Indian Journal of Chemistry
Vol. 47A, April 2008, pp. 538-541

PI, Szeged and edge Szeged indices of an infinite family of nanostar dendrimers

Ali Reza Ashrafi* & Mahsa Mirzargar

Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I R Iran

Email: ashrafi@kashanu.ac.ir

Received 21 November 2007; revised 28 February 2008

A topological index of a graph G is a numeric quantity related to G which describes the molecular graph G. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The PI and Szeged indices of a class of nanostar dendrimer are computed.

The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. It also shows good resistant to photo bleaching. The nanostar dendrimer promises great applications but first the structure and the energy transfer mechanism must be understood. Experimental and theoretical insight is needed in order to understand the energy transfer mechanism.

Methodology

Some algebraic definitions used for the study are given. 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 a chemical graph, vertices represent atoms and edges represent bonds. These graphs have been used for affinity diagrams showing a relationship between chemical substances.

Numbers reflecting certain structural features of a molecule that are obtained from its chemical graph are usually called topological indices. The Wiener index, W, one of widely used descriptors of molecular topology, was introduced in 1947 by Wiener[1] as the half-sum of all topological distances in the hydrogen-depleted graph representing the skeleton of the molecule. Here, we denote by d(u,v), the topological distance between vertices u and v of the graph G, which is the length of a minimum path between these vertices. We encourage the readers to consult two survey articles by Dobrynin and his co-authors[2,3] and references therein for background material and historical aspect of Wiener index.

Diudea[4-10] was the first scientist who investigated the mathematical properties of nanostructures. He and his team studied several nanostructures by computing their topological indices and designed a package named TopoCluj[11] for computing topological indices of the molecular graphs of nanostructures.

Khadikar and co-authors[12-15] defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. It is defined as $PI(G) = \sum_{e=uv\in G}[m_u(e) + m_v(e)]$, where $m_u(e)$ is the number of edges of G lying closer to u than to v and $m_v(e)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted.

The Szeged index is another topological index introduced by Ivan Gutman.[16-18] 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 $Sz(G) = \sum_{e=uv\in E(G)}[n_u(e)n_v(e)]$. It may be noted that vertices equidistance from u and v are not taken into account. The edge Szeged index of G is defined similarly by $Sz_e(G) = \sum_{e=uv\in E(G)}[m_u(e)m_v(e)]$.[19]

Recently, the first author of this paper continued the pioneering work of Diudea and his team to compute PI and Szeged indices of some classes of nanostructures.[20-25] We also encourage the reader to consult papers by Iranmanesh[26-28] and Taeri[29,30] for more information on this subject. Our notation is standard and taken from literature.[31-34]

Results and discussion

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. In this section we compute PI and Szeged indices of a nanostar dendrimer NS[n], (Fig. 1). Using a simple calculation, one can show that $|V(NS[n])| = 120.2^n - 108$ and $|E(NS[n])| = 140.2^n - 127$. We begin by computing $n_u(e)$ and $n_v(e)$ for the edges $e = E_j^i$,

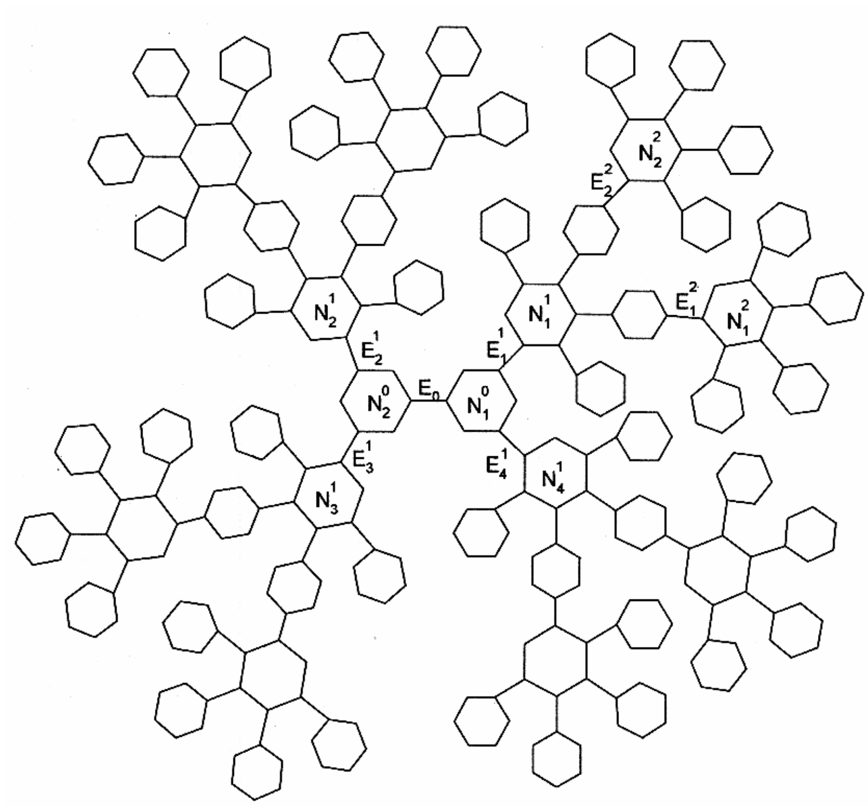

Fig. 1—The nanostar dendrimer NS[2].

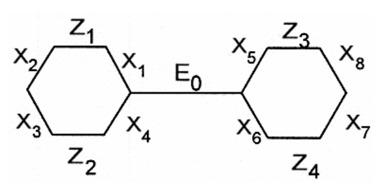

Fig. 2—A part of the core of NS[n].

$1 \leq i \leq n$, $1 \leq j \leq 2^{i+1}$ (Fig. 1). Here $e = E_i^j$ denotes an arbitrary edge connecting two branches of dendrimer NS[n]. If $e = uv = E_j^i$, $1 \leq i \leq n$, $1 \leq j \leq 2^{i+1}$ then by an inductive argument $n_u(e) = 30.(2^{n-i+1} - 1)$.

For $e=uv = E_0$, $n_u(e) = \dfrac{|V(NS[n])|}{2} = 3(5.2^{n+2} - 18)$, (Fig. 2). If $e = uv$ is an edge from two central hexagons then for eight edges $e = X_1 = a_1b_1,\ldots,X_8 = a_8b_8$ of the hexagons N_1^0 and N_2^0, $n_{a_t}(x_t) = 30(2^n - 1) +3 = 3(10.2^n - 9)$, $1 \leq t \leq 8$, and for four edges $Z_1 = c_1d_1,\ldots,Z_4 = c_4d_4$ $n_{c_s}(z_s) = 60.(2^n - 1)+3=3.(20.2^n - 19)$, $1 \leq s \leq 4$. We now consider an arbitrary hexagon N in the i[th] branch of NS[n] and assume that $e = uv \in N$, (Fig. 3). For four edges, $e = l_1=g_1h_1$, …, $l_4 = g_4h_4$, $n_{g_t}(l_t) = 60.(2^{n-i} - 1) + 21 = 60.2^{n-i} - 39$, $1 \leq t \leq 4$, and for two edges, $e = w_1 = r_1s_1$, $w_2 = r_2s_2$, $n_{r_1}(w_1) = n_{r_2}(w_2) = 30.(2^{n-i} - 1) + 15 = 30.2^{n-i} - 15$.

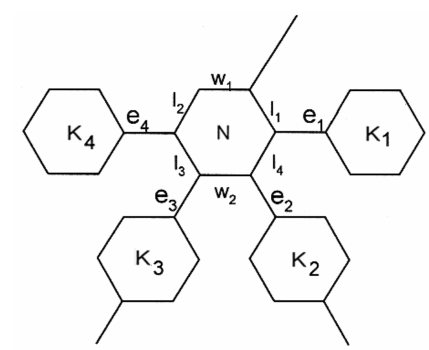

Fig. 3—A part of a branch of NS[n].

We now consider edges of the hexagons K_1 and K_4, (Fig. 3). One can see that for an arbitrary edge $e = uv$ of this type, $n_u(e) = 3$. On the other hand, for edges of the hexagons K_2 and K_3, $n_u(e) = 30.(2^{n-i} - 1) + 3 = 30.2^{n-i} - 27$. Also, for two edges $e_1 = u_1v_1$ and $e_4 = u_4v_4$, $n_{u_1}(e_1) = n_{u_4}(e_4) = 6$ and for two other edges $e_2 = u_2v_2$ and $e_3 = u_3v_3$, $n_{u_2}(e_2) = n_{u_3}(e_3) = 30.(2^{n-i}-1) + 6 = 30.2^{n-i} - 24$. Using these calculations, we have:

Theorem 1: The Szeged index of the dendrimer NS[n] is computed as follows:

$$Sz(NS[n]) = -284400.4^n + 187200.n.4^n - 75600.n.2^n + 415944\ 2^n - 131184.$$

Proof: By our calculations given above, we have:

$$
\begin{aligned}
&Sz\,(NS[n]) \\
&= \sum_{e=uv} n_u(e) n_v(e) \\
&= 9(5.2^{n+2} - 18)^2 + 180 \sum_{i=1}^{n} 2^{i+1}. \\
&\times (5.2^{n+2} - 5.2^{n-i+1} - 13)\,(2^{n-i+1} - 1) \\
&+216.(10.2^n - 9)^2 + 36(20.2^n - 19)(20.2^n - 17) \\
&+4 \sum_{i=1}^{n} 2^{i+1}\,(60.2^{n-i} - 39)(120.2^n - 60.2^{n-i} - 69) \\
&+2 \sum_{i=1}^{n} 2^{i+1}\,(30.2^{n-i} - 15)(120.2^n - 30.2^{n-i} - 93) \\
&+144.(2^n - 1)\,(120.2^n - 111) \\
&+12 \sum_{i=1}^{n} 2^{i+1}\,(30.2^{n-i} - 27)(120.2^n - 30.2^{n-i} - 81) \\
&+48.(2^n - 1)\,(120.2^n - 114) \\
&+2 \sum_{i=1}^{n} 2^{i+1}\,(30.2^{n-i} - 24)(120.2^n - 30.2^{n-i} - 84) \\
&= -284400.4^n + 187200.n.4^n - 75600.n.2^n \\
&\quad +415944.2^n - 131184,
\end{aligned}
$$

which proves the theorem.

We now compute the PI index of a nanostar dendrimer NS[n]. We begin with computing $m_u(e)$ and $m_v(e)$ for the edges $e = E_j^i$, $1 \le i \le n$, $1 \le j \le 2^{i+1}$ (Fig. 1). Suppose $e = uv = E_j^i$, $1 \le i \le n$, $1 \le j \le 2^{i+1}$. Then by an inductive argument $m_u(e) = 34.(2^{n-i+1} - 1) + (2^{n-i+1} - 2) = 35.2^{n-i+1} - 36$. For $e = uv = E_0$, $m_u(E_0) = \dfrac{|E(NS[n])| - 1}{2} = 70.2^n - 64$ and if e = uv is an edge from two central hexagons then for eight edges $X_1 = a_1b_1, \ldots, X_8 = a_8b_8$ of hexagons N_1^0 and N_2^0, $m_{a_t}(x_t) = 34(2^n - 1) + (2^n - 1) + 2 = 35.2^n - 33$, $1 \le t \le 8$, and for four edges $Z_1 = c_1d_1, \ldots, Z_4 = c_4d_4$, $m_{c_s}(z_s) = 68.(2^n - 1) + 2(2^n - 1) + 2 = 70.2^n - 68$, $1 \le s \le 4$. We now consider an arbitrary hexagon N in the i^th^ branch of NS[n], and $e = uv \in N$, (Fig. 3). For edges $e = l_1 = g_1h_1, \ldots, l_4 = g_4h_4$, $m_{g_t}(l_t) = 68.(2^{n-i} - 1) + (2^{n-i+1} - 2) + 23 = 70.2^{n-i} - 47$, $1 \le t \le 4$, and for edges $w_1 = r_1s_1$, $w_2 = r_2s_2$, we have $m_{r_1}(w_1) = m_{r_2}(w_2) = 34.(2^{n-i} - 1) + (2^{n-i+1} - 2) + 16 = 36.2^{n-i} - 20$.

Now consider Fig. 3, for edges e = uv of the hexagons K_1 and K_4, $m_u(e) = 2$ and for edges e = uv of hexagons K_2 and K_3, $m_u(e) = 34.(2^{n-i} - 1) + (2^{n-i+1} - 2) + 2 = 36.2^{n-i} - 34$. Finally, for two edges $e_1 = u_1v_1$ and $e_4 = u_4v_4$, $m_{u_1}(e_1) = m_{u_4}(e_4) = 6$ and for two edges $e_2 = u_2v_2$ and $e_3 = u_3v_3$, $m_{u_2}(e_2) = m_{u_3}(e_3) = 34.(2^{n-i} - 1) + (2^{n-i+1} - 2) + 6 = 36.2^{n-i} - 30$. Therefore,

Theorem 2: The PI index of the nanostar dendrimer NS[n] is computed as follows:
$$PI(NS[n]) = 19600.4^n - 35820.2^n + 16364.$$

Proof: By our calculations given above, we have:

$$
\begin{aligned}
PI(NS[n]) &= \sum_{e=uv} [m_u(e) + m_v(e)] \\
&= (120(2^n - 1) + 12)(140.2^n - 129) \\
&\quad + (20(2^n - 1) + 1)(140.2^n - 128) \\
&= 19600.4^n - 35820.2^n + 16364,
\end{aligned}
$$

which proves the theorem.

We are now ready to compute the edge Szeged index of a nanostar dendrimer.

Theorem 3: The edge Szeged index of the nanostar dendrimer NS[n] is computed as follows:

$$Sz_e(NS[n]) = -426332.4^n + 259280.n.4^n - 102752.n.2^n + 632456.2^n - 205872.$$

Proof: By calculations before Theorem 2, one can see that

$$
\begin{aligned}
Sz_e(NS[n]) &= \sum_{e=uv} [m_u(e) m_v(e)] \\
&= (70.2^n - 64)^2 + \sum_{i=1}^{n} 2^{i+1}.(35.2^{n-i+1} - 36) \\
&\times (140.2^n - 35.2^{n-i+1} - 92) \\
&+ 8(35.2^n - 33)(105.2^n - 96) \\
&+ 4(70.2^n - 68)(70.2^n - 61) \\
&+ 4 \sum_{i=1}^{n} 2^{i+1}(70.2^{n-i} - 47)(140.2^n - 70.2^{n-i} - 82) \\
&+ 2 \sum_{i=1}^{n} 2^{i+1}.(36.2^{n-i} - 20)(140.2^n - 36.2^{n-i} - 109) \\
&+ 96(2^n - 1)(140.2^n - 131) \\
&+ 12 \sum_{i=1}^{n} 2^{i+1}.(36.2^{n-i} - 34)(140.2^n - 36.2^{n-i} - 95) \\
&+ 48(2^n - 1)(140.2^n - 134) \\
&+ 2 \sum_{i=1}^{n} 2^{i+1}(36.2^{n-i} - 30)(140.2^n - 36.2^{n-i} - 98) \\
&= 426332.4^n + 259280.n.4^n - 102752.n.2^n \\
&+ 632456.2^n - 205872,
\end{aligned}
$$

proving our theorem.

Acknowledgement

This research was in part supported by a grant from the Center of Excellence of Algebraic Methods and Applications of Isfahan University of Technology.

References

1 Wiener H, *J Am Chem Soc,* 69 (1947) 17.
2 Dobrynin A A, Entringer R & Gutman I, *Acta Appl Math,* 66 (2001) 211.
3 Dobrynin A A, Gutman I, Klavzar S & Zigert P, *Acta Appl Math*, 72 (2002) 247.
4 John P E & Diudea M V, *Croat Chem Acta*, 77 (2004) 127.
5 Diudea M V, Stefu M, Pârv B & John P E, *Croat Chem Acta*, 77 (2004) 111.
6 Diudea M V, Parv B & Kirby E C, *MATCH Commun Math Comput Chem,* 47 (2003) 53.
7 Diudea M V, *Bull Chem Soc Japan*, 75 (2002) 487.
8 Diudea M V, *MATCH Commun Math Comput Chem,* 45 (2002) 109.
9 Diudea M V & John P E, *MATCH Commun Math Comput Chem*, 44 (2001) 103.
10 Diudea M V & Kirby E C, *Fullerene Sci Technol*, 9 (2001) 445.
11 Diudea M V, Ursu O & Nagy Cs L, *Topocluj 2.0-Calculations in Molecular Topology*, (B-B University), 2002.
12 Khadikar P V, *Nat Acad Sci Lett*, 23 (2000) 113.
13 Khadikar P V, Kale P P, Deshpande N V, Karmarkar S & Agrawal V K, *J Math Chem*, 29 (2001) 143.
14 Khadikar P V & Karmarkar S, *J Chem Inf Comput Sci*, 41 (2001) 934.
15 Khadikar P V, Karmarkar S & Varma R G, *Acta Chim Slov*, 49 (2002) 755.
16 Diudea M V & Gutman I, *Croat Chem Acta*, 71 (1998) 21.
17 Gutman I, *Graph Theory Notes of New York,* 27 (1994) 9.
18 Minailiuc O M, Katona G, Diudea M V, Strunje M, Graovac A & Gutman I, *Croat Chem Acta,* 71 (1998) 473.
19 Gutman I & Ashrafi A R, *Croat Chem Acta*, 81 (2008) (in press).
20 Ashrafi A R & Saati H, *J Comput Theor Nanosci*, 4 (2007) 761.
21 Ashrafi A R & Loghman A, *MATCH Commun Math Comput Chem*, 55 (2006) 447.
22 Ashrafi A R & Loghman A, *J Comput Theor Nanosci*, 3 (2006) 378.
23 Ashrafi A R & Rezaei F, *MATCH Commun Math Comput Chem*, 57 (2007) 243.
24 Ashrafi A R & Loghman A, *Ars Combinatoria*, 80 (2006) 193.
25 Yousefi-Azari H, Manoochehrian B & Ashrafi A R, *Ars Combinatoria*, 84 (2007) 255.
26 Iranmanesh A & Soleimani B, *MATCH Commun Math Comput Chem*, 57 (2007) 251
27 Iranmanesh, A Soleimani B & Ahmadi A, *J Comput Theor Nanosci*, 4 (2007) 147.
28 Iranmanesh A & Ashrafi A R, *J Comput Theor Nanosci*, 4 (2007) 514.
29 Heydari A & Taeri B, *MATCH Commun Math Comput Chem*, 57 (2007) 463.
30 Eliasi M & Taeri B, *MATCH Commun Math Comput Chem*, 59 (2008) 437.
31 Knop J V, Muller W R, Szymanski K & Trinajstic N, *Computer Generation of Certain Classes of Molecules* (SKTH, Zagreb), 1985.
32 Gutman I & Polansky O E, *Mathematical Concepts in Organic Chemistry*, (Springer-Verlag, New York), 1986.
33 Mirzagar M, *Laplacian Energy of Graphs* (MSc Thesis, University of Kashan), 2007.
34 Newkome G R, Moorefield C N & Vogtlen F, *Dendrimers and Dendrons. Concepts, Syntheses, Applications* (Wiley-VCH Verlag GmbH & Co. KGaA), 2002.