqrt{2}) - (2\sqrt{2} + \frac{5}{2}) \end{aligned}$$

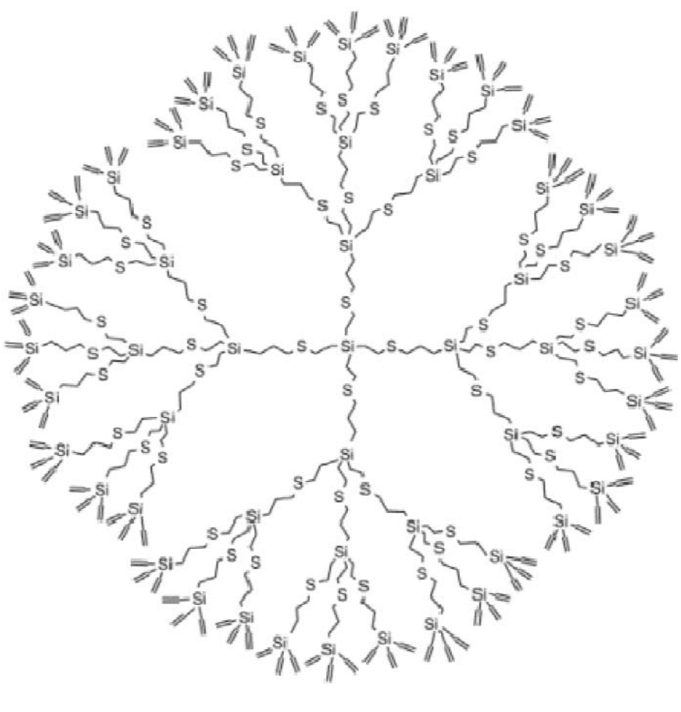

Fig. 2. G_3 dendrimer

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