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2-CONNECTIVITY INDEX AND ITS COMPUTATION FOR TWO KINDS OF NANOSTARS

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ABSTRACT. Dendrimers are highly branched organic macromo-lecules with successive layers or generations of branch units surrounding a central core [1]. These are key molecules in nanotechnology and can be used, e.g., in medicine as drug carrier molecules or contrast agents. In this article, we compute the 2-connectivity indices of three infinite classes of dendrimers.

Keywords: *Connectivity index, Randić index, Second-order Connectivity, dendrimer nanostars.*

INTRODUCTION

Molecular connectivity indices are associated to the molecular accessibility. The first and second-order connectivity indices model molecular accessibility areas and volumes, respectively, whereas the higher order indices represent magnitudes in higher dimensional spaces [2].

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

$$^{m}\chi\,(G) = \sum_{i_1..to..i_{m+1}} \frac{1}{\sqrt{d_{i_1} d_{i_2} \dots d_{i_{m+1}}}}$$

where $i_1, i_2, \dots, i_{m+1}$ runs over all paths of length *m* in *G* and d_i denotes the degree of the vertex *i*. In particular, 2-connectivity index is defined as follows:

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

Milan Randić introduced the branching index (now called Randić index) as,

$$^{1}\chi(G) = \chi(G) = \sum_{i,j} \frac{1}{\sqrt{d_i d_j}}$$

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where *i,j* range 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 $\chi(G)$ and the boiling point of the substance [3, 4, 5].

Dendrimer is a synthetic 3-dimentional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. 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., M. Ghorbani et al. and M. V. Diudea et al. [6-14]. In this article we compute the 2-connectivity index for two types of dendrimer nanostars.

RESULTS AND DISCUSSION

Consider a graph *G* on *n* vertices, where *n*≥*2*. The maximum possible vertex degree in such graph is *n-1*. Define d_{ijk} as the number of 2-edges paths with 3 vertices of degree *i, j* and *k* respectively. It is clear that $d_{ijk} = d_{jik} = d_{kij} = d_{jki} = d_{ikj}$, then

$$^{2}\chi\,(G) = \sum_{1\le i\le j\le k\le n-1} \frac{d_{ijk}}{\sqrt{ijk}} \qquad (1)$$

We now consider two infinite classes $NS_1[n]$ and $NS_2[n]$ of dendrimer nanostars, of type Polyamidoamine (PAMAM) and Polypropylen-iminoctamine, respectively, Figures 1 and 2.

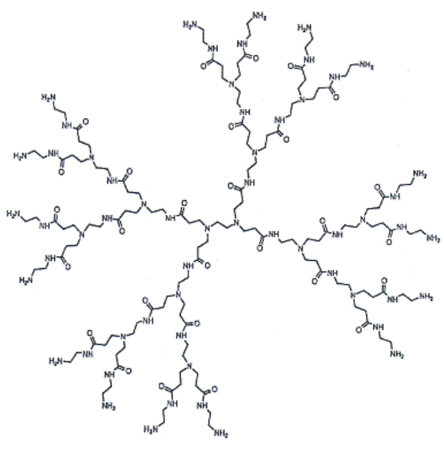

Figure 1. PAMAM Dendrimer

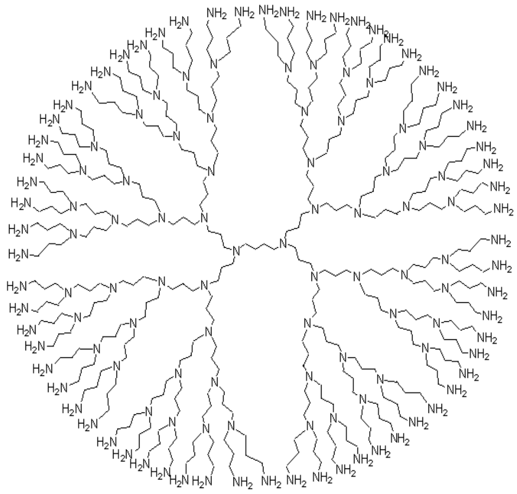

Figure 2. Polypropyleniminoctamine Dendrimer

The aim of this section is to compute the 2-connectivity index of these dendrimer nanostars.

For computing this index of the molecular graph of $G(n) = NS_1[n]$, where *n* represents the steps of growth in this type of dendrimer nanostar (Figure 1), define y_{123} to be the number of 2-edges paths with 3 vertices of degree 1, 2 and 3, y_{223} to be the number of 2-edges paths with two vertices of degree 2 and a vertex of degree 3, y_{222} to be the number of 2-edges paths with three vertices of degree 2, and y_{122} to be the number of 2-edges paths with a vertex of degree 1 and two vertices of degree 2. Since $NS_1[n]$ has four similar branches and three extra edges for *n=1 we have*,

$$y_{ijk} = \begin{cases} 4, & ijk = 122 \\ 8, & ijk = 123 \\ 8, & ijk = 222 \\ 24, & ijk = 223 \end{cases}$$

for n=2, we have

$$y_{ijk} = \begin{cases} 8, & ijk = 122 \\ 24, & ijk = 123 \\ 12, & ijk = 222 \\ 64, & ijk = 223 \end{cases}$$

and for n=3, we get

$$y_{ijk} = \begin{cases} 16, & ijk = 122 \\ 56, & ijk = 123 \\ 28, & ijk = 222 \\ 144, & ijk = 223 \end{cases}$$

In Figures 3 and 4 below, one branch of PAMAM dendrimer and the generation for n=1 is shown:

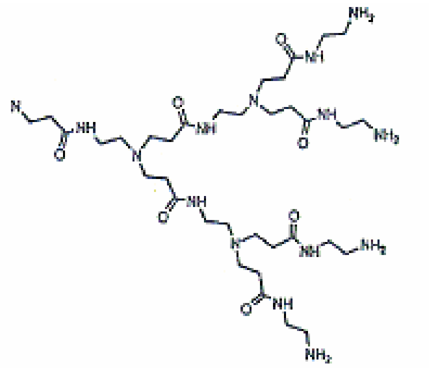

Figure 3. One branch of PAMAM dendrimer

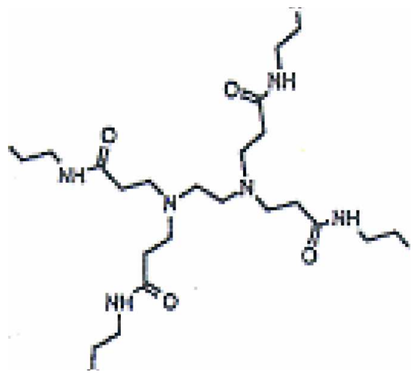

Figure 4. PAMAM dendrimer $NS_1[n]$ at generation n=1

By induction argument and a simple calculation, one can prove that $y_{123} = 2\cdot 2^n$, $y_{123} = 8\cdot 2^n - 8$, $y_{222} = 4\cdot 2^n - 4$ and $y_{223} = 20\cdot 2^n - 16$. Now we have the following result:

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

$$^2\chi(G) = (\frac{4}{3}\sqrt{6} + \frac{10}{3}\sqrt{3} + \sqrt{2} + 1)2^n - (\frac{4}{3}\sqrt{3} + \frac{10}{3}\sqrt{6} + \sqrt{2})$$

Proof. According to (1) and the above calculations we have

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

$$= \frac{2.2^n}{\sqrt{1.2.2}} + \frac{4.2^n - 4}{\sqrt{2.2.2}} + \frac{8.2^n - 8}{\sqrt{1.2.3}} + \frac{20.2^n - 16}{\sqrt{2.2.3}}$$

$$= (\frac{4}{3}\sqrt{6} + \frac{10}{3}\sqrt{3} + \sqrt{2} + 1)2^n - (\frac{4}{3}\sqrt{3} + \frac{10}{3}\sqrt{6} + \sqrt{2})$$

And we get the result.

For computing 2-connectivity index of the second class of dendrimer nanostars, we consider $H(n) = NS_2[n]$ with four similar branches and five extra edges, *n* represents the steps of growth of this dendrimer nanostar (Figure 2).

In Figures 5 and 6 below, one branch is shown and the dendrimer at generation n=1:

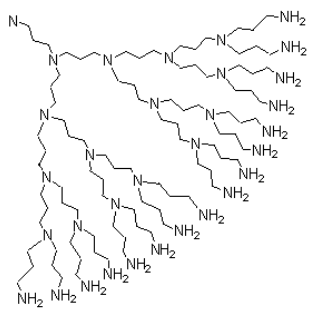

Figure 5. One branch of polypropyleniminoctamin dendrimer

Figure 6. Polypropyleniminoctamin dendrimer $NS_2[n]$ at generation n=1

Again, define z_{223} to be the number of 2-edges paths with two vertices of degree 2 and a vertex of degree 3, z_{222} to be the number of 2-edges paths with three vertices of degree 2, and z_{122} to be the number of 2-edges paths with a vertex of degree 1 and two vertices of degree 2. For n=1 we have:

$$z_{ijk} = \begin{cases} 4, & ijk = 122 \\ 6, & ijk = 222 \\ 12, & ijk = 223 \end{cases}$$

for n=2 we have:

$$z_{ijk} = \begin{cases} 8, & ijk = 122 \\ 14, & ijk = 222 \\ 36, & ijk = 223 \end{cases}$$

and finally for n=3 we get:

$$z_{ijk} = \begin{cases} 16, & ijk = 122 \\ 30, & ijk = 222 \\ 84, & ijk = 223 \end{cases}$$

Using a similar argument as in theorem 1, one can see that $z_{122} = 2.2^n$, $z_{222} = 4.2^n - 2$, and $z_{223} = 12.2^n - 12$.

Now we can state the final result.

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

$$^2\chi\,(H[n]) = (2\sqrt{3} + \sqrt{2} + 1)2^n - (\frac{\sqrt{2}}{2} + 2\sqrt{3})$$

Proof. Using formula (1) above and some simple calculations we see that

$$^2\chi\,(H[n]) = \sum_{1 \le i \le j \le k \le n-1} \frac{z_{ijk}}{\sqrt{ijk}}$$

$$= \frac{2.2^n}{\sqrt{1.2.2}} + \frac{4.2^n - 2}{\sqrt{2.2.2}} + \frac{12.2^n - 12}{\sqrt{2.2.3}}$$

$$= (2\sqrt{3} + \sqrt{2} + 1)2^n - (\frac{\sqrt{2}}{2} + 2\sqrt{3})$$

and the result is obtained.

In Table 1, the 2-connectivity indices of $NS_1[n]$ and $NS_2[n]$ arecomputed for n=1,…, 10.

Table1. *Computing 2-connectivity index for dendrimers* $NS_1[n]$ *and* $NS_2[n]$

n	***2-connectuvity index of NS₁[n]***	***2-connectuvity index of NS₂[n]***
1	12.5618	7.5854
2	35.5592	19.3421
3	81.3740	42.8553
4	173.0037	89.8818
5	356.2629	183.9349
6	722.7814	372.0410
7	1455.8000	748.2531
8	2921.9000	1500.7000
9	5854.0000	3005.5000
10	11718.0000	6015.2000

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