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THE SZEGED AND WIENER NUMBERS OF WATER-SOLUBLE POLYARYL ETHER DENDRIMER NANOSTARS

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A topological index of a graph G is a number Top(G) which is invariant under graph isomorphism. The Wiener and Szeged indices are two important distances based topological index applicable in nanoscience. The aim of this paper is to compute these numbers for a new class of nanostar dendrimers.

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1. Introduction

Dendrimers are macromolecules comprised of a series of branches extending outward from an inner core. The word dendrimer originates from the Greek dendron, meaning "tree". These mkolecules1 have attracted much attention because of their various electrical and optical properties.

Suppose G is a simple graph, a graph without multiple edges and loops. The set of vertices and edges of G are denoted by V(G) and E(G), respectively. A topological index is a numeric quantity derived from the structural graph of a molecule. The number of vertices and edges are the simplest topological indices of graphs. The distance $d_G(u,v)$ (d(u,v) for short) between two vertices $u, v \in V(G)$ is the length of a shortest path connecting them.

The concept of "topological index" was first proposed by Haro Hosoya[1] for characterizing the topological nature of a graph. Such graph invariants are usually related to the distance function and so named distance based topological index. The first topological index of this type was proposed in 1947 by the chemist Harold Wiener.[2] It is defined as the sum of all distances between vertices of the graph under consideration.

The Szeged index is a topological index introduced by Ivan Gutman[3]. 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 than v and $n_v(e)$ is the number of vertices of G lying closer to v than u. 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 equidistant from u and v are not taken into account.

The aim of this paper is to compute the Wiener and Szeged indices of a water-soluble polyaryl ether dendrimer[4] G[n], see Figure 1. We encourage the reader to consult papers published bi Diudea and co-authors[5-11] and our earlier papers[12-20] for background material as well as basic computational techniques. Our notations are standard and taken mainly from the standard book of graph theory.

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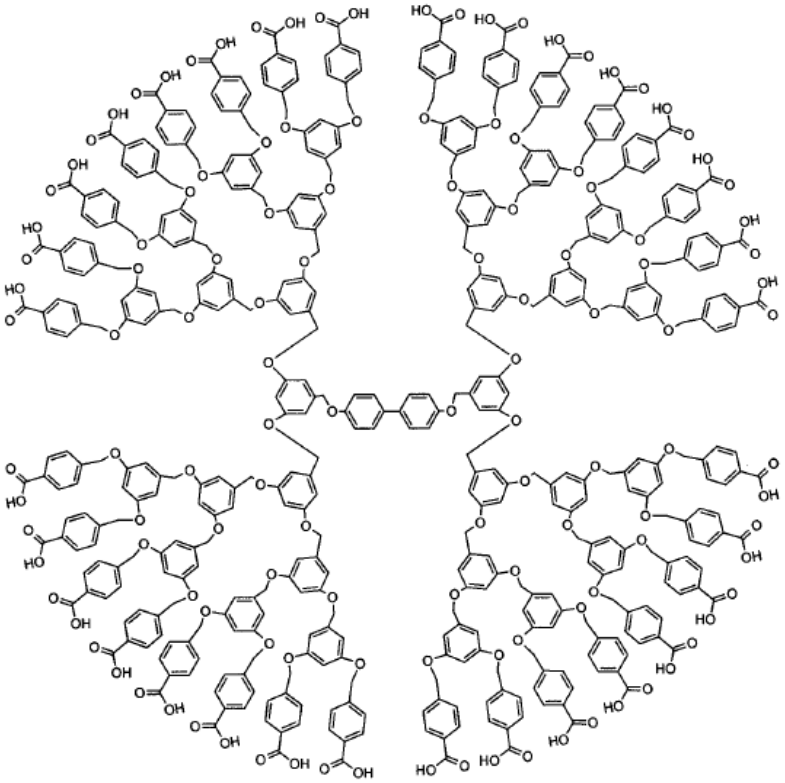

Fig. 1. The Molecular Graph of Dendrimer Nanostar G[4].

2. Main Results and discussion

In this section the Wiener index of the molecular graph G[n] is computed. Let G be graph. A subgraph S of G is called convex if for each vertex x,y ∈ V(H) there exists no shortest path in G from x to y which involves a vertex w ∈ V(G) − V(H). If G and H are graphs such that V(H) ⊆ V(G) and E(H) ⊆ E(G) then H is said to be a subgraph of G.

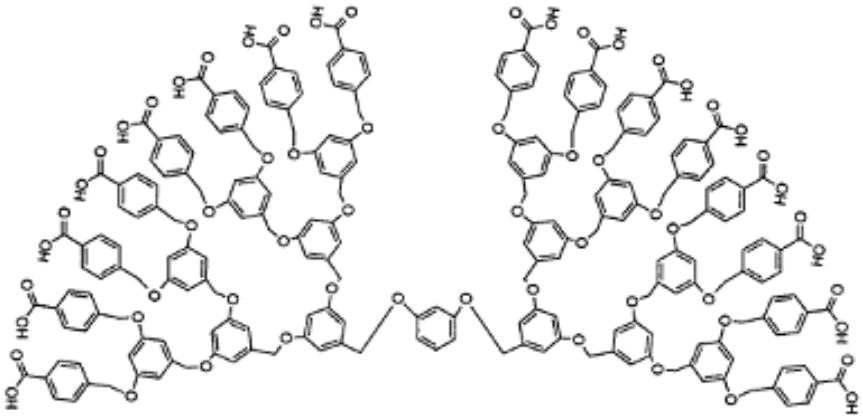

Fig. 2. The Graph of H[4].

Define H[n] to be the graph constructed from G[n] by deleting almost on half of its vertices and edges, see Figure 2. In an earlier paper[21], we proved that if $\{F_i\}_{1\le i\le k}$ is a partition of E(G) such that for each i, $1 \le i \le k$, $G - F_i$ is a two component graph such that both of components are convex then $W(G) = \Sigma_{1\le i\le k} |V(GF_i(1))|.|V(GF_i(2))|$, where $GF_i(1)$ and $GF_i(2)$ are two

components of $G - F_i$. If we omit an edge outside hexagons of G[n] then the components of new graph are easily convex. On the other hand, the graphs obtained from G[n] by deleting two non-adjacent parallel edges of a hexagon are also convex. These subsets constitute a partition $\{F_i\}_{1\le i\le k}$ of E(G) and $H[n] = G[n] - F_i$ has the required properties of the mentioned theorem. Define $g_n = |V(G[n])|$ and $h_n = |V(H[n])|$. Then $h_n = \sum_{i=0}^{n} 6\times 2^i + \sum_{i=1}^{n} 2^{i+1} + 4\times 2^n = 5(2^{n+2} - 2)$ and $g_n = 2h_n + 16 = 5\times 2^{n+3} - 4$. Suppose $a^* = a(g_n - a)$. Then we have:

Theorem 1. The Wiener index of G[n] is computed as follows:

$$W(G[n]) = 502 - 3440.4^n + 8000.n.4^n + 28000.n.2^n + 8548.2^n$$

Proof. Consider a hexagon C_6 in $H[n] \le G[n]$. From Figure 3, one can see that $G[n] - \{e_1,e_4\}$ has exactly two components, both of them are convex and one of the components has h_α - 3 vertices, $0 \le \alpha \le n$. We notice that the number of such hexagons is $2^{n-\alpha}$. Similarly, $G[n] - \{e_2,e_5\}$ and $G[n] - \{e_3,e_6\}$ have also two components, both of them are convex and one of their components has $h_{\alpha-1} + 5$ vertices, $0 \le \alpha \le n$. Suppose e is an edge outside cycles of G[n]. Then G[n] – e has exactly two convex component. One of these components has h_β, $h_\beta + 1$ or $h_\beta + 2$ vertices and the number of such edges is $2^{n-\beta}$, $1 \le \beta \le n$. For $\alpha = 0$, one can see that there is 2^n hexagons and $G[n] - \{e_1,e_4\}$, $G[n] - \{e_2,e_5\}$ and $G[n] - \{e_3,e_6\}$ have exactly two components, where both of them are convex and one of them has 7 vertices. There is a similar argument for other edges of G[n] and so there is a partition $\{F_i\}_{1\le i\le r}$ in which $G - F_i$ has two convex components. Therefore,

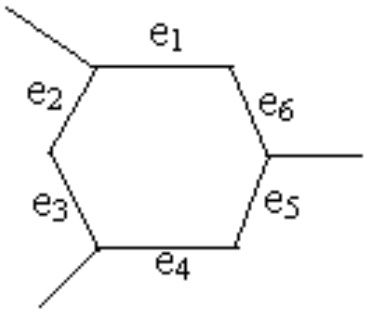

Fig. 3. The Position of Edges in a Hexagon.

Fig. 4. The Core of G[n].

$$\begin{aligned}\sum_{e\in H[n]} m(e) = &\sum_{i=0}^{n-1} 2^i[(h_{n-i} - 3)^* + 2(h_{n-i-1} + 5)^*] + 2^n.3.(g_{n-7})^* \\ &+ \sum_{i=1}^{n} 2^i[(h_{n-i} + 2)^* + (h_{n-i} + 1)^* + (h_{n-i})^*] \\ &+ 2^n[2(g_n - 1)^* + (g_n - 2)^* + (g_n - 4)^*]\end{aligned}$$

On the other hand, if S is the core of G[n], then we have:

$$\sum_{e\in S} m(e) = 2[h_n^* + (h_n+1)^* + (h_n+2)^* + 3(h_n+5)^*] + \left(\frac{g_n}{n}\right)^*.$$

Therefore, $W(G[n]) = 2\Sigma_{e\in H[n]}m(e) + \Sigma_{e\in S}m(e) = 502 - 3440.4^n + 8000.n.4^n + 28000.n.2^n + 8548.2^n$. This completes our proof. ■

Theorem 2. The Szeged index of G[n] is computed as follows:

$$Sz(G[n]) = 726 + 11200n4^n + 3920.n.2^n - 3600.4^n + 11592.2^n$$

Proof. Choose the set F = {uv}, where uv is an edge outside hexagons of G[n]. By definition of the Szeged index and partition of edges described in the proof of Theorem 1, $n_u(e)n_v(e) = |V(GF(1))|.|V(GF(2))|$. Similarly, if F = {uv,ab} then $n_u(e)n_v(e) = n_a(e)n_b(e) = |V(GF(1))|.|V(GF(2))|$. So, by a similar argument as Theorem 1,

$$\sum_{e=uv\in E(H[n])} n_u(e)n_v(e) = 2\sum_{i=0}^{n-1} 2^i[(h_{n-i}-3)^* + 2(h_{n-i-1}+5)^*] + 2^{n+1}.3.(g_{n-7})^*$$
$$+ \sum_{i=1}^{n} 2^i[(h_{n-i}+2)^* + (h_{n-i}+1)^* + (h_{n-i})^*]$$
$$+ 2^n[2(g_n-1)^* + (g_n-2)^* + (g_n-4)^*],$$

$$\sum_{e=uv\in E(S)} n_u(e)n_v(e) = 2[h_n^* + (h_n+1)^* + (h_n+2)^* + 3.2(h_n+5)^*] + \left(\frac{g_n}{n}\right)^*.$$

Therefore, $Sz(G[n]) = 2\Sigma_{e=uv\in E(H[n])}n_u(e)n_v(e) + \Sigma_{e=uv\in E(S)}n_u(e)n_v(e) = 726 + 11200n4^n + 3920.n.2^n - 3600.4^n + 11592.2^n$, which completes our argument. ■

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