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Computing the Szeged Index of Styrylbenzene Dendrimer and Triarylamine Dendrimer of Generation 1 − 3

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Abstract

Let e be an edge of a G connecting the vertices u and v. Define two sets $N_1(e|G)$ and $N_2(e|G)$ as $N_1(e|G)=\{x \in V(G) \mid d(x,u)<d(x,v)\}$ and $N_2(e|G)=\{x \in V(G) \mid d(x,v)<d(x,u)\}$. The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$ respectively. The Szeged index of the graph G is defined as $Sz(G)=\sum_{e\in E(G)} n_1(e|G)n_2(e|G)$. In this paper we compute the Szeged index of the two-type of dendrimers.

1. INTRODUCTION

Dendrimers are large and complex molecules with very well-defined chemical structures. They are nearly perfect monodisperse macromolecules with a regular and highly branched three-dimensional architecture. They consist of three major architectural components: core, branches, and end groups. Dendrimers are versatile molecular structures due to their multifunctionality and specific shape. These unique properties make them attractive molecules for their use as building blocks in larger, organized structures of higher complexity [1-3].

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edges-shapes of which are represented by V(G) and E(G), respectively. The graph G is said to be connected if for every vertices x and y in V(G) there exist a path between x and y. In this paper all of graphs are connected.

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A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labeling or pictorial representation of a graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules. Here, we consider only one topological index containing Szeged index of dendrimers. In the follow we define Wiener index.

The Wiener index W(G) [4,5] of a molecular graph G is defined as the sum of the distances between all pairs of vertices. In other words,

$$W(G) = \frac{1}{2}\left(\sum_{i=1}^{n} P_i\right)$$

where length of the path that contains the least number of is edges between vertex i and vertex j in graph G and n is the maximum possible number of i and j. In [6-17] topological indices of some nanotubes is computed. The goal of this article is to obtain a formula for the Szeged index of some dendrimers.

2. COMPUTING THE SZEGED INDEX OF STYRYLBENZENE DENDRIMER

Figure 1 shows a Styrylbenzene dendrimer which has grown n stages.

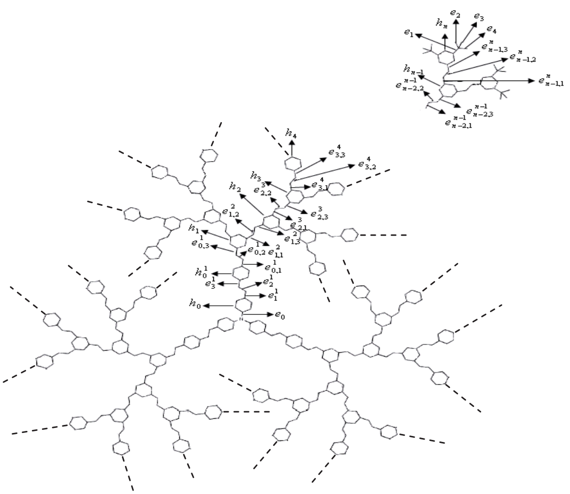

Figure 1. Styrylbenzene Dendrimer

Let h_i be a hexagon which is in stage i. Since this dendrimer has grown in stage 1 in a different way from other stages, therefore h_0 is central hexagon and h_0^1 is hexagon between h_0 and h_1. And $e_{i-1,j}^i$ be j-th edge of between h_i and h_{i-1} such that $1 \le j \le 3,\ 2 \le i \le n$. Also for the first stage the edges are denoted as is shown in figure 1.

At first we compute $n_1(e|G)$ for hexagons. Now assume that e is an edge of h_n for 4 of these edges we have $n_1(e|G) = 3+4 = 7$ and for the other 2 edges we have $n_1(e|G) = 3+8 = 11$, also the number of these hexagons is $3\times 2^{n-1}$. If e is an edge of h_{n-1}, for 4 of these edges we have $n_1(e|G) = 1\times 6 + 1\times 2 + 1\times 8 + 3 = 19$ and for the other 2 edges we have $n_1(e|G) = 2\times 6 + 2\times 2 + 2\times 8 + 3 = 35$, also the number of these hexagons is $3\times 2^{n-2}$. We continue until achieve to stage 1. Suppose that e is an edge of h_1, for 4 of these edges we have

$$n_1(e|G) = \left(2^{n-2} + 2^{n-3} + \ldots + 1\right)\times 6 +$$
$$\left(2^{n-2} + 2^{n-3} + \ldots + 1\right)\times 2 + 2^{n-2}\times 8 + 3$$
$$= \left(2^n - 1\right)\times 6 + \left(2^n - 1\right)\times 2 + 2^{n-2}\times 8 + 3$$

and for the other 2 edges we have

$$n_1(e|G) = \left(2^{n-1} + 2^{n-2} + \ldots + 2\right)\times 6 +$$
$$\left(2^{n-1} + 2^{n-2} + \ldots + 2\right)\times 2 + 2^{n-1}\times 8 + 3$$
$$= \left(2^n - 2\right)\times 6 + \left(2^n - 2\right)\times 2 + 2^{n-1}\times 8 + 3$$

also the number of these hexagons is 3. If e is an edge of the hexagon h_0^1, for all of edges of h_0^1 we have

$$n_1(e|G) = \left(2^{n-1} + 2^{n-2} + \ldots + 2 + 1\right)\times 6 +$$
$$\left(2^{n-1} + 2^{n-2} + \ldots + 2 + 1\right)\times 2 + 2^{n-1}\times 8 + 3$$
$$= \left(2^n - 1\right)\times 6 + \left(2^n - 1\right)\times 2 + 2^{n-1}\times 8 + 3$$

also the number of these hexagons is 3. If e is an edge of the hexagon h_0, for all of edges of h_0 we have

$$n_1(e|G) = (2^{n-1} + 2^{n-2} + ... + 2 + 2) \times 6 +$$
$$(2^{n-1} + 2^{n-2} + ... + 2 + 2) \times 2 + 2^{n-1} \times 8 + 3$$
$$= 2^n \times 6 + 2^n \times 2 + 2^{n-1} \times 8 + 3$$

also the number of these hexagons is 3.

Now $n_1(e|G)$ is computed for $e^i_{i-1,j}$. Suppose that e is the edge $e^n_{n-1,3}$, we have $n_1(e|G) = 1\times 6 + 1\times 8 = 14$, for the edge $e^n_{n-1,2}$ we have $n_1(e|G) = 15$, for the edge $e^n_{n-1,1}$ we have $n_1(e|G) = 16$, the number of these edges is $3 \times 2^{n-1}$. We continue until achieve to stage 1. Suppose that e is the edge $e^1_{0,3}$ we have

$$n_1(e|G) = (2^{n-1} + 2^{n-2} + ... + 2 + 1) \times 6 + 2^{n-1} \times 8 +$$
$$(2^{n-1} + 2^{n-2} + ... + 2) \times 2$$
$$= (2^n - 1) \times 6 + 2^{n-1} \times 8 + (2^n - 2) \times 2$$

Also

$$n_1(e|G) = (2^{n-1} + 2^{n-2} + ... + 2 + 1) \times 6 + 2^{n-1} \times 8 +$$
$$(2^{n-1} + 2^{n-2} + ... + 2) \times 2 + 1$$
$$= (2^n - 1) \times 6 + 2^{n-1} \times 8 + (2^n - 2) \times 2 + 1$$

and

$$n_1(e|G) = (2^{n-1} + 2^{n-2} + ... + 2 + 1) \times 6 + 2^{n-1} \times 8 +$$
$$(2^{n-1} + 2^{n-2} + ... + 2) \times 2 + 2$$
$$= (2^n - 1) \times 6 + 2^{n-1} \times 8 + (2^n - 2) \times 2 + 2$$

the number of these edges is 3. If e is the edge e^1_3 we have

$$n_1(e^1_3|G) = (2^{n-1} + 2^{n-2} + ... + 2 + 2) \times 6 + 2^{n-1} \times 8 +$$
$$(2^{n-1} + 2^{n-2} + ... + 2 + 1) \times 2$$
$$= 2^n \times 6 + 2^{n-1} \times 8 + (2^n - 1) \times 2 = a$$

if e is the edge e^1_2 we have $n_1(e^1_2|G) = a + 1$, if e is the edge e^1_1 we have $n_1(e|G) = a + 2$, the number of these edges is 3. Suppose that e is the edge e_0 we have

$$n_1(e_0 \mid G) = \left(2^{n-1} + 2^{n-2} + \ldots + 2 + 3\right) \times 6 + 2^{n-1} \times 8 +$$
$$\left(2^{n-1} + 2^{n-2} + \ldots + 2 + 2\right) \times 2$$
$$= \left(2^n + 1\right) \times 6 + 2^{n-1} \times 8 + 2^n \times 2$$

the number of these edges is 3.

Suppose that $e = e_1$ in the figure 1, then $n_1(e \mid G) = 4$, the number of these edges is 3×2^n. Now, let e be one of e_2, e_3 or e_4, then $n_1(e_2 \mid G) = n_1(e_3 \mid G) = n_1(e_4 \mid G) = 1$, the number of these edges is $3 \times 2^{n-1} \times 6$. Now the Szeged index of this dendrimer when it grows n stages is computed:

$$Sz(G_n) = \sum_{i=0}^{n-1} 3 \times 2^i \times \left[\begin{array}{l} 2 \times \underbrace{\left(\left(2^{n-i} - 2\right) \times 6 + \left(2^{n-i} - 2\right) \times 2 + 2^{n-1-i} \times 8 + 3\right)}_{a_1} \times \left(r - a_1\right) \\ +4 \times \underbrace{\left(\left(2^{n-1-i} - 1\right) \times 6 + \left(2^{n-1-i} - 1\right) \times 2 + 2^{n-2-i} \times 8 + 3\right)}_{a_2} \times \left(r - a_2\right) \end{array}\right]$$
$$+ 3 \times 6 \times \left[\underbrace{\left(\left(2^n - 1\right) \times 6 + \left(2^n - 1\right) \times 2 + 2^{n-1} \times 8 + 3\right)}_{a_3} \times \left(r - a_3\right)\right]$$
$$+ 3 \times 6 \times \left[\underbrace{\left(2^n \times 6 + 2^n \times 2 + 2^{n-1} \times 8 + 3\right)}_{a_4} \times \left(r - a_4\right)\right]$$
$$+ \sum_{i=0}^{n-1} 3 \times 2^i \times \left[\begin{array}{l} \underbrace{\left(\left(2^{n-i} - 1\right) \times 6 + 2^{n-1-i} \times 8 + \left(2^{n-i} - 2\right) \times 2\right)}_{a_5} \times \left(r - a_5\right) \\ + \left(a_5 + 1\right) \times \left(r - a_5 - 1\right) + \left(a_5 + 2\right) \times \left(r - a_5 - 2\right) \end{array}\right]$$
$$+ 3 \times \left[\begin{array}{l} \underbrace{\left(2^n \times 6 + 2^{n-1} \times 8 + \left(2^n - 1\right) \times 2\right)}_{a_6} \times \left(r - a_6\right) \\ + \left(a_6 + 1\right) \times \left(r - a_6 - 1\right) + \left(a_6 + 2\right) \times \left(r - a_6 - 2\right) \end{array}\right]$$
$$+ 3 \times \left[\underbrace{\left(\left(2^n + 1\right) \times 6 + 2^{n-1} \times 8 + 2^n \times 2\right)}_{a_7} \times \left(r - a_7\right)\right]$$
$$+ 3 \times 2^n \times 4 \times (r - 4) + 3 \times 2^{n-1} \times 6 \times (r - 1)$$

Since $r = 3 \times \left(\left(2^n + 1\right) \times 6 + 2^n \times 2 + 2^{n-1} \times 8\right) + 1 = 3 \times \left(12 \times 2^n + 6\right) + 1$ is the number of vertices of this graph, we have

$$Sz(G_n) = 17820 \times 2^n + 1512 \times 4^n + 9324 \times n \times 2^n + 9072 \times n \times 4^n + 4962$$

3. COMPUTING THE SZEGED INDEX OF TRIARYLAMINE DENDRIMER OF GENERATION 1 −3

Figure 2 shows a Triarylamine Dendrimer of Generation 1 − 3 which has grown n stages.

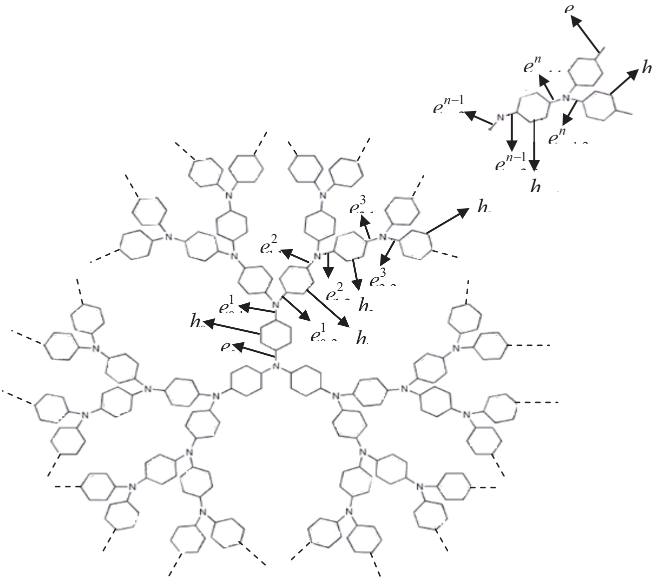

Figure 2. Triarylamine Dendrimer of Generation 1 − 3

Let h_i be a hexagon which is in the stage i. Also, let $e_{i-1,j}^{i}$ be j-th edge of between h_i and h_{i-1} such that $1 \le j \le 2, 1 \le i \le n$. At first we compute $n_1(e|G)$ for hexagons. Now assume that e is an edge of h_n for all 6 edges: $n_1(e|G) = 3+1 = 4$, the number of these hexagons is 3×2^n. if e is an edge of h_{n-1} for all 6 edges: $n_1(e|G) = 2\times 6+3+1+2 = 18$, the number of these hexagons is $3\times 2^{n-1}$. We continue until achieve to stage 1. If e is an edge of the hexagon h_1, for all of edges of h_1 we have

$$\begin{aligned} n_1(e|G) &= \left(2^{n-1}+2^{n-2}+\ldots+2\right)\times 6+3+1+2+\ldots+2^{n-1} \\ &= \left(2^n-2\right)\times 6+3+\left(2^n-1\right) \end{aligned}$$

Also the number of these hexagons is 3×2. If e is an edge of the hexagon h_0, for all of edges of h_0 we have

$$n_1(e|G)=\left(2^n+2^{n-1}+\ldots+2\right)\times 6+3+1+2+\ldots+2^n$$
$$=\left(2^{n+1}-2\right)\times 6+3+\left(2^{n+1}-1\right)$$

Also the number of these hexagons is 3. Suppose that e is the edge e_n we have $n_1(e|G)=1$, the number of these edges is 3×2^n. Now $n_1(e|G)$ is computed for $e^i_{i-1,j}$. Suppose that e is the edge $e^n_{n-1,2}$ we have $n_1(e|G)=6+1=7$, the number of these edges is 3×2^n. If e is the edge $e^n_{n-1,1}$ we have $n_1(e|G)=2\times 6+1+2=15$, the number of these edges is $3\times 2^{n-1}$. We continue until achieve to stage 1. If e is the edge $e^1_{0,2}$ we have

$$n_1(e|G)=\left(2^{n-1}+2^{n-2}+\ldots+2+1\right)\times 6+1+2+\ldots+2^{n-1}$$
$$=\left(2^n-1\right)\times 6+\left(2^n-1\right)$$

The number of these edges is 3×2. If e is the edge $e^1_{0,1}$ we have

$$n_1(e|G)=\left(2^n+2^{n-1}+\ldots+2^2+2\right)\times 6+1+2+\ldots+2^{n-1}+2^n$$
$$=\left(2^{n+1}-2\right)\times 6+\left(2^{n+1}-1\right)$$

the number of these edges is 3. Suppose that e is the edge e_0 we have

$$n_1(e|G)=\left(2^n+2^{n-1}+\ldots+2^2+2+1\right)\times 6+1+2+\ldots+2^{n-1}+2^n$$
$$=\left(2^{n+1}-1\right)\times 6+\left(2^{n+1}-1\right)$$

the number of these edges is 3. Now the Szeged index of this dendrimer when it grows n stages is computed in follows:

$$Sz(G_n)=\sum_{i=0}^{n}3\times 2^i\times\left[6\times\underbrace{\left(\left(2^{n+1-i}-2\right)\times 6+3+\left(2^{n+1-i}-1\right)\right)}_{a_1}\times(r-a_1)\right]$$
$$+\sum_{i=0}^{n}3\times 2^i\times\left[\underbrace{\left(\left(2^{n+1-i}-1\right)\times 6+\left(2^{n+1-i}-1\right)\right)}_{a_2}\times(r-a_2)\right]$$
$$+\sum_{i=1}^{n}3\times 2^{i-1}\times\left[\underbrace{\left(\left(2^{n+2-i}-2\right)\times 6+\left(2^{n+2-i}-1\right)\right)}_{a_3}\times(r-a_3)\right]$$

Since $r=21\times\left(2^{n+1}-1\right)+1$ is the number of vertices of this graph, we have

$Sz\left(G_n\right)=14112\times n\times 4^n-15456\times 4^n+19476\times 2^n-2346$

The Szeged index of the Triarylamine Dendrimer of Generation 1 − 3 which have grown 10 stages is summarized in the following table:

n	$r=21\times\left(2^{n+1}-1\right)+1$	$Sz\left(G_n\right)$
1	64	30852
2	148	278082
3	316	1866222
4	652	10771974
5	1324	56920374
6	2668	284240790
7	5356	1365680214
8	10732	6382569942
9	21484	29219658966
10	42988	131656139478

Szeged index of the Triarylamine Dendrimer of Generation 1 − 3

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