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RESEARCH ARTICLE

The Wiener, Szeged, and PI Indices of a Dendrimer Nanostar

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Let $G = (V, E)$ be a simple connected graph. The distance between two vertices of G is defined to be the length of the shortest path between the two vertices. There are topological indices assigned to G and based on the distance function which are invariant under the action of the automorphism group of G. Some important indices assigned to G are the Wiener, Szeged, and PI index which we will find them for a certain chemical graph called dendrimer nanostar.

Keywords: Nanostar, Topological Index, Wiener Index, Szeged Index, PI-Index.

1. INTRODUCTION

The graphs considered in this paper are simple and connected. Let $G = (V, E)$ be a graph with vertex set V and edge set E. We will assume that G is a finite graph, i.e., both V and E are finite sets. For $u, v \in V$, the length of the shortest path from u to v is denoted by $d(u, v)$ and is called the topological distance between u and v. The Wiener index of G is denoted by $W(G)$ and is defined by:

$$W(G) = \sum_{\{u,v\}\subseteq V} d(u, v)$$

If for a vertex $v \in V$ the sum of distances between v and all other vertices of G is denoted by $d(v)$, i.e., $d(v) = \sum_{x\in V} d(v, x)$, then $W(G) = 1/2 \sum_{v\in V} d(v)$.

Wiener was the first one who considered the above index in connection with chemical graphs.[24] The Wiener index is one of the oldest descriptors concerned with the molecular graph and is concerned with the determination of the boiling points of paraffins. We remark that Wiener defined this index only for acylic molecules in a different way, but the definition of $W(G)$ in terms of distances between vertices of a graph G was first defined by Hosoya in Ref. [14].

In mathematical research, the Wiener index has been first studied in Ref. [8], and for a long time mathematicians were not aware of the importance of the Wiener index in mathematical chemistry. However, because of the chemical facts about the Wiener index and also because it is an invariant of the graph, that is: it is invariant under the automorphism of the graph, hence various researchers found methods to calculate this index. Among the important works on finding the Wiener index of a general graph the reader is referred to the papers by Gutman et al.[7,5,11,12]

In theoretical chemistry molecular structure descriptor, also called topological indices, are used to understand properties of chemical compounds. By now there exist many different types of such indices for a general graph $G = (V, E)$. Here, apart from the Wiener index, we are interested in indices such as the Szeged and the Padmakar-Ivan index, the so called PI-index of a graph.

The Szeged index[9,10,17] is a topological index closely related to the Wiener index of a graph $G = (V, E)$. Let $e = uv$ be an edge of G. By $n_u(e \mid G)$ we mean the number of vertices lying closer to u than v and similarly we define $n_v(e \mid G)$. Therefore if we define the following sets: $N_u(e|G) = \{w \in V \mid d(w, u) < d(w, v)\}$ and $N_v(e \mid G) = \{w \in V \mid d(w, v) < d(w, u)\}$. Then $n_u(e \mid G) = |N_u(e \mid G)|$ and $n_v(e \mid G) = |N_v(e \mid G)|$. The Szeged index of G is defined by the following formula:

$$Sz(G) = \sum_{e=uv\in E} n_u(e \mid G)n_v(e \mid G)$$

In Ref. [20] basic properties of Szeged index and its analogy to the Wiener index is discussed. It is proved that for a tree T the Wiener index of T is equal to its Szeged index.

Since the Szeged index takes into account how the vertices of the graph G are distributed, it is natural to define an index that takes into account the distribution of the edges of G. The padmakar-Ivan (PI) index,[16,18], is another important index which is assigned to a graph G and takes into account the distribution of edges of the graph and therefore complements the Szeged index in a certain sense.

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Let the number of edges in the graphs induced by $N_u(e \mid G)$ and $N_v(e \mid G)$ be denoted by $n_{\text{eu}}(e \mid G)$ and $n_{\text{ev}}(e \mid G)$, respectively. The PI index of G is defined by:

$$PI(G) = \sum_{e \in E} (n_{\text{eu}}(e \mid G) + n_{\text{ev}}(e \mid G))$$

We remark that the edges equidistant from both ends of the edge uv are not counted in the above expression for $PI(G)$. It is easy to see that if $N(e)$ denotes the number of all the edges equidistance from e, then $N(e) + n_{\text{eu}}(e \mid G) + n_{\text{ev}}(e \mid G) = |E|$, hence we have: $PI(G) = \sum_{e \in E}(E - N(e)) = |E|^2 - \sum_{e \in E} N(e)$. Therefore to compute $PI(G)$ it is enough to know the number of edges of G and the numbers $N(e)$ for each edge e of G.

All the indices mentioned above, when applied to chemical graphs have many chemical applications and it was shown that the PI index is related to the Szeged and the Wiener index of a graph, and all of them have connections with the physicochemical properties of many complex compounds.

For the topological indices associated to a graph two groups of problems can be distinguished in the theory of topological indices. One is to ask the dependence of the index to the graph and the other is the calculation of these indices efficiently. The greatest progress in solving the above problems was made for trees and hexagonal systems by Gutman et al. in Refs. [5, 7]. Because of the importance of the above indices important methods have been developed to compute them. For example one can refer to Refs. [1–4, 6, 13, 19, 21–23]

In this paper we will consider the graph of a certain dendrimer nanostar and find its topological indices such as the Wiener, Szeged, and PI indices. The Wiener index of this dendrimer is calculated in Ref. [15], but in this paper we find it using a different method. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The nanostar dendrimer is part of a new group of molecules that appears to be photon funnels just like artificial antennas.

2. PRELIMINARIES

Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. We recall that the distance between two vertices u and v is denoted by $d(u, v)$ and it is the length of the shortest path from u to v. If we want to specify the graph in question then the distance between u and v is denoted by $d_{\text{G}}(u, v)$. If H is a subgraph of G, then this fact is denoted by the symbol $H \leq G$ and H is called an isometric subgraph if $d_{\text{H}}(u, v) = d_{\text{G}}(u, v)$ for all vertices u and v of H, and if this is the case then we write $H \ll G$.

Let V_1 and V_2 be non-empty subsets of the vertex set V of G. The distance between V_1 and V_2 is denoted by $d_{\text{G}}(V_1, V_2)$ and is defined as follows $d_{\text{G}}(V_1, V_2) = \sum_{u \in V_1} \sum_{v \in V_2} d_{\text{G}}(u, v)$. If $V_2 = V$ then we write $d_{\text{G}}(V_1, V) = d(V_1, G)$. With this notation the Wiener index of the graph G can be written as $W(G) = (1/2) d_{\text{G}}(V, G)$.

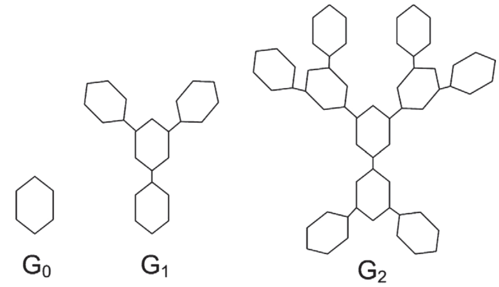

Fig. 1. A dendrimer nanostar.

If $\{F_i\}_{i=1}^r$ is a partition of the vertex set V, then it is easy to see that: $W(G) = 1/2 \sum_{i=1}^r \sum_{j=1}^r d_{\text{G}}(F_i, F_j)$. Also if $H \ll G$, then: $W(H) = (1/2) d_{\text{H}}(V(H), V(H))$ and $W(G) = (1/2) d(V(G), G)$, where $V(H)$ and $V(G)$ denote the vertex sets of H and G, respectively.

In this paper we will consider a graph which is denoted by G_n, $n \geq 0$. This a kind of dendrimer nanostar. The shape of this graph is as follows. For $n = 0$, G_0 is a hexagon, and for $n = 1$, G_1 is emerged from three non-adjacent vertices of G_0 in such a way that three hexagons are build from them and so on, see Figure 1.

3. MAIN RESULTS

Theorem 1. $W(G_n) = 972 n 4^n - 1458.4^n + 1755.2^n - 270$, $n \geq 0$.

Proof. If we replace each hexagon in G_n by a point, a tree is obtained which is denoted by T_n. Here we draw T_2 in Figure 2.

The hexagon C_6 corresponding to the vertex v_i in T_n is denoted by C_{v_i}. It is easy to verify that if $v_i \neq v_j$, then $d_{G_n}(C_{v_i}, C_{v_j}) = 36(d(v_i, v_j) + 2(d(v_i, v_j) - 1)) + 108 = 108 d(v_i, v_j) + 36$, and $d(C_{v_i}, C_{v_i}) = 27$ for all i, j. As we mentioned earlier, if $\{V_i\}_{i=1}^r$ is a partition of the vertex set of a graph G, then $W(G) = \sum_{v \in V_i} \sum_{v \in V_j} d_{\text{G}}(u, v)$.

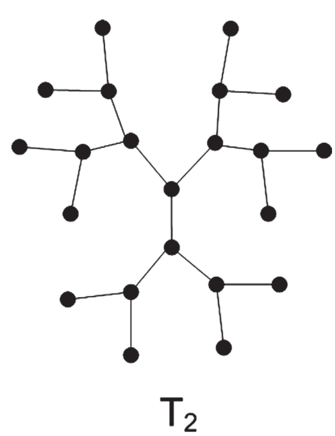

Fig. 2. A tree associated to G_n.

Now considering G_n we can compute $W(G_n)$ as follows:

$$
\begin{aligned}
W(G_n) &= \sum_{\{u,v\}\subseteq V(G_n)} d_{G_n}(u, v) \\
&= \sum_{\{u,v\}\subseteq V(T_n)} d_{G_n}(V(C_u), V(C_v)) \\
&\quad + \frac{1}{2} \sum_{v\in V(T_n)} d_{G_n} V(C_u), V(C_v) \\
&= \sum_{\{u,v\}\subseteq V(T_n)} (108 d_{T_n}(u, v) + 36) + 27|V(T_n)| \\
&= \sum_{\{u,v\}\subseteq V(T_n)} 108 d_{T_n}(u, v) \\
&\quad + 36\binom{|V(T_n)|}{2} + 27|V(T_n)| \\
&= 108W(T_n) + 36\binom{|V(T_n)|}{2} + 27|V(T_n)| \qquad (1)
\end{aligned}
$$

But clearly the number of vertices of the tree T_n is $|V(T_n)| = 1 + 3\sum_{i=0}^{n-1} 2^i = 3.2^n - 2$ for $n \geq 0$, hence it is enough to calculate $W(T_n)$. But the Wiener index of a tree is equal to its Szeged index. Hence we calculate $Sz(T_n)$. For any edge of T_n, the number of vertices closer to one end of this edge is equal to $2^{n-i} - 1$ and the rest of vertices are closer to the other end of the edge. Since the number of edges at each step is 3.2^i, $0 \leq i \leq n$, we have $Sz(T_n) = \sum_{i=0}^{n} (2^{n-i} - 1)(3.2^n - 2 - (2^{n-i} - 1)) \cdot 3.2^i = 9n4^n - 15.4^n + 18.2^n - 3$. Now substituting the above value in (1) we obtain $W(G_n) = 972n4^n - 1458.4^n + 1755.2^n - 270$, $n \geq 0$. and the theorem is proved. □

Next we calculate the Szeged index of G_n.

Theorem 2. $Sz(T_n) = 1620n.4^n - 2376.4^n + 2862.2^n - 432$, $n \geq 0$.

Proof. First we introduce a graph H_0 as follows. H_0 is the null graph, H_1 is a hexagon and H_2 is the following graph in Figure 3. And the graph H_3 is built using H_2 by adding two hexagons on each of the two hexagons, see Figure 3.

In this manner a general graph H_n is constructed such that if we add three copy of it to the central hexagon the graph G_n is obtained as demonstrated above in G_2 in Figure 3. It is clear that $t_n = |V(H_n)| = 6(2^n - 1)$ and $u_n = |V(G_n)| = 3|V(H_n)| + 6 = 18.2^n - 12$, $n \geq 0$.

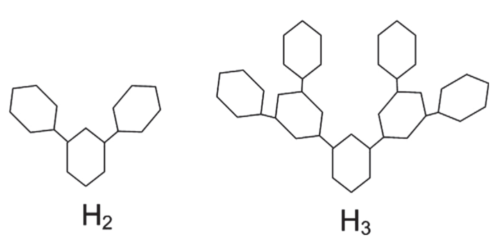

Fig. 3. A hexagonal graph.

Since the only circuits in G_n are the hexagons, the graph is bipartite and for the edge $e = uv$ we have $n_u(e \mid G) + n_v(e \mid G) = u_n$. In calculating $Sz(G_n)$ there are three summations to be considered:

(a) By considering each edge, which is a cut edge (an edge not contained in a circuit or by its deletion the graph becomes bipartite), one of $n_u(e \mid G)$ or $n_v(e|G)$ is equal to t_{n-i} and the other one is $u_n - t_{n-i}$. By the structure of the graph G_n the number of edges of G_n that one of whose end points in closer to t_i vertices is equal to 3.2^i, $0 \leq i \leq n-1$. Therefore $A = 3\sum_{i=0}^{n-1} 2^i t_{n-i}(u_n - t_{n-i}) = 108(3n.4^n - 5.4^n + 6.2^n - 1)$.

(b) For each C_6, except the central C_6, the edges involved in a circuit, there are 4 vertices each of which is closer to $t_{n-i-1} + 3$ vertices and for the other two vertices each is closer to $t_{n-i} - 3$ vertices. Since the number of such hexagons is 3.2^i we obtain the following portion of $Sz(G_n)$.

$$
\begin{aligned}
B &= 3\sum_{i=0}^{n-1} 2^i [2(t_{n-i} - 3)(u_n - t_{n-i} + 3) \\
&\qquad + 4(t_{n-i-1} + 3)(u_n - t_{n-i-1} - 3)] \\
&= 6[216n.4^n - 378.4^n + 459.2^n - 81]
\end{aligned}
$$

(c) For the edges in the central hexagon the following term is contributed to $Sz(G_n)$:

$$C = 6(t_n + 3)(u_n - t_n - 3) = 54(8.4^n - 10.2^n + 3)$$

Finally the Szeged index of G_n is equal to $Sz(G) = A + B + C = 1620n.4^n - 2376.4^n + 2862.2^n - 432$, $n \geq 0$. □

In the end we will calculate the PI index of G_n.

Theorem 3. $PI(G_n) = 441.4^n - 639.2^n + 232$, $n \geq 0$.

Proof. By definition of the PI-index, as indicated in the introduction, we can write: $PI(G_n) = |E(G_n)|^2 - \sum_{e\in E} N(e)$, where $N(e)$ is the number of edges of G_n equidistance from e. Now it is easy to see that if e is an edge of a hexagon, then $N(e) = 2$, and if e is an edge joining any two hexagons, then $N(e) = 1$. But the number of hexagons in G_n is equal to $3.2^n - 2$ and the number of edges joining hexagons is $3(2^n - 1)$. Since the number of edges of G_n is $21.2^n - 15$ we obtain:

$$
\begin{aligned}
PI(G_n) &= (21.2^n - 15)^2 - 2(3.2^n - 2) - 3(2^n - 1) \\
&= 441.4^n - 639.2^n + 232, \quad n \geq 0 \quad □
\end{aligned}
$$

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