Digest Journal of Nanomaterials and Biostructures Vol. 4, No.2, June 2009, p. 269 – 273

CONNECTIVITY INDEX OF THE FAMILY OF DENDRIMER NANOSTARS

ALI REZA ASHRAFI*, PARISA NIKZAD
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran

The nanostar dendrimer is a synthesized molecule built up from branched unit called monomers. In this paper, we focus our attention to achieve Randic index of infinite family of nanostar dendrimers.

(Received March 20, 2009; accepted April 4, 2009)

Keyword: Connectivity index, dendrimer nanostars.

1. Introduction

Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application, connectivity index is one of them. In this article many attempt have been made to compute this index for three types of dendrimer nanostars. 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.[1] We encourage the readers to consult papers by one of us (ARA)[2-9] and papers by Diudea and his co-authors[10-14] for background materials, as well as basic computational techniques.

Let G be a simple graph and consider the m-connectivity index ${}^{m}\chi(G) = \sum_{i_1-i_2-\ldots-i_{m+1}} 1/\sqrt{d_{i_1}d_{i_2}\ldots d_{i_m}}$, 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 the vertex i. Randic[15] introduce the 1-connectivity index (now called Randic index) as ${}^{1}\chi(G) = \sum_{i-j} 1/\sqrt{d_i d_j}$, where i-j ranging over all pairs of adjacent vertices of G. This index has been successfully correlated with physo-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.[17-21]

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

2. Main results and discussion

Considered a graph G on n vertices, $n \geq 2$. The maximum possible vertex degree in such a graph is n-1. Suppose d_{ij} denote the number of edges of G connecting vertices of degrees i and j. Clearly, $d_{ij} = d_{ji}$. Then 1-connectivity index can be written as $\chi(G) = \sum_{1 \leq i \leq j \leq n-1} \frac{d_{ij}}{\sqrt{ij}}$. Therefore, if the graph G consists of components $G_1, G_2, \ldots, G_p$ then $\chi(G) = \chi(G_1) + \chi(G_2) + \ldots + \chi(G_p)$.

We now consider three infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ of dendrimer nanostars, Figures 1-3. The aim of this section is to compute the connectivity index of these dendrimer nanostars.

2.1 Connectivity Index of the First Class of Dendrimer Nanostars

Consider the molecular graph of $G(n) = NS_1[n]$, 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 a vertex of degree 2 with a vertex of degree 3 and x_{22} to be the number of edges connecting two vertices of degree 2. 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 $x_{23} = 3x'_{23}$. On the other hand a simple calculation shows that $x'_{23} = 6.2^n - 4$. Therefore, $x_{23} = 3(6.2^n - 4) = 18.2^n - 12$. Using a similar argument, one can see that $x'_{22} = 3.2^n + 1$ and then $x_{22} = 3(3.2^n + 1) = 9.2^n + 3$.

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

$$\chi(G(n)) = 2 + \frac{\sqrt{3}}{2} + 3\sqrt{3}.2^{(n+1/2)} - 2\sqrt{6} + 9.2^{(n-1)}.$$

Proof. Since $NS_1[n]$ has three similar branches and four extras edges that one of them degree 3 and 4, so $x_{14} = 1$ and $x_{34} = 3$. Therefore,

$$\begin{aligned}\chi(G(n)) &= \frac{1}{\sqrt{1.3}} + \frac{3}{\sqrt{3.4}} + \frac{18.2^n - 12}{\sqrt{2.3}} + \frac{9.2^n + 3}{\sqrt{2.2}} \\ &= \frac{\sqrt{3}}{3} + \frac{\sqrt{3}}{2} + \frac{18.2^n - 12}{\sqrt{6}} + \frac{9.2^n + 3}{2} \\ &= 2 + \frac{\sqrt{3}}{2} + 3\sqrt{3}.2^{(n+1/2)} - 2\sqrt{6} + 9.2^{(n-1)}\end{aligned}$$

2.2 Connectivity 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 and w_{22} is the number of edges of H[n] connecting two vertices degrees 2. The molecular graph of $NS_2[n]$ has two similar branches and so it is enough to compute the number of such edges, say z_{23}, in one branch. By a routine calculation, one can prove $z_{23} = 12.2^n - 4$ and so $y_{23} = 2(12.2^n - 4) = 24.2^n - 8$. A Similar argument shows that [n] is computed as follows:

$$\chi(G(n)) = \frac{4}{3} + 4\sqrt{6}.2^n - \frac{85}{6}\sqrt{6} + 6.2^n.$$

Proof. Since $NS_2[n]$ has two similar branches and one extras edge that connect vertices of degree 3 and 3, so $x_{33} = 1$ and we have:

$$\chi(G(n)) = \frac{1}{\sqrt{3.3}} + \frac{24.2^n - 8}{\sqrt{2.3}} + \frac{12.2^n + 2}{\sqrt{2.2}}$$

$$= \frac{1}{3} + \frac{24.2^n - 8}{\sqrt{6}} + \frac{12.2^n + 2}{2}$$
$$= \frac{4}{3} + 4\sqrt{6}.2^n - \frac{85}{6}\sqrt{6} + 6.2^n.$$

2.3 Connectivity Index of the Third Class of Dendrimer Nanostars

In the end of this paper, we consider the molecular graph of 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_{33} to be the number of edges connecting two vertices of degree 3 and t_{13} to be the number of edges connecting a vertex of degree 1 with a vertex of degree 3.

The molecular graph $NS_3[n]$ has four similar branches and so it is enough to compute the values of u_{13}, u_{23}, u_{22} and u_{33} in one branch of K(n). On the other hand, there are two edges connecting vertices of degree 2 and 3 outside these branches. A similar calculation as above shows that $u_{23} = 7.2^n - 2$ and $u_{22} = 11.2^{n-1} - 2$. Therefore, $t_{23} = 4(7.2^n - 2) + 2 = 28.2^n - 6$ and since there is one edges connecting two vertices of degree 2 outside our branches, $t_{22} = 4(11.2^{n-1} - 2) + 1 = 22.2^n - 7.$

The method for computing other two kinds of edges are similar to what is said above and we have $t_{33} = 6.2^n$ and $t_{13} = 2^{n+1}.$

Theorem 3. The connectivity index of K(n) is computed as follows:

$$\chi(G(n)) = 13.2^n + \frac{\sqrt{3}}{3}2^{n+1} + 14\frac{\sqrt{3}}{3}.2^{n+1/2} - \sqrt{6} - \frac{7}{2}.$$

Proof. Since $NS_3[n]$ has four similar branches and three extras edges, so

$$\chi(G(n)) = \frac{6.2^n}{\sqrt{3.3}} + \frac{2^{n+1}}{\sqrt{1.3}} + \frac{28.2^n - 6}{\sqrt{2.3}} + \frac{22.2^n - 7}{\sqrt{2.2}}$$
$$= \frac{6.2^n}{3} + \frac{2^{n+1}}{\sqrt{3}} + \frac{28.2^n - 6}{\sqrt{6}} + \frac{22.2^n - 7}{2}$$
$$= 13.2^n + \frac{\sqrt{3}}{3}2^{n+1} + 14\frac{\sqrt{3}}{3}.2^{n+1/2} - \sqrt{6} - \frac{7}{2}.$$

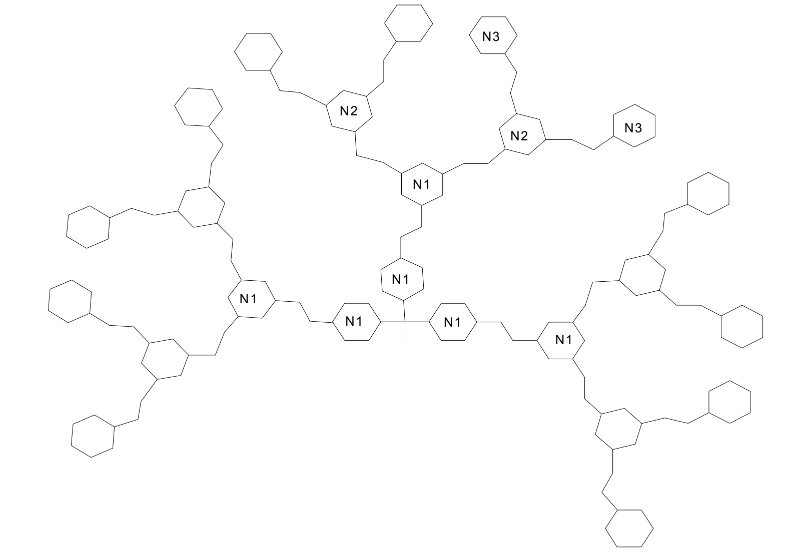

Figure 1. The Molecular Graph of $NS_1[3]$.

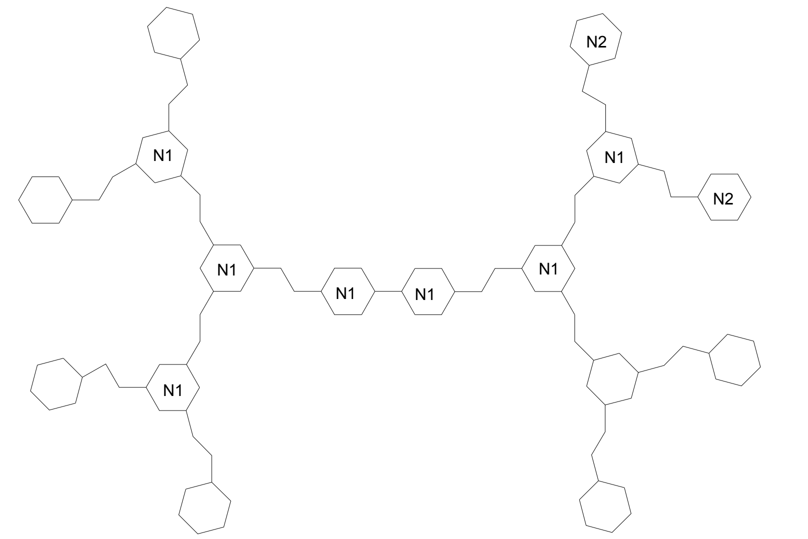

Figure 2. The Molecular Graph of $NS_2[2]$.

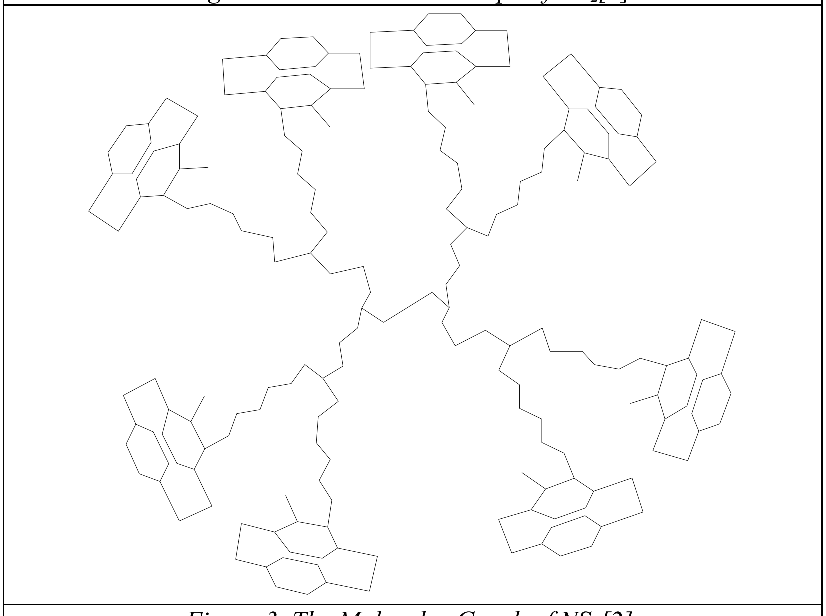

Figure 3. The Molecular Graph of $NS_2[2]$.

References

[1] G. R. Newkome, Moorefield C N & Vogtlen F, Dendrimers and Dendrons. Concepts, Syntheses, Applications (Wiley-VCH Verlag GmbH & Co. KGaA), 2002.
[2] A. R. Ashrafi, Mirzargar M., Indian J. Chem., **47A**(4), 535 (2008),.
[3] H. Yousefi-Azari, A. R. Ashrafi, M. H. Khalifeh, Digest Journal of Nanomaterials and Biostructures, **3**(4), 315 (2008).
[4] H. Yousefi-Azari, A. R. Ashrafi, M. H. Khalife, Digest Journal of Nanomaterials and Biostructures, **3**(4), 251 (2008).
[5] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Digest Journal of Nanomaterials and Biostructures, **4**(1), 63 (2009).
[6] S. Yousefi, A. R. Ashrafi, MATCH Commun. Math. Comput. Chem., **56**, 169 (2006),.
[7] S. Yousefi, A. R. Ashrafi, J. Math. Chem., **42**, 1031 (2007).
[8] S. Yousefi, A. R. Ashrafi, Current Nanoscience, **4**, 161 (2008),.
[9] A. R. Ashrafi, S. Yousefi, MATCH Commun. Math. Comput. Chem. **57**, 403 (2007),.
[10] A. R. Ashrafi, S. Yousefi, Nanoscale Res Lett., **2,** 202 (2007),.
[11] M. V. Diudea, A. Graovac, MATCH Commun. Math. Comput. Chem., **44**, 93 (2001),.
[12] M. V. Diudea, John P. E., MATCH Commun. Math. Comput. Chem., **44**, 103 (2001),.
[13] Diudea M. V., Bull. Chem. Soc. Jpn., **75**, 487 (2002),.
[14] Diudea M. V., MATCH Commun. Math. Comput. Chem., **45**, 109 (2002),.
[15] Randic, M., J. Am. Chem. Soc., **97**, 6609 (1975),.
[16] Bollobas, B., Erdos, P., Ars Combinatoria, **50**, 225 (1998).
[17] Mihali Z., Trinajstic N., J. Chem. Educ., **69**(9), 701 (1992).
[18] Morales D., Araujo O., J. Math. Chem. **13**, 95 (1993).
[19] Randic M., Hansen P. J., Jurs P.C., J. Chem. Inf. Comput. Sci., **28**, 60 (1988),.
[20] Estrada, E., Chem. Phys. Lett., **312**, 556 (1999).
[21] Estrada, E., J. Chem. Inf. Comput. Sci., **35**, 1022 (1995).