

## Some Topological Indices of Nanostar Dendrimers

MODJTABA GHORBANI\* AND MAHIN SONGHORI

Department of Mathematics, Faculty of Science, Shahid Rajaei Teacher Training University, Tehran, 16785-136, I. R. Iran

(Received September 25, 2010)

### ABSTRACT

Wiener index is a topological index based on distance between every pair of vertices in a graph  $G$ . It was introduced in 1947 by one of the pioneer of this area *e.g.*, Harold Wiener. In the present paper, by using a new method introduced by Klavžar, we compute the Wiener, Szeged, GA, ABS, connectivity and Zagreb group indices of some nanostar dendrimers.

**Keywords:** Wiener index, Szeged index, Randić index, Zagreb index, ABC index, GA index, Nanostar dendrimers.

### 1. INTRODUCTION

Topological indices are numbers associated with molecular graphs for the purpose of allowing quantitative structure-activity/property/toxicity relationships. The Wiener index is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds. It has been also much researched from the purely mathematical viewpoint, giving rise to a vast corpus of literature over the last decades. A number of derivative invariants have been investigated and many formulas for particular classes of graphs were obtained. We refer the reader to a comprehensive survey of results for trees by Dobrynin, Entringer and Gutman as an illustration of that effort [1]. Typical results of such work are usually formulas expressing the Wiener index of graphs from the considered class via some other graph invariants. For trees (acyclic graphs) Wiener defined  $W$  as the sum of products

\*Author to whom correspondence should be addressed.(e-mail:mghorbani@srttu.edu)

of the numbers of vertices on the two sides of each edge; for more details about Wiener index see [2 - 5]. Here our notation is standard and mainly taken from standard books of graph theory such as, e.g., [6]. All graphs considered in this paper are simple and connected.

The vertex and edge sets of a graph  $G$  are denoted by  $V(G)$  and  $E(G)$ , respectively. The distance  $d_G(x, y)$  between two vertices  $x$  and  $y$  of  $V(G)$  is defined as the length of any shortest path in  $G$  connecting  $x$  and  $y$ . The Wiener index  $W(G)$  of a graph  $G$  is defined as [7]

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v).$$

The Szeged index is another topological index which is introduced by Ivan Gutman [8, 9]. It is defined as the sum of  $[n_u(e|G) n_v(e|G)]$ , over all edges of  $G$ . Here,  $n_u(e|G)$  is the number of vertices of  $G$  lying closer to  $u$  than to  $v$  and  $n_v(e|G)$  is the number of vertices of  $G$  lying closer to  $v$  than to  $u$ . Notice that vertices equidistance from  $u$  and  $v$  are not taken into account. A subgraph  $H$  of a graph  $G$  is called isometric if  $d_H(u, v) = d_G(u, v)$  for all  $u, v$  in  $V(H)$ . Isometric subgraphs of hypercubes are called partial cubes. Clearly, all trees are partial cube. The goal of this paper is computing the Wiener and Szeged indices of some bipartite chemical graphs by using cut method.

## 2. MAIN RESULTS AND DISCUSSION

### 2.1 Wiener and Szeged Indices

The Djoković–Winkler relation  $\Theta$  is defined on the edge set of a graph in the following way [10–12].

Edges  $e = xy$  and  $f = uv$  of a graph  $G$  are in relation  $\Theta$  if  $d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u)$ . Winkler [12] proved that among bipartite graphs,  $\Theta$  is transitive precisely for partial cubes; hence the relation  $\Theta$ , partitions the edge set of a partial cube. Let  $G$  be a partial cube and  $\Gamma = \{F_1, F_2, \dots, F_r\}$  be the partition of its edge set induced by the relation  $\Theta$ . Then we say that  $\Gamma$  is the  $\Theta$ -partition of  $G$ .

Let now  $G$  be a partial cube,  $\Gamma$  be its  $\Theta$ -partition and  $F \in \Gamma$ . Denoted by  $G_1(F)$  and  $G_2(F)$  means the connected components of  $G \setminus F$ . Set  $n_1(F) = |G_1(F)|$ ,  $n_2(F) = |G_2(F)|$  and we have the following Theorem proved by Klavžar in [11]:

**Theorem 1.** Let  $G$  be a partial cube and  $\Gamma$  its  $\Theta$ -partition. Then

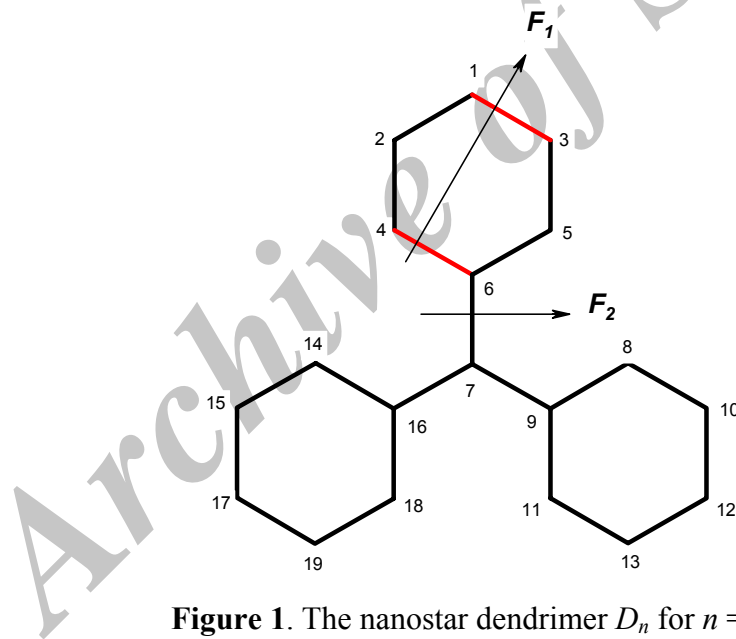
$$W(G) = \sum_{F \in \Gamma} n_1(F)n_2(F)$$

and

$$Sz(G) = \sum_{F \in \Gamma} |F| n_1(F)n_2(F).$$

In the next section we apply this Theorem to compute the mentioned topological indices of dendrimers, see [13 – 18] for more information on the Wiener and Szeged indices of graphs.

Consider a nanostar dendrimer  $D_n$  depicted in Figure 1.



**Figure 1.** The nanostar dendrimer  $D_n$  for  $n = 1$ .

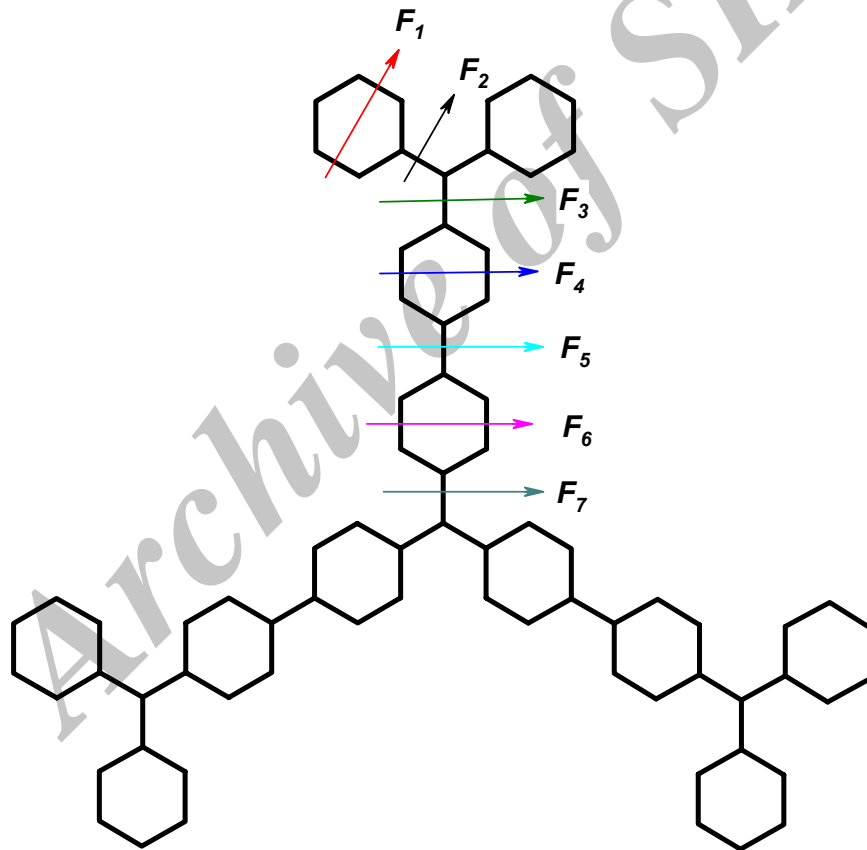
One can see that the nanostar dendrimer graph is a partial cube. In this section by using Klavžar Theorem we can compute the Wiener and Szeged indices of this infinite class of dendrimers. To do this, consider the following Examples:

**Example 2.** Consider the nano dendrimer depicted in Fig. 1. The  $\Theta$  - partition of edge set is  $\Gamma = \{F_1, F_2\}$ , where  $F_1 = \{\{1, 3\}, \{4, 6\}\}$  and  $F_2 = \{\{6, 7\}\}$ . On the other hand, there are nine partitions equivalent with  $F_1$  and  $F_2$  is unique. So, according to Theorem 1 we have:

$$W(G) = 9 \times 3 \times 16 + 3 \times 6 \times 13 = 666,$$

$$Sz(G) = 2 \times 9 \times 3 \times 16 + 3 \times 6 \times 13 = 1098.$$

**Example 2.** Consider the nanostar dendrimer  $D_n$ , for  $n = 2$  (Fig. 2). The  $\Theta$  - partition of edge set is  $\Gamma = \{F_1, F_2, \dots, F_7\}$ , where  $|F_1| = |F_4| = |F_6| = 2$ ,  $|F_2| = |F_3| = |F_5| = |F_7| = 1$ . On the other hand there are 18 partitions equivalent with  $F_1$ , 6 with  $F_2$ , 3 with  $F_3$ , 9 with  $F_4$ , 3 with  $F_5$ , 9 with  $F_6$  and 3 with  $F_7$ , respectively. Thus, according to Theorem 1 we have:



**Figure 2.** The nanostar dendrimer for  $n = 2$ .

By continuing this method, we can prove the following Theorem:

**Theorem 3.** Consider the nanostar dendrimer  $D_n$ . Then the Wiener and Szeged indices of  $D_n$  are as follows:

**Proof.** For computing Wiener and Szeged indices we should to compute all strips in  $D_n$ . To do this it is enough to consider five types of  $\Theta$  – partitions, *e. g.*  $F_1, F_2, \dots, F_5$ . In other words there exist  $9 \times 2^{n-i}$  ( $1 \leq i \leq n$ ) cuts of type  $F_1$ ,  $3 \times 2^{n-i}$  ( $1 \leq i \leq n$ ) cuts of type  $F_2$ ,  $3 \times 2^{n-i}$  ( $2 \leq i \leq n$ ) cuts of type  $F_3$ ,  $9 \times 2^{n-i}$  ( $2 \leq i \leq n$ ) cuts of type  $F_4$  and  $3 \times 2^{n-i}$  ( $2 \leq i \leq n$ ) cuts of type  $F_5$ , respectively. On the other hand  $|F_1| = |F_4| = 2$  and  $|F_2| = |F_3| = |F_5| = 1$ . So, by using Theorem 1 we should compute Wiener and Szeged indices for every case, separately:

- **Case 1** (Components of  $G \setminus F_1$ ): In this case the values of Wiener and Szeged indices are:

$$W_1 = 9 \sum_{i=1}^n 2^{n-i} ((19 \times 2^{i-1} - 16) |V(D_n)| - (19 \times 2^{i-1} - 16)^2),$$

$$S_1 = 18 \sum_{i=1}^n 2^{n-i} ((19 \times 2^{i-1} - 16) |V(D_n)| - (19 \times 2^{i-1} - 16)^2).$$

- **Case 2** (Components of  $G \setminus F_2$ ): In this case the values of Wiener and Szeged indices are:

$$W_2 = 3 \sum_{i=1}^n 2^{n-i} ((19 \times 2^{i-1} - 13) |V(D_n)| - (19 \times 2^{i-1} - 13)^2),$$

$$S_2 = 3 \sum_{i=1}^n 2^{n-i} ((19 \times 2^{i-1} - 13) |V(D_n)| - (19 \times 2^{i-1} - 13)^2).$$

- **Case 3** (Components of  $G \setminus F_3$ ): In this case the values of Wiener and Szeged indices are:

$$W_3 = 3 \sum_{i=2}^n 2^{n-i} ((19 \times 2^{i-1} - 25) |V(D_n)| - (19 \times 2^{i-1} - 25)^2),$$

$$S_3 = 3 \sum_{i=2}^n 2^{n-i} ((19 \times 2^{i-1} - 25) |V(D_n)| - (19 \times 2^{i-1} - 25)^2).$$

- **Case 4** (Components of  $G \setminus F_4$ ): In this case the values of Wiener and Szeged indices are:

$$W_4 = 9 \sum_{i=2}^n 2^{n-i} ((19 \times 2^{i-1} - 22) |V(D_n)| - (19 \times 2^{i-1} - 22)^2),$$

$$S_4 = 18 \sum_{i=2}^n 2^{n-i} ((19 \times 2^{i-1} - 22) |V(D_n)| - (19 \times 2^{i-1} - 22)^2).$$

- **Case 5** (Components of  $G \setminus F_5$ ): In this case the values of Wiener and Szeged indices are:

$$W_5 = 3 \sum_{i=2}^n 2^{n-i} ((19 \times 2^{i-1} - 19) |V(D_n)| - (19 \times 2^{i-1} - 19)^2),$$

$$S_5 = 3 \sum_{i=2}^n 2^{n-i} ((19 \times 2^{i-1} - 19) |V(D_n)| - (19 \times 2^{i-1} - 19)^2).$$

In all cases  $|V(D_n)| = 57 \times 2^{n-1} - 38$ . By summation of values of  $w_i$  ( $1 \leq i \leq 5$ ) we have:

$$W(D_n) = \frac{29241}{4} n 2^{2n} - 19494 \times 2^{2n} + 28863 \times 2^n - 9369,$$

$$Sz(D_n) = \frac{48735}{4} n 2^{2n} - 32490 \times 2^{2n} + 48195 \times 2^n - 15705.$$

## 2.2 Zagreb Indices, Geometric – Arithmetic Index, ABC Index and Randic Index

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [19]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where  $d_u$  and  $d_v$  are the degrees of  $u$  and  $v$ .

The connectivity index was introduced in 1975 by Milan Randić [20, 21] who has shown this index to reflect molecular branching. Randić index (Randić molecular connectivity index) was defined as follows:

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

Another topological index namely, geometric – arithmetic index (GA) defined by Vukicević and Furtula [22] as follows:

$$GA(G) = \sum_{uv \in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

Recently Furtula et al. [6] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

In the following Theorem we compute these topological indices of nanostar dendrimers.

**Theorem 4.** Consider nanostar dendrimer  $D_n$ , then

$$\begin{aligned} M_1(G) &= 318 \times 2^{n-1} - 240, \\ M_2(G) &= 384 \times 2^{n-1} - 327, \\ GA(G) &= (36 + 12\sqrt{6})2^{n-1} - \frac{12}{5}\sqrt{6} - 39, \\ ABC(G) &= (27\sqrt{2} + 8)2^{n-1} - 9\sqrt{2} - 18, \\ \chi(G) &= (16 + 5\sqrt{6})2^{n-1} + \sqrt{6} - 15. \end{aligned}$$

**Proof.** It is easy to see that this graph has  $|V(D_n)| = 57 \times 2^{n-1} - 38$  vertices,  $|E(D_n)| = 33 \times 2^{n-1} - 45$  edges and the edge set of graph can be divided to three partitions, e.g.  $[e_1]$ ,  $[e_2]$  and  $[e_3]$ . For every  $e = uv$  belong to  $[e_1]$ ,  $d_u = d_v = 2$ . Similarly, for every  $e = uv$  belong to  $[e_2]$ ,  $d_u = d_v = 3$ . Finally, if  $e = uv$  be an edge of  $[e_3]$ , then  $d_u = 2$  and  $d_v = 3$ . On the other hand, there are  $24 \times 2^{n-1} - 12$ ,  $30 \times 2^{n-1} - 6$  and  $12 \times 2^{n-1} - 27$  edges of type  $e_1$ ,  $e_2$  and  $e_3$ , respectively. By using the following table the proof is completed:

Endpoints of Edges	(2, 2)	(2, 3)	(3, 3)
Number of Edges	$24 \times 2^{n-1} - 12$	$30 \times 2^{n-1} - 6$	$12 \times 2^{n-1} - 27$

## REFERENCES

1. A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.*, **2001**, 66, 211 - 249.
2. A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.*, **2002**, 72, 247 - 294.
3. I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.*, **1997**, 36A, 128 - 132.
4. S. Klavžar, I. Gutman, Wiener number of vertex-weighted graphs and a chemical application, *Discrete Appl. Math.*, **1997**, 80, 73 - 81.
5. H. Y. Zhu, D. J. Klein, I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Comput. Sci.*, **1996**, 36, 420 - 428.
6. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, **1992**.
7. H. Wiener, Structural determination of the paraffin boiling points, *J. Amer. Chem. Soc.*, **1947**, 69, 17 - 20.
8. I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y.*, **1994**, 27, 9 - 15.
9. I. Gutman, A. A. Dobrynin, The Szeged index - A success story, *Graph Theory Notes N. Y.*, **1998**, 34, 37 - 44.
10. S. Klavžar, I. Gutman, A theorem on Wiener-type invariants for isometric subgraphs of hypercubes, *Applied Mathematics Letters*, **2006**, 19, 1129 - 1133.
11. D. Djoković, Distance preserving subgraphs of hypercubes, *J. Combin. Theory Ser. B*, **1973**, 14, 263 - 267.
12. M. Jalali, M. Ghorbani, On Omega polynomial of  $C_{40n+6}$  fullerenes, *Studia Universitatis Babeş-Bolyai, Chimia*, **2009**, 4(2), 25 - 32.
13. P. Winkler, Isometric embeddings in products of complete graphs, *Discrete Appl. Math.*, **1984**, 7, 221 - 225.
14. V. Chepoi, S. Klavžar, The Wiener index and the Szeged index of benzenoid systems in linear time, *J. Chem. Inf. Comput. Sci.*, **1997**, 37, 752 - 755.
15. A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.*, **2002**, 72, 247 - 294.
16. I. Gutman, A. A. Dobrynin, S. Klavžar, L. Pavlović, Wiener-type invariants of trees and their relation, *Bull. Inst. Combin. Appl.*, **2004**, 40, 23 - 30.
17. S. Klavžar, I. Gutman, B. Mohar, Labeling of benzenoid systems which reflects the vertex-distance relations, *J. Chem. Inf. Comput. Sci.*, **1995**, 35, 590 - 593.
18. S. Klavžar, H. M. Mulder, Partial cubes and crossing graphs, *SIAM J. Discrete Math.*, **2002**, 15, 235 - 251.



19. I. Gutman, D. Vukičević, J. Žerovnik, A class of modified Wiener indices, *Croat. Chem. Acta*, **2004**, 77, 103 – 109.
20. M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.*, **1975**, 97, 6609 – 6615.
21. P. Yu, An upper bound on the Randić of trees, *J. Math. Study (Chinese)*, **1998**, 31, 225 – 230.
22. D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, **2009**, 46, 1369 – 1376.
23. B. Furtula, A. Graovac and D. Vukičević, Atom-bond connectivity index of trees, *Discrete Appl. Math.*, **2009**, 157, 2828 – 2835.
24. M. Ghorbani, Computing Vertex PI, Omega and Sadhana Polynomials of  $F_{12(2n+1)}$  Fullerenes, *Iranian J. Math. Chem.*, **2010**, 1, 105 – 110.
25. M. V. Diudea, A. D. Manikpuri and S. Karmakar, Padmakar V Khadikar-Curriculum, *Iranian J. Math. Chem.*, **2010**, 1, 1 – 6.
26. P. V. Khadikar, Padmakar - Ivan Index in Nanotechnology, *Iranian J. Math. Chem.*, **2010**, 1, 7 – 42.

Archive of SID