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Computing the Szeged Index of Two Type Dendrimer Nanostars

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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 $N_1(e|G) = \{x \in V(G) | d(x,u) < d(x,v)\}$ and $N_2(e|G) = \{x \in V(G) | d(x,v) < d(x,u)\}$. 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 $Sz(G) = \sum_{e \in E} n_1(e|G)\, n_2(e|G)$. In this paper we compute the szeged index of the first and second type of dendrimer nanostar.

INTRODUCTION

Dendrimers are large and complex molecules with very well-defined chemical structures. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse (basically meaning of a consistent size and form) macromolecules with a regular and highly branched three-dimensional architecture. They consist of three major architectural components: core, branches and end groups. Dendrimers are produced in an iterative sequence of reaction steps.[1] We can consider the figure of dendrimers as the shape of molecular graph.

A graph G consist of a set of vertices V(G) and a set of edges E(G). In chemical graph, each vertex represented an atom of the molecule, and covalent bonds between atoms are represented by edges between the corresponding vertices. This shape derive from a chemical compound is often called its molecular graph, and can be a path, a tree or in general a graph.

A topological index is a single number, derived following a certain rule, which can be used to characterize the molecule.[2] Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener[3] introduced Wiener index to demonstrate correlations between physico-chemical properties of organic compounds and the index of their molecular graphs. Wiener originally defined his index (W) on trees and studied its use for correlation of physico chemical properties of alkanes, alcohols, amines and their analogous compounds.[4] A number of successful QSAR studies have been made based on the Wiener index and its decomposition forms.[5] Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz.[6] The Szeged index, is a modification of Wiener index to cycle molecules. The Szeged index was conceived by Gutman at the Attila Jozsef University in Szeged. This index received considerable attention. It has attractive mathematical characteristics.[7]

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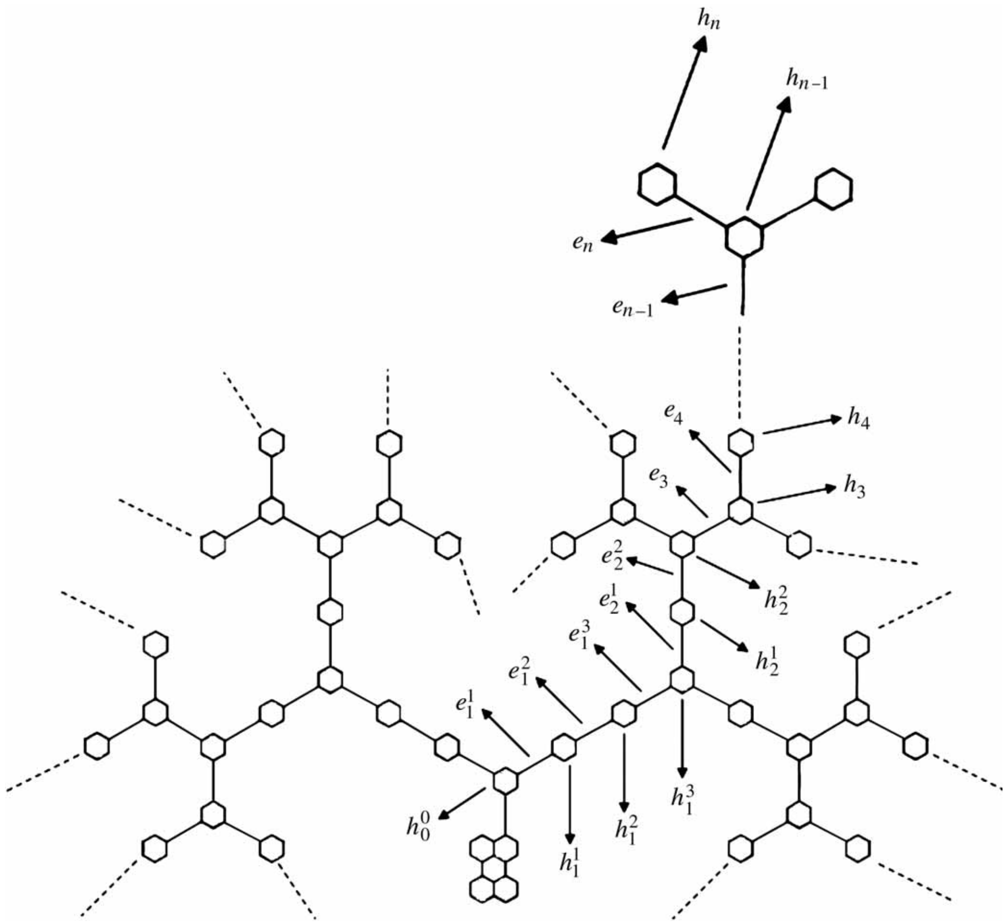

Figure 1. First-type nanostar.

In a connected graph Wiener index is equal to sum distances between all different vertices from that graph. So the Wiener number of graph G is defined by: $W(\mathrm{G}) = \frac{1}{2}\sum_{v,w\in \mathrm{V}} d(v,w)$ in Refs. 8–11.

In this paper, we compute the Szeged index of the first and second type of dendrimer nanostars.

COMPUTING THE SZEGED INDEX OF FIRST-TYPE NANOSTAR

Figure 1 shows a first-type nanostar which has grown n stages.

In Figure 1, we show the graph of this nanostar. In this figure we have 1 nucleus and a central hexagon denoted by h_0^0. In the stages 1 and 2, denoted the hexagons and edges by h_i^j, where $1 \le i \le 2$, $1 \le j \le 3$ and in the other stages, we denoted the hexagons and edges by h_j and e_j. The grown of this nanostar from the stage 3 is the same and we have only two hexagons in each stage. Now, we start the computing of the Szeged index of this nanostar from stage n. Suppose that e is an edge of the hexagon h_n, for all of edges of h_n we have $n_1(e|\mathrm{G}) = 3$, also the number of these hexagons is 2^n. Suppose further that e is an edge of h_{n-1}, for 4 of these edges we have $n_1(e|\mathrm{G}) = 1 \times 6 + 3$ and for the other 2 edges we have $n_1(e|\mathrm{G}) = 2 \times 6 + 3$, also the number of these hexagons is 2^{n-1}. Now assume that e is an edge of h_k so that $3 \le k \le n$, in this case, for 4 of the edges we have $n_1(e|\mathrm{G}) = (2^{n-k} - 1) \times 6 + 3$ and for the other 2 edges we have $n_1(e|\mathrm{G}) = 2 \times (2^{n-k} - 1) \times 6 + 3$, the number of these hexagons is 2^k. If e is an edge of h_2^2, for 4 of the edges we have $n_1(e|\mathrm{G}) = (2^{n-2} - 1) \times 6 + 3$ and for the other 2 edges we have $n_1(e|\mathrm{G}) = 2 \times (2^{n-2} - 1) \times 6 + 3$, the number of these hexagons is 2^2. If e is an edge of h_2^1, for all 6 edges: $n_1(e|\mathrm{G}) = (2^{n-1} - 1) \times 6 + 3$, the number of these hexagons is 2^2. If e is an edge of h_1^3, for 4 of the edges we have $n_1(e|\mathrm{G}) = 2^{n-1} \times 6 + 3$ and for the other 2 edges we have $n_1(e|\mathrm{G}) = 2^n \times 6 + 3$, the number of these hexagons is 2. If e is an edge of h_1^2, for all 6 edges: $n_1(e|\mathrm{G}) = (2^n + 1) \times 6 + 3$, the number of these hexagons is 2. If e is an edge of h_1^1, for all 6 edges: $n_1(e|\mathrm{G}) = (2^n + 2) \times 6 + 3$, the number of these hexagons is 2. If e is an edge of h_0^0, for 4 of the edges we have $n_1(e|\mathrm{G}) = (2^n + 3) \times 6 + 3$ and for the other 2 edges we have $n_1(e|\mathrm{G}) = 2 \times (2^n + 3) \times 6 + 3$. Now assume that e is the edge e_n we have $n_1(e|\mathrm{G}) = 6$ and the number of these edges is 2^n. For the edge e_{n-1} we have $n_1(e_{n-1}|\mathrm{G}) = (2 + 1)\times 6$ and the number of these edges is 2^{n-1}. For the edge e_k in a way that $3 \le k \le n$ we have $n_1(e_k|\mathrm{G}) = (2^{n-k+1} - 1)\times 6$, the number of these edges is 2^k. For the edge e_2^2 we have $n_1(e_2^2|\mathrm{G}) = (2^{n-1} - 1)\times 6$. For the edge e_2^1 we have $n_1(e_2^1|\mathrm{G}) = 2^{n-1}\times 6$, the number of these edges is 2^2. For the edge e_1^3 we have $n_1(e_1^3|\mathrm{G}) = (2^n + 1)\times 6$. For the edge e_1^2 we have $n_1(e_1^2|\mathrm{G}) = (2^n + 2)\times 6$. For the edge e_1^1 we have $n_1(e_1^1|\mathrm{G}) = (2^n + 3)\times 6$, the number of these edges in stage one is 2. For the edge between the nucleus and central hexagon (h_0^0), we have $n_1(e|\mathrm{G}) = (2^{n+1} + 7)\times 6$.

Now we obtain $n_1(e|\mathrm{G})$ for the edges of the nucleus.

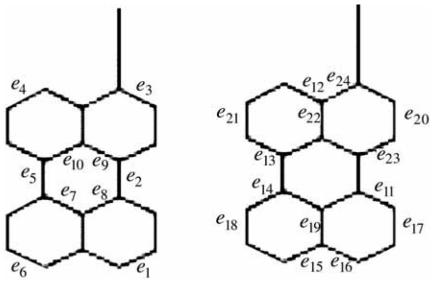

Figure 2. Nucleus.

According to the Figure 2, we have $n_1(e_i|\mathrm{G}) = 10$ for i = 1,2,3,4,5,6,7,8,9,10, for i = 11,12,13,14,15,16 we have $n_1(e_i|\mathrm{G}) = 3$, for i = 17,18,19, $n_1(e_i|\mathrm{G}) = 5$, for i = 20,21,22, $n_1(e_i|\mathrm{G}) = 15$ and for i = 23,24, $n_1(e_i|\mathrm{G}) = 17$.

The number of the vertices of this nanostar is equal to $r = (2^{n+1} + 7)\times 6 + 20$. But we know that $n_2(e|\mathrm{G}) = r - n_1(e|\mathrm{G})$ for any of edge e. Now the Szeged index of the above nanostar is obtained in the following way:

$$
\begin{aligned}
Sz(\mathrm{G}_n) = {} & \\
& \sum_{k=3}^{n}\left[2^k\begin{pmatrix}4\times((2^{n-k}-1)\times 6+3)(r-(2^{n-k}-1)\times 6-3)\ + \\ 2\times(2(2^{n-k}-1)\times 6+3)(r-2(2^{n-k}-1)\times 6-3)\end{pmatrix}\right]+ \\
& 2^2\begin{bmatrix}4\times((2^{n-2}-1)\times 6+3)(r-(2^{n-2}-1)\times 6-3)+ \\ 2(2(2^{n-2}-1)\times 6+3)(r-2(2^{n-2}-1)\times 6-3)\end{bmatrix} \\
& 2^2\,[6((2^{n-1}-1)\times 6+3)(r-(2^{n-1}-1)\times 6-3)]\ + \\
& 2\begin{bmatrix}4(2^{n-1}\times 6+3)(r-2^{n-1}\times 6-3)+ \\ 2(2^n\times 6+3)(r-2^n\times 6-3)\end{bmatrix}+ \\
& 2\,[6((2^n+1)\times 6+3)(r-(2^n+1)\times 6-3)]\ + \\
& 2\,[6((2^n+2)\times 6+3)(r-(2^n+2)\times 6-3)]\ + \\
& 4((2^n+3)\times 6+3)(r-(2^n+3)\times 6-3)\ + \\
& 2((2(2^n+3)\times 6+3))(r-2(2^n+3)\times 6-3)\ + \\
& \sum_{k=3}^{n}[2^k((2^{n-k+1}-1)\times 6(r-(2^{n-k+1}-1)\times 6))]+ \\
& 2^2\,[(2^{n-1}-1)\times 6(r-(2^{n-1}-1)\times 6)]\ + \\
& 2^2\,[2^{n-1}\times 6(r-2^{n-1}\times 6)]\ + \\
& 2\,[(2^n+1)\times 6\,(r-(2^n+1)\times 6)]\ + \\
& 2\,[(2^n+2)\times 6\,(r-(2^n+2)\times 6)]\ + \\
& 2\,[(2^n+3)\times 6\,(r-(2^n+3)\times 6)]\ + \\
& (2^{n+1}+7)\times 6\,(r-(2^{n+1}+7)\times 6) \\
& 10\times 10\times(r-10)+6\times 3\times(r-3)\ + \\
& 3\times 5\times(r-5)+3\times 15\times(r-15)+2\times 17\times(r-17) = \\
& 41788+16812\times 2^n+4440\times 2^n\times n\ + \\
& 468\times 4^n+720\times n\times 4^n.
\end{aligned}
$$

The Szeged index of the first-type nanostars which have grown 10 stages is summarized in table I.

TABLE I. The Szeged index of the first-type nanostars

n	$r = (2^{n+1} + 7) \times 6 + 20$	$Sz(\mathrm{G}_n)$
3	158	451036
4	254	1452028
5	446	5455804
6	830	22434364
7	1598	96415036
8	3134	421596988
9	6206	1850485564
10	12350	8103203644

COMPUTING THE SZEGED INDEX OF SECOND-TYPE NANOSTAR

Figure 3 shows a second-type nanostar which has grown n stages.

Let h_i^i be the hexagon between hexagons h_i and h_{i-1}. Let e_i^j be j-th edge of between two hexagons in the stage i, $1 \le i \le n$, $1 \le j \le 2$. In the first step we compute $n_1(e|\mathrm{G})$ for h_i's. For the h_n we have $n_1(e|\mathrm{G}) = 3$ which is the same for all of its six edges, the number of these hexagons is 2^n. If e is an edge of h_{n-1}, for 2 of the edges of the hexagon, we have $n_1(e|\mathrm{G}) = 2\times 2\times 6 + 3$ and for the other 4 edges we have $n_1(e|\mathrm{G}) = 2\times 6 + 3$, the number of these hexagon is 2^{n-1}. Now assume that e is an edge of h_{k-1}, $1 \le k \le n$, for 2 of the edges we have $n_1(e|\mathrm{G}) = 2\times(2^{n-(k-1)} + 2^{n-k} + ... + 2)\times 6 + 3 = 2\times(2^{n-k+2} - 2)\times 6 + 3$ and for the other 4: $n_1(e|\mathrm{G}) = (2^{n-(k-1)} + 2^{n-k} + ... + 2)\times 6 + 3 = (2^{n-k+2} - 2)\times 6 + 3$, the number of these hexagons is $2^{(k-1)}$. Now we compute $n_1(e|\mathrm{G})$ for h_i^i's. For all of six edges of

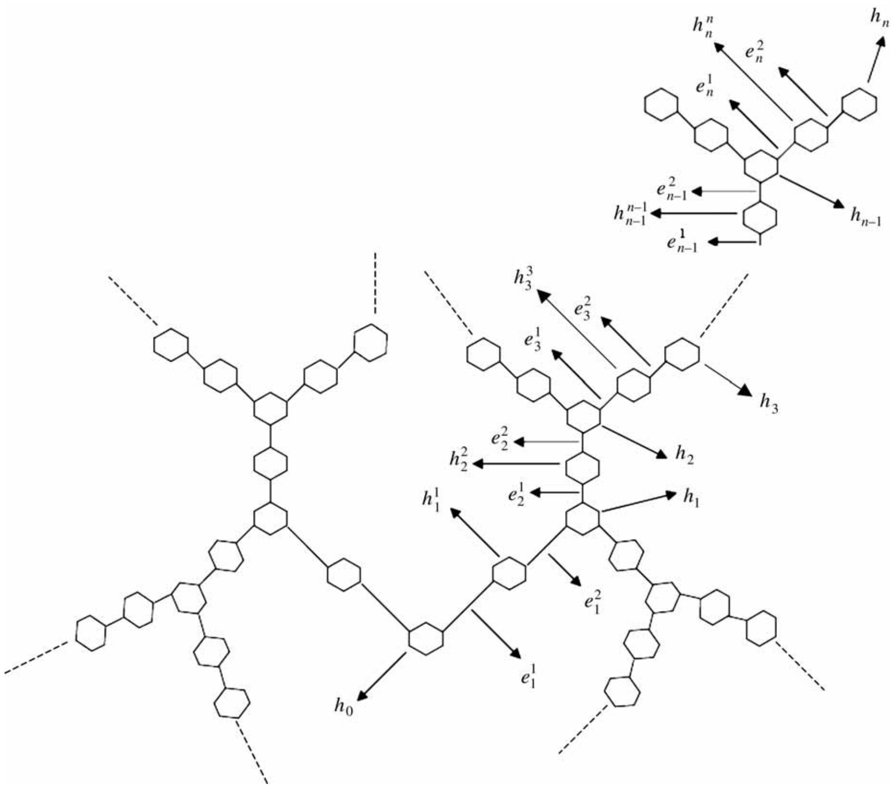

Figure 3. Second-type nanostar.

the h_n^n we have $n_1(e|G) = 9$, the number of these hexagons is 2^n. If e is an edge of h_{n-1}^{n-1}, for all six edges: $n_1(e|G) = (2^2 + 1)\times 6 + 3$, the number of this hexagon is 2^{n-1}. If e is an edge of h_k^k, $1 \le k \le n-1$, for all of the six edges, $n_1(e|G) = (2^{n-k+1} + 2^{n-k} + ... + 2^2 + 1) \times 6 + 3 = (2^{n-k+2} - 3) \times 6 + 3$, the number of these hexagons is 2^k. Now $n_1(e|G)$ is computed for e_i^j. For the edge e_n^2, $n_1(e_n^2|G) = 1 \times 6$. For the edge e_n^1, $n_1(e_n^1|G) = 2 \times 6$, the number of these edges is 2^n. For the edge e_{n-1}^2, $n_1(e_{n-1}^2|G) = (2^2 + 1) \times 6$. For the edge e_{n-1}^1, $n_1(e_{n-1}^1|G) = (2^2 + 2) \times 6$, the number of these edges is 2^{n-1}. For the edge e_k^2 we have $n_1(e_k^2|G) = (2^{n-k+2} - 3) \times 6$ and $n_1(e|G)$ for the edges e_i^1 is as follows: for the edge e_k^1 we have $n_1(e_k^1|G) = (2^{n-k+2} - 2) \times 6$, the number of these edges is 2^k. Therefore we have computed $n_1(e|G)$ for all of the edges of this nanostar. The number of the vertices of this nanostar is equal to $r = (2^{n+2} - 3) \times 6$. But we know that $n_2(e|G) = r - n_1(e|G)$ for any of edge e. Now its Szeged index is obtained easily.

$$Sz(G_n) =$$

$$\sum_{k=1}^{n}\left[2^{k-1}\times\begin{pmatrix}2\times(2\times(2^{n-k+2}-2)\times 6+3)(r-2\times(2^{n-k+2}-2)\times 6-3)\\ +4\times((2^{n-k+2}-2)\times 6+3)(r-(2^{n-k+2}-2)\times 6-3\end{pmatrix}\right]+$$

$$\sum_{k=1}^{n-1}[2^k(6\times((2^{n-k+2}-3)\times 6+3))(r-(2^{n-k+2}-3)\times 6-3)]+$$

$$2^n(6\times(9(r-9)+3(r-3)))+$$

$$\sum_{k=1}^{n}[2^k((2^{n-k+2}-3)\times 6)(r-(2^{n-k+2}-3)\times 6)]+$$

$$\sum_{k=1}^{n}[2^k((2^{n-k+2}-2)\times 6)(r-(2^{n-k+2}-2)\times 6)]=$$

$$-882+6912\times 4^n\times n-15264\times 4^n+3456\times 2^n\times n+16200\times 2^n.$$

The Szeged index of the second-type nanostar when it has grown eight stages, is shown in the following table II.

TABLE II. The Szeged index of the second-type nanostar

n	$r = (2^{n+2} - 3) \times 6$	$Sz(G_n)$
2	78	68526
3	174	561870
4	366	3649806
5	750	20829582
6	1518	109710990
7	3054	547807374
8	6126	2634761358

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SAŽETAK

Račun szegedskog indeksa za dva tipa dendrimerskih nanozvijezda

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Neka je e grana u grafu G koja povezuje čvorove u i v. Definirajmo skupove: $N_1(e|G) = \{x \in V(G) | d(x,u) < d(x,v)\}$ i $N_2(e|G) = \{x \in V(G) | d(x,v) < d(x,u)\}$ a njihove kardinalitete označimo s: $n_1(e|G)$ i $n_2(e|G)$. Szegedski indeks, Sz(G), grafa G je definiran s: $Sz(G) = \sum_{e \in E} n_1(e|G)\, n_2(e|G)$. U radu je izračunat Sz za dva tipa dendrimerskih nanozvijezda.