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SZEGED INDEX OF AN INFINITE FAMILY OF NANOSTAR DENDRIMERS

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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 macromolecules that appear to be photon funnels just like artificial antennas. The aim of this paper is topological study of such molecules. Our main result is computing Szeged index of an infinite class of nanostars. It is proved that the method is general and can be applied for other nanostars.

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1. Introduction

Nanobiotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. Dendrimers are one of the main objects of this new area of science. Here a dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a step-wise fashion from simple branched monomer units, the nature and functionality of which can be easily controlled and varied. The nanostar dendrimer is part of a new group of macromolecules that the structure and the energy transfer mechanism must be understood.

A map taking graphs as arguments is called a graph invariant or topological index if it assigns equal values to isomorphic graphs. 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.

The Szeged index is a topological index introduced by Ivan Gutman. The aim of this paper is to present a novel method for computing this topological index for dendrimer nanostars. The presented method is general and can be used for other distance based topological indices.

2. Definitions

Some algebraic definitions used for the study are given. Let G be a graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of G is denoted by d(u,v) and it is defined as the number of edges in a minimal path connecting the vertices u and v.

A molecular graph is a graph such that vertices represent atoms and edges represent bonds. These graphs have been used for affinity diagrams showing a relationship between chemical substances. Obviously, the degree of each atom in a molecular graph is at most four.

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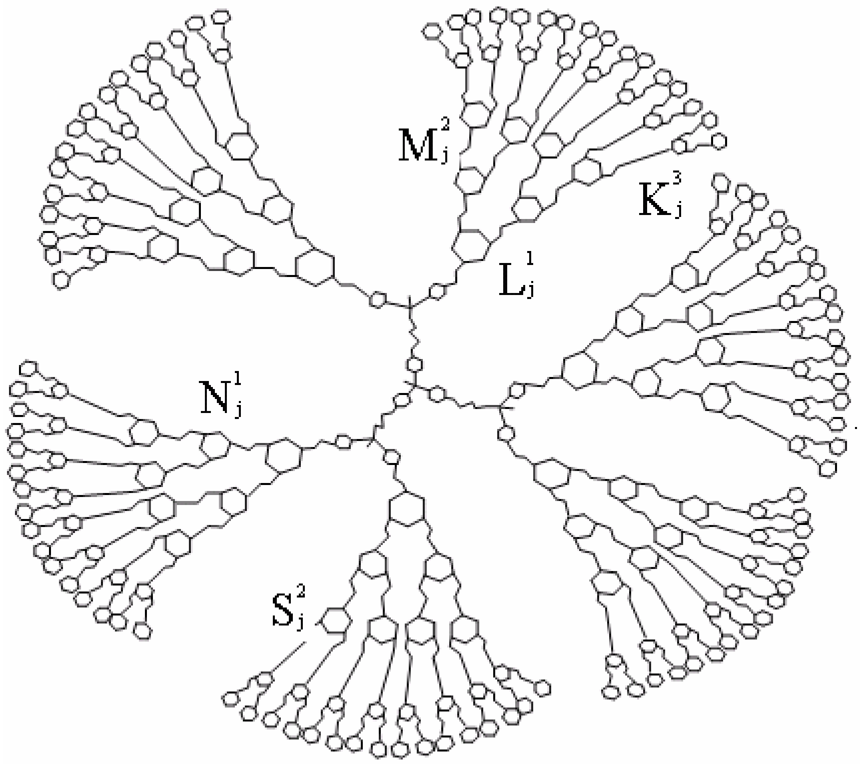

Fig. 1. The molecular graph of the nanostar dendrimer NS[4].

The Wiener index is the first distance based topological index was introduced in 1947 by chemist Harold Wiener[1] as the half-sum of all topological distances in the hydrogen-depleted graph representing the skeleton of the molecule. We encourage the readers to consult papers[2,3] and references therein for background material and historical aspect of the Wiener index.

The Szeged index is another topological index introduced by Ivan Gutman.[4-7] 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 and $n_v(e)$ is the number of vertices of G lying closer to v. 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. We encourage the reader to consult our earlier paper[8-12] for background material as well as basic computational techniques. Our notations are standard and taken mainly from the standard book of graph theory.

3. Theorem and Proof

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. Throughout this section NS[n] denotes the molecular graph of a nanostar dendrimer with exactly n generation, Fig. 1. The Szeged index of this nanostar is computed for the first time. The aim of this section is to prove the following theorem:

Theorem. The Szeged index of the nanostar dendrimer NS[n] is computed as follows:

$$18432n.4^n + 9984n.2^n - 33024.4^n + 20856.2^n + 12168.$$

Proof. To prove the theorem we partition the edges of NS[n] into 20 classes as follows:

$$E_i^0, i = 1,...,4 \;;\; E_j^0, j = 1,...,6 \;;\; E_k^0, k = 1,2,3$$

$E_{l_1}^0, l_1 = 1, 2,3$; $E_{l_2}^0, l_2 = 1, 2,3$; $E_{l_3}^0, l_3 = 1, 2,3$

$E_{l_4}^0, l_4 = 1, 2,3$; $E_{l_5}^0, l_5 = 1, 2,3$;

$E_{m_1}^0, m_1 = 1,...,6$; $E_{m_2}^0, m_2 = 1,...,6$

$E_{m_3}^0, m_3 = 1,...,6$; $H_i^0, i = 1,...,18$

$F_i^o, i = 1,...,36$; $G_i^0, i = 1,...,24$; $G_j^0, j = 1,...,12$

$L_j^i, 1 \le i \le n, 1 \le j \le 3.2^{i+1}$; $M_j^i, 1 \le i \le n, 1 \le j \le 3.2^{i+1}$;

$K_j^i, 1 \le i \le n, 1 \le j \le 3.2^{i+1}$; $N_j^i, 1 \le i \le n, 1 \le j \le 3.2^{i+3}$;

$S_j^i, 1 \le i \le n, 1 \le j \le 3.2^{i+2}$.

In Fig. 2, these edges are depicted. For simplicity, we name these edges, type 1, type 2, …, type 20. To compute the Szeged index of NS[n], it is enough to compute $n_u(e)$ and $n_v(e)$ for above edges. In Table 1, these values for each type are reported.

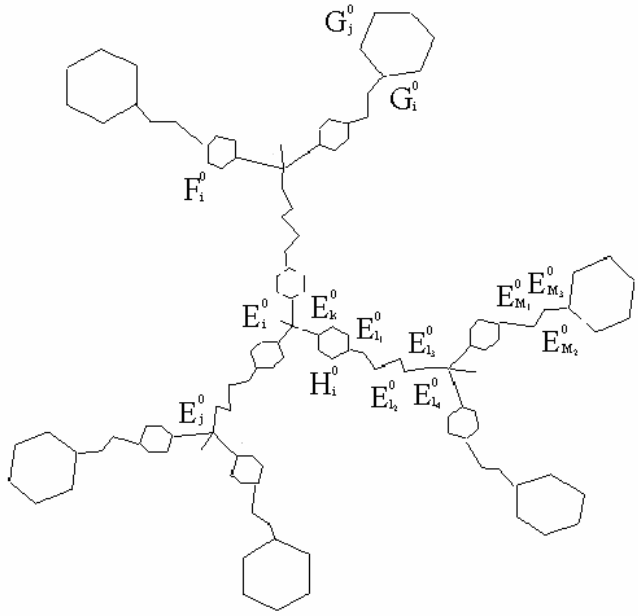

Fig. 2. The core of the nanostar dendrimer NS[n].

Table 1. The values of $n_u(e)$ and $n_v(e)$ for the edges of the nanostar dendrimer NS[n].

Edges	$\mathbf{n_u(e)}$	$\mathbf{n_v(e)}$	**Edges**	$\mathbf{n_u(e)}$	$\mathbf{n_v(e)}$
Type 1	$48.2^{n+1}+25$	1	Type 11	$2^{n+4} - 10$	$48.2^{n+1} + 36 – 2^{n+4}$
Type 2	$2^{n+4} - 2$	$48.2^{n+1} + 28 – 2^{n+4}$	Type 12	$2^{n+5} + 2$	$48.2^{n+1} + 24 – 2^{n+5}$
Type 3	$2^{n+5} + 8$	$48.2^{n+1} + 18 – 2^{n+5}$	Type 13	$2^{n+4} - 5$	$48.2^{n+1} + 31 – 2^{n+4}$
Type 4	$2^{n+5} + 2$	$48.2^{n+1} + 24 – 2^{n+5}$	Type 14	$2^{n+3} - 5$	$48.2^{n+1} + 31 – 2^{n+3}$
Type 5	$2^{n+5} + 1$	$48.2^{n+1} + 25 – 2^{n+5}$	Type 15	$2^{n+4} - 13$	$48.2^{n+1} + 39 – 2^{n+4}$
Type 6	2^{n+1}	$48.2^{n+1} + 26 – 2^{n+5}$	Type 16	$2^{n+4-i} - 8$	$48.2^{n+1} + 34 – 2^{n+4-i}$
Type 7	$2^{n+1} - 1$	$48.2^{n+1} + 27 – 2^{n+5}$	Type 17	$2^{n+4-i} - 9$	$48.2^{n+1} + 35 – 2^{n+4-i}$
Type 8	$2^{n+5} - 2$	$48.2^{n+1} + 28 – 2^{n+5}$	Type 18	$2^{n+4-i} - 10$	$48.2^{n+1} + 36 – 2^{n+4-i}$
Type 9	$2^{n+4} - 8$	$48.2^{n+1} + 34 – 2^{n+4}$	Type 19	$2^{n+3-i} - 5$	$48.2^{n+1} + 31 – 2^{n+3-i}$
Type 10	$2^{n+4} - 9$	$48.2^{n+1} + 35 – 2^{n+4}$	Type 20	$2^{n+4-i} - 13$	$48.2^{n+1} + 39 – 2^{n+4-i}$

Since edges of NS[n] is partitioned By calculations given in Table 1, on can see that

$$Sz(NS[n]) = \sum_{i=1}^{n} 3.2^{i+1}.(2^{n+4-i} - 8).(48.2^{n+1} + 34 - 2^{(n+4-i)}) + \sum_{i=1}^{n} 3.2^{i+1}.(2^{n+4-i} - 9).(48.2^{n+1} + 35 - 2^{(n+4-i)})$$
$$+ \sum_{i=1}^{n} 3.2^{i+1}.(2^{n+4-i} - 10).(48.2^{n+1} + 36 - 2^{(n+4-i)}) + \sum_{i=1}^{n} 3.2^{i+3}.(2^{n-i+3} - 5).(48.2^{n+1} + 31 - 2^{n+3-i})$$
$$+ \sum_{i=1}^{n} 3.2^{i+1}.(2^{n+4-i} - 13).(48.2^{n+1} + 39 - 2^{n+4-i}) + 6(2^{n+4} - 2)(482^{n+1} + 2^{n-4} + 28)$$
$$+ 3(2^{n+5} + 8)(48.2^{n+1} - 2^{n+5} + 18) + 3(2^{n+5} + 2)(48.2^{n+1} - 2^{n+5} + 24)$$
$$+ 3(2^{n+5} + 1)(48.2^{n+1} - 2^{n+5} + 25) + 3.2^{n+1}(48.2^{n+1} - 2^{n+5} + 26) +$$
$$+ 3.(2^{n+1} - 1)(48.2^{n+1} - 2^{n+5} + 27) + 3(2^{n+5} - 2)(48.2^{n+1} - 2^{n+5} + 28)$$
$$+ 6(2^{n+4} - 8)(48.2^{n+1} - 2^{n+4} + 34) + 6(2^{n+4} - 9)(48.2^{n+1} - 2^{n+4} + 35)$$
$$+ 6(2^{n+4} - 10)(48.2^{n+1} - 2^{n+4} + 36) + 24(2^{n+3} - 5)(48.2^{n+1} - 2^{n+3} + 31)$$
$$+ 12(2^{n+4} - 13)(48.2^{n+1} - 2^{n+4} + 39) + 18(2^{n+5} + 2)(48.2^{n+1} - 2^{n+5} + 24)$$
$$+ 36(2^{n+4} - 5)(48.2^{n+1} - 2^{n+4} + 31) + 4(48.2^{n+1} + 25)$$
$$= 18432n.4^{n} + 9984n.2^{n} - 33024.4^{n} + 20856.2^{n} + 12168.$$

This completes our proof.

References

[1] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[2] A. A. Dobrynin, R. Entringer and I. Gutman, Acta Appl. Math. **66**, 211 (2001).
[3] A. A. Dobrynin, I. Gutman, S. Klavzar and P. Zigert, Acta Appl. Math. **72**, 247 (2002).
[4] I. Gutman, Graph Theory Notes of New York **27**, 9 (1994).
[5] M. V. Diudea, I. Gutman, Croat. Chem. Acta **71**, 21 (1998).
[6] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, J. Singh, A. Shrivastava, I. Lukovits, M. V. Diudea, Lett. Drug. Des. Discov. **2**, 606 (2005).
[7] A. Iranmanesh, N. A. Gholami, Croat. Chem. Acta **81**, 299 (2008).
[8] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Linear Alg Appl. **429**, 2702 (2008).
[9] A. R. Ashrafi, M. Mirzargar, Int. J. Chem. Mod. **1**, 19 (2008).
[10] A. R. Ashrafi, M. Mirzargar, MATCH Commun. Math. Comput. Chem. **60**, 897 (2008).
[11] A. R. Ashrafi, M. Mirzargar, Indian J. Chem. **47A**, 535 (2008).
[12] A. R. Ashrafi, H. Saati, J. Comput. Theoret. Nanosci. **5**, 681 (2008).