Digest Journal of Nanomaterials and Biostructures Vol. 4, No.1, March 2009, p. 155 - 157

SZEGED INDEX OF NANOSTAR DENDRIMERS

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A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper the Szeged Index of an infinite class of nanostar dendrimers are computed.

(Received January 29, 2009; accepted February 13, 2009)

Keywords: Nanostar dendrimer, Szeged Index

1. Introduction

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. In such a graph, vertices represent atoms and edges represent bonds. The graph G is said to be connected if for every vertices x and y in V(G) there exists a path connecting x and y. The distance d(u,v) between vertices u and v of a connected graph G is the number of edges in a minimum path from u to v. A topological index is a real number related to a molecular graph, which is a graph invariant. There are several topological indices already defined. The Wiener index W is the first topological index that was introduced in 1947 by Harold Wiener.[1] It is defined as the sum of distances between all pairs of vertices in the graph under consideration. The Szeged index is another topological index which is acquaintance with Ivan Gutman.[2-4] To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Suppose $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)}[n_u(e)n_v(e)]$. Notice that vertices equidistance from u and v are not taken into account.

Diudea[5-10] was the first scientist investigated the mathematical properties of nanostructures. He and his team considered too many nanostructures into account by computing their topological indices and counting polynomials. The first author of this paper continued the works of Diudea by computing the topological indices of some new type of nanostructures.[11-16]

Throughout this paper $G[n] = NSC_5C_6[n]$ denotes the nanostar dendrimer of Figure 1. We encourage the reader to consult papers[17,18] and book[19] for further study on this topic. Our notation is standard and taken mainly from the standard book of graph theory.

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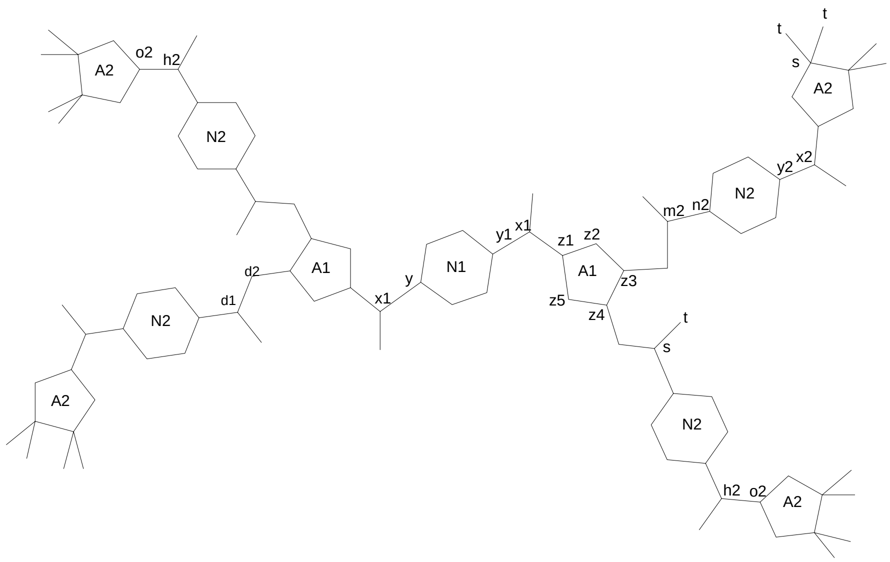

Fig. 1. The Nanostar Dendrimer NSC_5C_6 [2].

2. Main Results and discussion

The aim of this section is to compute the Szeged index of nanostar dendrimers $NSC_5C_6[n]$, depicted in Figures 1 and 2. This nanostar dendeimer has a core depicted in Figure 1. Using an inductive argument, one can show that $|V(NSC_5C_6 [n])| = 9.2^{n+2} – 44$.

We begin by computing values of $n_{u_i}(e)$ and $n_{v_i}(e)$ for an arbitrary edge $e = u_i v_i$ of the hexagon N_i, $1 \le i \le n$. Again apply an inductive argument to prove $n_{u_i}(e) = |V(G[n])| - n_{v_i}(e)$ and $n_{v_i}(e) = 9 \cdot 2^{n-i+2} - 22$. Values of other edges is computed in Table 1.

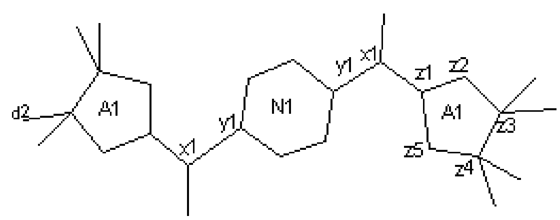

Fig.2. The Core of Nanostar Dendrimer $NSC_5C_6[n]$.

Consider the edges e = u_iv_i of pentagons A_i, $1 \le i \le n$. Then $n_{u_i}(e) = |V(G[n])| - n_{v_i}(e) - 9 \cdot 2^{n-i+1} + 15$ and $n_{v_i}(e) = 9 \cdot 2^{n-i+1} - 14$. Suppose e = u_iv_i is an edge of type z_2z_3 or z_4z_5 of pentagons A_i, $1 \le i \le n$. Then $n_{u_i}(e) = |V(G[n])| - n_{v_i}(e) - 1$ and $n_{v_i}(e) = 18 \cdot 2^{n-i+1} - 30$. To complete the investigation of of pentagons, we must consider the edge $e = z_3z_4$. A similar calculations show that $n_{u_i}(e) = n_{v_i}(e) = 9 \cdot 2^n - 14$.

Table 1. The Values of $N_u(e)$ of the Nanostar Dendrimer G[n].

Edges	The Values of $n_u(e)$
$e = uv = x_i y_i$	$n_u(e) = 18 \cdot 2^{n-i+1} - 25$
$e = uv = m_i n_i$	$n_u(e) = 9 \cdot 2^{n-i+2} - 19$
$e = uv = st$	$n_u(e) = 1$
$e = uv = o_i h_i$	$n_u(e) = 18 \cdot 2^{n-i+1} - 27$
$e = uv = d_1 d_2$ or $d_3 d_4$	$n_u(e) = 9 \cdot 2^{n-i+1} - 16$
$e = uv = g_1 g_2$	$n_u(e) = 9 \cdot 2^{n-i+1} - 17$

By computing the number of edges and some simple calculations by MAPLE, we can prove the following theorem:

Theorem. The Szeged index of the nanostar dendrimer $NSC_5C_6[n]$ is computed as $Sz(NSC_5C_6[n]) = -15846 + 41828.2^n - 21636.4^n - 4320.8^n + 2592.n.8^n - 4068.n.2^n + 11664.n.4^n$.

References

[1] H. Wiener, J. Am Chem Soc, **69,** 17 (1947).
[2] I. Gutman, Graph Theory Notes of New York, **27,** 9 (1994).
[3] M. V. Diudea and I. Gutman, Croat Chem Acta, **71,** 21 (1998).
[4] O. M. Minailiuc, G. Katona, M. V. Diudea, M. Strunje, A. Graovac and I. Gutman, Croat Chem Acta, **71,** 473 (1998).
[5] P. E. John and M. V. Diudea, Croat Chem Acta, **77**, 127 (2004).
[6] M. V. Diudea, M. Stefu, B. Pârv and P. E. John, Croat Chem Acta, **77,** 111 (2004).
[7] M. V. Diudea, B. Parv and E. C. Kirby, MATCH Commun Math Comput Chem, **47,** 53 (2003).
[8] M. V. Diudea, Bull Chem Soc Japan, **75,** 487 (2002).
[9] M. V. Diudea, MATCH Commun Math Comput Chem, **45,** 109 (2002).
[10] M .V. Diudea, P E John, MATCH Commun Math Comput Chem, **44**, 103 (2001).
[11] A. R. Ashrafi, H Saati, J Comput Theor Nanosci, **4,** 761 (2007).
[12] A. R. Ashrafi, A. Loghman, MATCH Commun Math Comput Chem, **55,** 447 (2006).
[13] A. R. Ashrafi, A Loghman, J Comput Theor Nanosci, **3,** 378 (2006).
[14] A. R. Ashrafi, Rezaei F, MATCH Commun Math Comput Chem, **57,** 243 (2007).
[15] A. R. Ashrafi, A. Loghman, Ars Combinatoria, **80,** 193 (2006).
[16] Yousefi-Azari H, Manoochehrian B & Ashrafi A R, Ars Combinatoria, **84,** 255 (2007).
[17] A. Heydari, B. Taeri B, MATCH Commun Math Comput Chem**, 57,** 463 (2007).
[18] M. Eliasi, B. Taeri, MATCH Commun Math Comput Chem, **59,** 437 (2008).
[19] Newkome G R, Moorefield C N & Vogtlen F, Dendrimers and Dendrons. Concepts, Syntheses, Applications (Wiley-VCH Verlag GmbH & Co. KGaA), 2002.