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The Wiener, Szeged, PI, vertex PI, the First and Second Zagreb Indices of N-branched Phenylacetylenes Dendrimers

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Abstract

A topological index of a molecular graph G is a numeric quantity related to G that is invariant under symmetry properties of G. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper the Wiener, PI, vertex PI, the first and second Zagreb indices of a class of nanostar dendrimer are computed.

1. Introduction

Throughout this section G is a simple connected graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of a connected graph G is denoted by $d_G(u,v)$ and it is defined as the number of edges in a minimal path connecting the vertices u and v. A topological index is a numeric quantity from the structure of a graph that is invariant under automorphisms of the graph under consideration. One of the most famous topological indices is the Wiener index introduced by Harold

Wiener [1]. The Wiener index of G is the sum of distances between all unordered pairs of vertices of G, $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)$.

The Szeged index is another topological index which is defined by Ivan Gutman [2] as $Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e)$, where $n_u(e)$ is the number of vertices of G lying closer to u than to v and $n_v(e)$ is the number of vertices of G lying closer to v than to u. If in the definition of Szeged index, we consider the sum of contributions, then we obtain a recently defined topological index, named vertex PI index. In mathematical language, the vertex PI index of G is defined as $PI_v(G) = \sum_{e=uv \in E(G)} [n_u(e) + n_v(e)]$ [3,4].

The Padmakar-Ivan (PI) index of the graph G is defined as $PI(G) = \sum_{e=uv \in E(G)} [m_u(e) + m_v(e)]$, 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 [5,6]. Finally, the first and second Zagreb indices of the graph G are defined as $Zg_1(G) = \sum_{u \in V(G)} \deg_G^2 u$ and $Zg_2(G) = \sum_{e=uv \in E(G)} \deg_G u \deg_G v$, respectively, see [7–9] and references therein for mathematical properties and chemical applications.

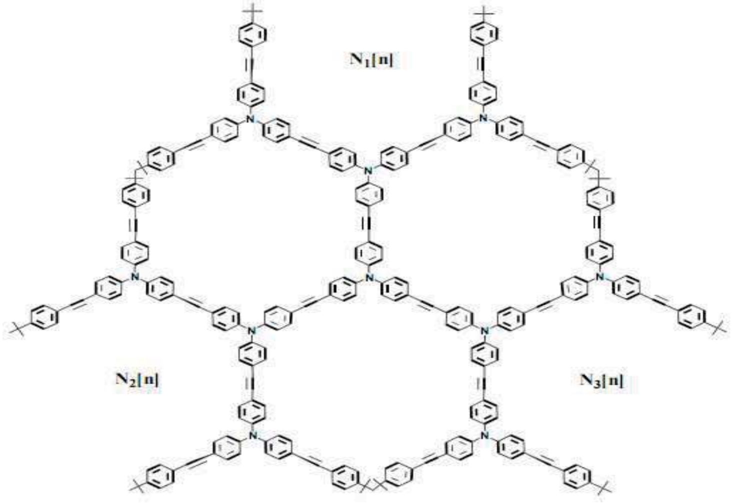

Figure 1. NSB[2].

2. Main Results

The nanostar dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and it is a great resistant of photo bleaching. Experimental and theoretical insight is needed in order to understand the energy transfer mechanism. In recent year, some people investigated the mathematical properties of this nanostructures into [10–14]. One type of nanostar dendrimers is N-branched phenylacetylenes, see [15,16]and it is shown by NSB[n], see Figure 1. In order to compute some topological indices of the nanostar dendrimer NSB[n], we first compute the number of vertices and edges of this nanostructure.

Lemma 1. The number of vertices and edges of dendrimer NSB[n] are given as:

$$|V(NSB[n])| = 87\times2^n - 38,$$
$$|E(NSB[n])| = 99\times2^n - 45.$$

Proof. At first we compute the number of vertices:

$$\begin{aligned}|V(NSB[n])| &= 19\,(1+3+\ldots+2^{n-1}\times3)+ 3\times2^n\times10\\ &= 19(1+3(2^n-1))+30\times2^n\\ &= 87\times2^n - 38.\end{aligned}$$

Now we obtain the number of edges:

$$\begin{aligned}|E(NSB[n])| &= 21\,(1+3+\ldots+3\times2^{n-1})+3(1+2+\ldots+2^n) + 3\times2^n\times10\\ &= 21\,(1+3(2^n-1)) +3(2^{n+1}-1) + 30\times2^n\\ &=99\times2^n - 45.\end{aligned}$$ ■□

For computing the Wiener index of NSB[n], we use the method of [17]. In what follows we recall some useful concepts. Let G be a connected graph. Then edges e = xy and f= uv of G are in the Djoković-Winkler relation Θ [18,19] if

$$d(x,u) + d(y,v) \neq d(x,v) + d(y,u).$$

The relation Θ is always reflexive and symmetric. Let Θ^* be the transitive closure of Θ. Then Θ^* is an equivalence relation on E(G) for any connected graph and it partitions the edge set of G into Θ^*-classes. For computing Θ^*-classes it is useful to know the following facts. Since two adjacent edges of G are in relation Θ if and only if they belong to a common triangle, all the edges of a given complete subgraph of G will be in the same Θ^*-class. Also, since an edge e of an isometric cycle C of G is in relation Θ with its antipodal edge(s) on C, all the edges of an odd cycle will be in the same Θ^*-class.

In what follows a powerful method given by Klavzar is described. Using this concept, it is possible to compute the Wiener index of nanostar dendrimers. Following Klavzar [17,20], the canonical metric representation α of a connected graph G is defined as follows:

- Let G be connected graph and $F_1, F_2, \ldots, F_k$ its Θ^*-classes.
- Define quotient graph G/F_i, i=1,…,k, as follows. Its vertices are the connected components of $G-F_i$, two vertices C and C' are adjacent if there exist vertices $x \in C$ and $y \in C'$ such that $xy \in F_i$.
- Define $\alpha : G \to \prod_{i=1}^{k} G/F_i$ with $\alpha : u \to (\alpha_1(u), .., \alpha_k(u))$, where $\alpha_i(u)$ is a connected component of $G-F_i$ that contains u. Let G be an arbitrary connected graph and

$$\alpha : G \to \prod_{i=1}^{k} G/F_i$$

is canonical metric representation of G. Let $(G/F_i, w_i)$ are natural weighted graphs, the weight of G/F_i is the number of vertices in the corresponding connected component of $G-F_i$. Then,

Theorem 2. [17] For any connected graph G, $W(G) = \sum_{i=1}^{k} W(G/F_i, w_i)$.

Theorem 3. The Wiener index of NSB[n] is given by follows:

$$W(NSB[n]) = 27\sum_{k=0}^{n} 2^{n-k}(\alpha_k |V| - \alpha_k^2 - 14) + 9 \times 2^n (87 \times 2^n - 39),$$

where $\alpha_n = 29 \times 2^n - 19$, $|V| = |V(NSB[n])|$.

Proof. We prove this theorem by applying Theorem 2. We may partition the molecular graph of NSB[n] into a core together with three isomorphic subgraphs $N_1[n]$, $N_2[n]$ and $N_3[n]$ (see Figure 1). We name each of $N_1[n]$, $N_2[n]$ and $N_3[n]$, to be a branch of NSB[n].

We partition Θ^*-classes of NSB[n] into three subsets A_1, A_2, A_3 where A_1, A_2, A_3 are contained Θ^*–classes of edges of hexagons, cut edges and edges which have a vertex of degree 1, respectively. It is easy to see that if an edge on a hexagon then $[e/\Theta^*]$ contains two elements, therefore each hexagon is partitioned to three Θ^*-classes and if e be a cut edge or has a vertex of degree 1, then $[e/\Theta^*]$ contains just one element, in this case $[e/\Theta^*]=\{e\}$. Therefore, the number of elements of A_1, A_2, A_3 are given by

$$|A_1| = 9\,(1+3+\ldots+3\times 2^{n-1}) + 9\times 2^n = 18(2^{n+1}-1),$$

$$|A_2| = 3\,(1+4+\ldots+4\times 2^{n-1}) + 2\times 3\times 2^n = 9(2^{n+1}-1),$$

$$|A_3| = 9\times 2^n.$$

The number of vertices of each branch of NSB[n] are $\alpha_n = |N_i[n]| = 29\times 2^n - 19$ for i = 1, 2, 3. We now define the values of W_1, W_2, W_3 as follows:

$$W_1 = \sum_{i=1}^{18(2^{n+1}-1)} W(NSB[n]/E_i, w_i), \text{ where } E_i \in A_1 \text{ for i = 1,…, } 18(2^{n+1}-1),$$

$$W_2 = \sum_{i=1}^{9(2^{n+1}-1)} W(NSB[n]/F_i, w_i), \text{ where } F_i \in A_2 \text{ for i = 1,…, } 9(2^{n+1}-1),$$

$$W_3 = \sum_{i=1}^{9\times 2^n} W(NSB[n]/G_i, w_i), \text{ where } G_i \in A_3 \text{ for i = 1,…, } 9\times 2^n.$$

By definition of W_1, W_2 and W_3 one can prove the following equalities:

$$\begin{aligned}
W_1 &= 3^2[(\alpha_n+3)(|V|-(\alpha_n+3))+(\alpha_n-3)(|V|-(\alpha_n-3))] \\
&\quad +3^2\times 2[(\alpha_{n-1}+3)(|V|-(\alpha_{n-1}+3))+(\alpha_{n-1}-3)(|V|-(\alpha_{n-1}-3))]+\ldots \\
&\quad +3^2\times 2^n[(10+3)(|V|-(10+3))+(10-3)(|V|-(10-3))] \\
&= 3^2\times 2(\alpha_n|V|-\alpha_n^2-9)+3^2\times 2^2(\alpha_{n-1}|V|-\alpha_{n-1}^2-9)+\ldots \\
&\quad +3^2\times 2^{n+1}(\alpha_0|V|-\alpha_0^2-9) = 3^2\sum_{k=0}^{n}2^{n-k+1}(\alpha_k|V|-\alpha_k^2-9).
\end{aligned}$$

$$\begin{aligned}
W_1 &= 3[(\alpha_n+6)(|V|-(\alpha_n+6))+\alpha_n(|V|-\alpha_n)+(\alpha_n-6)(|V|-(\alpha_n-6))] \\
&\quad +3\times 2[(\alpha_{n-1}+6)(|V|-(\alpha_{n-1}+6))+\alpha_{n-1}(|V|-\alpha_{n-1})+(\alpha_{n-1}-6)(|V|-(\alpha_{n-1}-6))]+\ldots \\
&\quad +3\times 2^n[(10+6)(|V|-(10+6))+10(|V|-10)+(10-6)(|V|-(10-6))] \\
&= 3^2(\alpha_n|V|-\alpha_n^2-24)+3^2\times 2(\alpha_{n-1}|V|-\alpha_{n-1}^2-24)+\ldots+3^2\times 2^n(\alpha_0|V|-\alpha_0^2-24) \\
&= 3^2\sum_{k=0}^{n}2^{n-k}(\alpha_k|V|-\alpha_k^2-24).
\end{aligned}$$

It is easy to see that $W_3 = 3^2 \times 2^n (87 \times 2^n - 39)$, where |V| = |V(NSB[n])|.

By these calculations, we can see that

$$W(NSB[n]) = W_1 + W_2 + W_3 = 27\sum_{k=0}^{n} 2^{n-k}(\alpha_k |V| - \alpha_k^2 - 14) + 9 \times 2^n (87 \times 2^n - 39).$$ ■□

Theorem 4. With notation of Theorem 3, the Szeged index of NSB[n] is given by :

$$Sz(NSB[n]) = 5 \times 3^2 \sum_{k=0}^{n} 2^{n-k} (\alpha_k |V| - \alpha_k^2 - 14) + 9 \times 2^n (87 \times 2^n - 39).$$

Proof. By definition of Szeged index and partition of edges as described in the proof of Theorem 3,

$$\sum_{e=uv\in A_1} n_u(e) n_v(e) = 2 \times 3^2 \sum_{k=0}^{n} 2^{n-k+1} (\alpha_k |V| - \alpha_k^2 - 9),$$

$$\sum_{e=uv\in A_2 \cup A_3} n_u(e) n_v(e) = 3^2 \sum_{k=0}^{n} 2^{n-k} (\alpha_k |V| - \alpha_k^2 - 24) + 3^2 \times 2^n (87 \times 2^n - 39),$$

Therefore, $Sz(NSB[n]) = 5 \times 3^2 \sum_{k=0}^{n} 2^{n-k} (\alpha_k |V| - \alpha_k^2 - 14) + 9 \times 2^n (87 \times 2^n - 39)$. ■□

Theorem 5. The PI index of the dendrimer NSB[n] is obtained by:

$$PI(NSB[n]) = 9801 \times 2^{2n} - 9081 \times 2^n + 2106.$$

Proof. By definition, we have

$$PI(NSB[n]) = \sum_{e=uv} m_u(e) m_v(e) = 3 \times (99 \times 2^n - 46)(1+4+4\times 2+\ldots+4\times 2^{n-1}+5\times 2^n)$$

$$+3\times(99\times 2^n - 47)(6 + 6\times 3 + 6\times 3\times 2 +\ldots+ 6\times 3\times 2^{n-1}+2^n)$$

$$= 3\times(99\times 2^n - 46)(9\times 2^n) + 3\times(99\times 2^n - 47)(24\times 2^n-12)$$

$$= 9801 \times 2^{2n} - 9081 \times 2^n + 2106.$$ ■□

Theorem 6. The vertex PI index of the dendrimer NSB[n] is obtained as follows:

$$PI_v(NSB[n]) = 8613\times 2^{2n} - 7677 \times 2^n + 1710.$$

Proof. It is easy to see that this nanostar is bipartite graphs, then

$$PI_v(NSB[n]) = |V(NSB[n])||E(NSB[n])|$$

$$= (87\times 2^n - 38)(99\times 2^n - 45)$$

$$= 8613\times 2^{2n} - 7677 \times 2^n + 1710.$$ ■□

Theorem 7. The first and second Zagreb indices of NBS[n] are computed as follows:

$$Zg_1(NSB[n]) = 492\times 2^n - 222, \quad Zg_2(NSB[n]) = 591 \times 2^n - 273.$$

Proof. At first we compute the first Zagreb index as follow:

$$\begin{aligned} Zg_1(NSB[n]) = 9 &+3\times 3^2[(2^n-1)+2+6(1+\ldots+2^{n-1})+2^{n+1}] \\ &+3\times 2^2[4+4\times 3(1+2+\ldots+2^{n-1})+ 4 \times 2^n] \\ &+3\times 4^2\times 2^n + 3\times 3 \times 1^2\times 2^n \\ &= 492\times 2^n - 222, \end{aligned}$$

Now we obtain the second Zagreb index.

$$\begin{aligned} Zg_2(NSB[n]) = 3\times &[4\times 3\times 2^n + 3\times 3(1+4+4\times 2+\ldots+4\times 2^{n-1}+2^n) \\ &+3\times 2(4+4\times 3+4\times 3\times 2+\ldots+4\times 3\times 2^{n-1}+4\times 2^n) \\ &+2\times 2(2+3\times 2+3\times 2\times 2+\ldots+3\times 2\times 2^{n-1}+2\times 2^n)+4\times 1\times 3\times 2^n] \\ &= 591 \times 2^n - 273. \end{aligned}$$ ■

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