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The Wiener and Szeged indices of hexagonal cored dendrimers

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Abstract. A topological index of a molecule graph G is a real number which is invariant under graph isomorphism. The Wiener and Szeged indices are two important distance based topological indices applicable in nano sciences. In this paper, these topological indices are computed for hexagonal cored dendrimers.

Keywords. Wiener index, Szeged index, dendrimers, nano particles.
2010 Mathematics Subject Classification. 05C12

1 Introduction

Let G be a simple connected graph. The sets of vertices and edges of G are denoted by $V(G)$ and $E(G)$, respectively. For vertices u and v in $V(G)$, we denote by $d(u,v)$ the topological distance i.e., the number of edges on a shortest path, joining the two vertices of G. Since G is connected, $d(u,v)$ exists for all vertices $u,v \in V(G)$. A topological index is a numeric quantity derived from the structural graph of a molecule. The first topological index of this type was proposed in 1947 by the chemist Harold Wiener [1]. It is defined as the half of the sum of all distances between vertices of the graph as follows:

$$W(G) = \frac{1}{2} \sum_{i,j \in V(G)} d(i,j). \tag{1}$$

The Szeged index is a topological index introduced by Ivan Gutman [2]. To define the Szeged index of a graph G, we assume that $e = uv$ is an edge connecting the vertices u and v.

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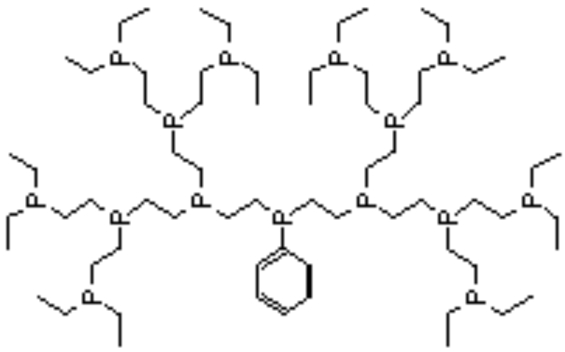

Figure 1. A tertiary phosphine dendrimer.

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

$$SZ(G) = \sum_{e=uv\in E(G)} n_u(e).n_v(e). \tag{2}$$

Notice that vertices equidistant from u and v are not taken into account. Dendrimers are macromolecules comprised of a series of branches extending outward from an inner core which have attracted much attention because of their various electrical and optical properties [4–8]. In this paper we consider a class of dendrimers such as tertiary phosphine dendrimers in which their graphs contain a hexagonal cycle and branches extending outward from hexagonal core are balanced tree (Figure 1).

We denote these described graphs by $D_{p,r}$ where r is number of generation and r is the classic degree of branching vertices of the graph (Figure 2). In this paper the computation of the Wiener and Szeged indices of hexagonal cored dendrimer are proposed.

2 Main Results

In this section at first, the Wiener index of $D_{p,r}$ will be calculated in terms of positive integer numbers p and r. For this purpose, we use of a method where introduced by Ashrafi et al. in [7]. Recall that a subgraph H of G is called convex if for each vertex $x, y \in V(H)$ there exists no shortest path in G from x to y which involves a vertex $w \in V(G) - V(H)$. Now let $\{F_i\}_{i=1}^{k}$ is a partition of $E(G)$ such that , $G - F_i$ is a two component graph such that both of components are convex for $1 \leq i \leq k$. Then the Wiener index of G is computed as

$$W(G) = \sum_{i=1}^{k} |V(GF_i(1)|.|V(GF_i(2)|, \tag{3}$$

where $GF_i(1)$ and $GF_i(2)$ are two components of $G - F_i$ for $1 \leq i \leq k$. Therefore to compute the Wiener index of $G = D_{p,r}$ the suitable partition of $E(G)$ must be introduced. Let C_6 denote the hexagonal core of the graph. One can see that $G - \{e\}$ has exactly two convex components

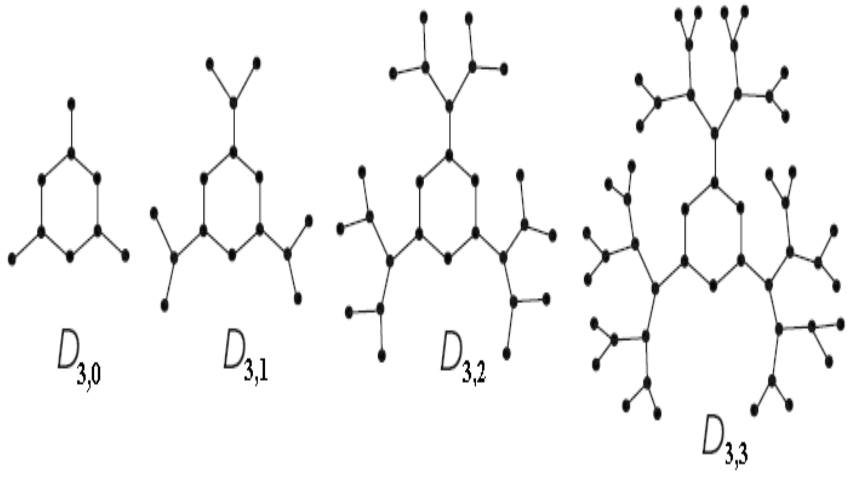

Figure 2. The graph of hexagonal cored dendrimers with generation numbers 0, 1, 2, 3.

for each $e \in E(G) - C_6$. Also for each edge of hexagonal core of the graph, the subgraphs $G - \{e_1, e_4\}$, $G - \{e_2, e_5\}$ and $G - \{e_3, e_6\}$, have exactly two convex components (see Figure 3).

Theorem 2.1. *Let $p \geq 3$. The Wiener index of hexagonal cored dendrimer computed as follows:*

$$W(G) = \frac{3}{(p-2)^2}[((p-1)^{r+1} + 6p - 13)(r(p-1)^{r+1} - \frac{(p-1)^{r+1} - p + 1}{p-2})$$
$$-\frac{(p-1)^{2r+2} - (p-1)^{r+1} - (p-1)^{r+2} + p - 1}{p-2}] + 12(\frac{(p-1)^{r+1} - 1}{p-2})^2$$
$$+45\frac{(p-1)^{r+1} - 1}{p-2} + 27.$$

Proof. Let T be one of the three acyclic branching subgraph of G, then

$$n = |V(T) = \sum_{i=1}^{r}(p-1)^i| = \frac{(p-1)^{r+1} - 1}{p-2}.$$

Now let e_i be one of the $3(p-1)^i$ edges of generation number i, then $F_i = G - \{e_i\}$ has two convex components $GF_i(1)$ and $GF_i(2)$, such that $n_i(1) = |GF_i(1)| = \sum_{j=1}^{r-i+1}(p-1)^j$ and $n_i(2) = |GF_i(2)| = 3n - 6 - n_i(1)$. For tree dotted edges shown in Figure 2 where are adjacent to C_6, we have $|GF_i(1)| = n$ and $|GF_i(2)| = 2n + 6$. Finally, foe $e \in F = G - \{e1, e_4\}$, we have $|GF_i(1)| = n + 3$ and $|GF_i(2)| = 2n + 3$.

The last equations can be used for $e \in F = G - \{e2, e_5\}$ and $e \in F = G - \{e3, e_6\}$. Thus by using Eq. 3, we have

$$W(G) = \sum_{i=1}^{k}|V(GF_i(1)|.|V(GF_i(2)| = \sum_{i=1}^{r}3(p-1)^i n_i(1).n_i(2) + 3n(2n+6) + 3(n+3)(2n+3).$$

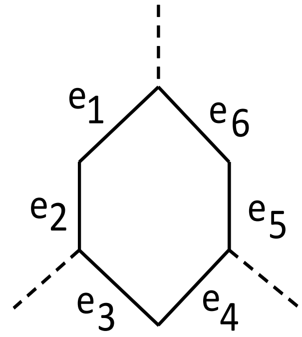

Figure 3. The graph of hexagonal cored dendrimer with generation numbers 0.

Thus

$$W(G) = \frac{3}{(p-2)^2}[((p-1)^{r+1} + 6p - 13)(r(p-1)^{r+1} - \frac{(p-1)^{r+1} - p + 1}{p-2}) \\ - \frac{(p-1)^{2r+2} - (p-1)^{r+1} - (p-1)^{r+2} + p - 1}{p-2}] + 12(\frac{(p-1)^{r+1} - 1}{p-2})^2 \\ +45\frac{(p-1)^{r+1} - 1}{p-2} + 27.$$

Therefore proof is completed. □

In what follows, by using computations in the Theorem 2.1, we obtain an exact formula for computation of the Szeged index of $D_{p,r}$, in terms of positive integer numbers p and r.

Theorem 2.2. *Let $p \geq 3$. The Szeged index of the hexagonal cored dendrimer is computed as follows:*

$$Sz(G) = \frac{3}{(p-2)^2}[((p-1)^{r+1} + 6p - 13)(r(p-1)^{r+1} - \frac{(p-1)^{r+1} - p + 1}{p-2}) \\ - \frac{(p-1)^{2r+2} - (p-1)^{r+1} - (p-1)^{r+2} + p - 1}{p-2}] + 18(\frac{(p-1)^{r+1} - 1}{p-2})^2 \\ +72\frac{(p-1)^{r+1} - 1}{p-2} + 54.$$

Proof. Let $e = uv \in F = E(G) - C_6$. Then $n_u(e) = |GF(1)|$ and $n_v(e) = |GF(2)|$. If $e = uv \in C_6$ then $n_u(e) = n + 3$ and $n_v(e) = 2n + 3$. Therefore by using Eq. 2 and the used methods in the Theorem 2.1, we have

$$SZ(G) = \sum_{e=uv \in E(G)-C_6} n_u(e).n_v(e) + \sum_{e=uv \in C_6} n_u(e).n_v(e) \\ = \sum_{i=1}^{r} 3(p-1)^i n_i(1).n_i(2) + 6(n+3)(2n+3).$$

The result can be obtained by replacing the value of n, $n_i(1)$ and $n_i(2)$ for $1 \leq i \leq r$, in the last equation. Therefore proof is completed. □

In Table 1, the numerical data for the Wiener and Szeged indices of hexagonal cored dendrimers of various value of number of generations and degree for branching vertices are given.

Table 1

p	r	$W(D_{p,r})$	$SZ(D_{p,r})$
3	1	354	516
3	2	1674	2184
3	4	39858	46488
4	4	632244	723384
4	6	71890536	79087968
5	5	98965752	110181984
6	6	24035368674	26324655804

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