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Some Topological Indices of Nanostar Dendrimers

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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 and Szeged 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

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other graph invariants. For trees (acyclic graphs) Wiener defined W as the sum of products 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] $W(G) = \sum_{\{u,v\}} d_G(u,v)$.

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 Θ 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 Θ 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, Θ is transitive precisely for partial cubes; hence the relation Θ, partitions the edge set of a partial cube. Let G be a partial cube and $\Gamma = \{F_1, F_2, \ldots, F_r\}$ be the partition of its edge set induced by the relation Θ. Then we say that Γ is the Θ-partition of G.

Let now G be a partial cube, Γ be its Θ-partition and $F \in \Gamma$. Denoted by $G_1(F)$ and $G_2(F)$ means the connected components of $G \backslash F$. 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 Γ its Θ-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.

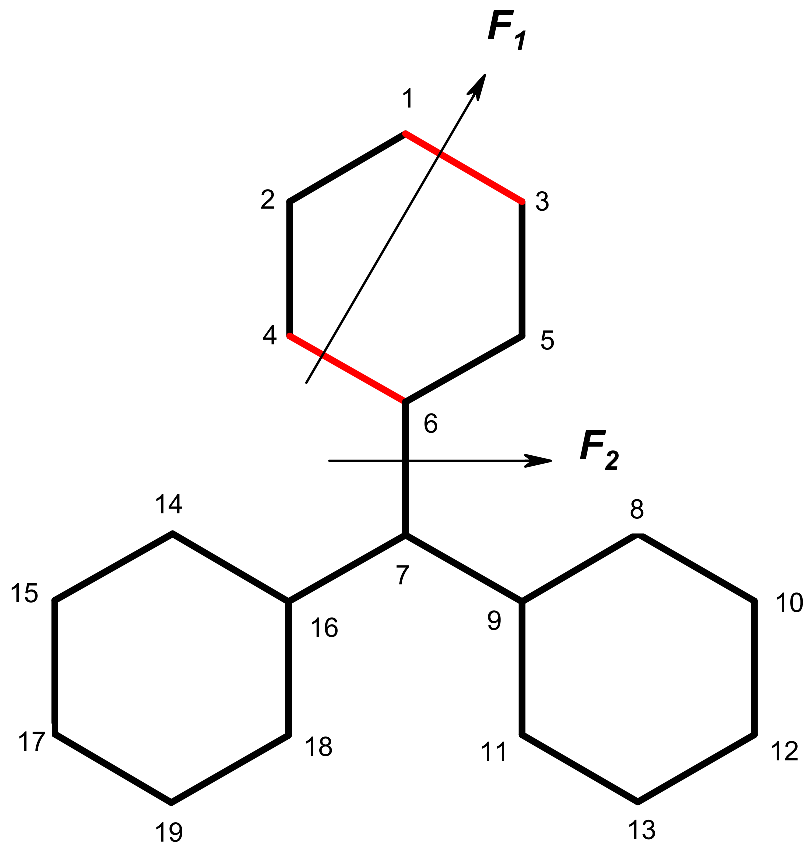

Figure 1. The nanostar dendrimer D_n for $n = 1$.

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 Θ - partition of edge set is Γ = $\{F_1,F_2\}$, 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:

$$W(G) = 9\times3\times16 + 3\times6\times13 = 666,$$
$$Sz(G) = 2\times9\times3\times16 + 3\times6\times13 = 1098.$$

Example 2. Consider the nanostar dendrimer D_n, for $n = 2$ (*Fig.* 2). The Θ - partition of edge set is $\Gamma = \{F_1, F_2, \ldots ,F_7,\}$, 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:

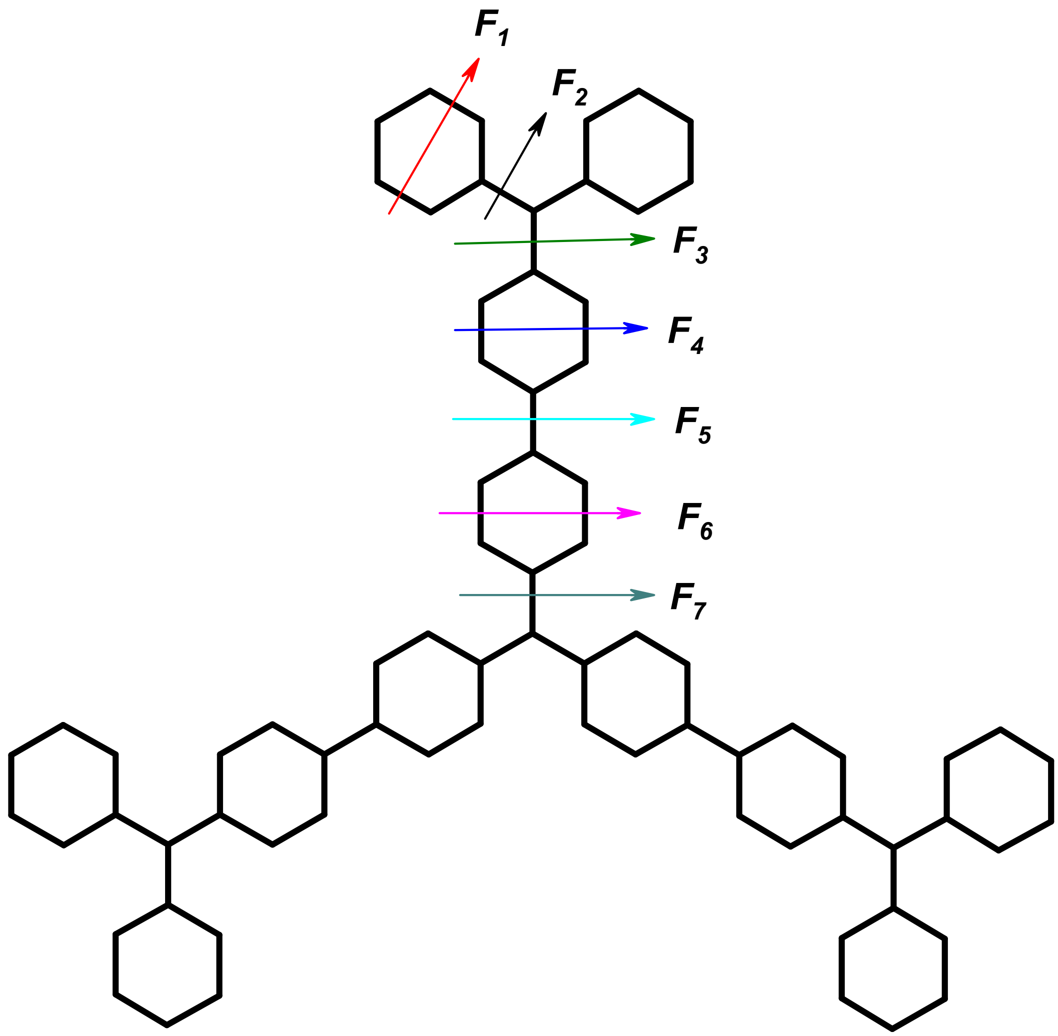

Figure 2. The nanostar dendrimer for $n = 2$.

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 Θ – partitions, *e. g.* $F_1, F_2, \ldots, F_5$. In other words there exist $9\times 2^{n-i}\,(1\le i\le n)$ cuts of type F_1, $3\times 2^{n-i}\,(1\le i\le n)$ cuts of type F_2,

$3\times 2^{n-i}\,(2\le i\le n)$ cuts of type F_3, $9\times 2^{n-i}\,(2\le i\le n)$ cuts of type F_4 and $3\times 2^{n-i}\,(2\le i\le n)$ 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\\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\\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\\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\\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\\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 ($1 \le i \le 5$) we have:

$$W(D_n) = \frac{29241}{4} n2^{2n} - 19494\times 2^{2n} + 28863\times 2^n - 9369,$$

$$Sz(D_n) = \frac{48735}{4} n2^{2n} - 32490\times 2^{2n} + 48195\times 2^n - 15705.$$

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:

$$M_1(G) = \sum_{v\in V(G)} (\mathrm{d}_v)^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} \mathrm{d}_u\,\mathrm{d}_v\,,$$

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:

$$GA(G) = \sum_{uv\in E} \frac{2\sqrt{\mathrm{d}_u\,\mathrm{d}_v}}{\mathrm{d}_u + \mathrm{d}_v}.$$

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:

$$ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{\mathrm{d}_u + \mathrm{d}_v - 2}{\mathrm{d}_u\,\mathrm{d}_u}}.$$

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

Theorem 4. Consider nanostar dendrimer D_n, then

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

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	$24\times 2^{n-1} - 12$	$30\times 2^{n-1} - 6$	$12\times 2^{n-1} - 27$

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