PI, Szeged and edge Szeged indices of an infinite family of nanostar dendrimers

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A topological index of a graph G is a numeric quantity related to G which describes the molecular graph G. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The PI and Szeged indices of a class of nanostar dendrimer are computed.

The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. It also shows good resistant to photo bleaching. The nanostar dendrimer promises great applications but first the structure and the energy transfer mechanism must be understood. Experimental and theoretical insight is needed in order to understand the energy transfer mechanism.

Methodology

Some algebraic definitions used for the study are given. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. In a chemical graph, vertices represent atoms and edges represent bonds. These graphs have been used for affinity diagrams showing a relationship between chemical substances.

Numbers reflecting certain structural features of a molecule that are obtained from its chemical graph are usually called topological indices. The Wiener index, W, one of widely used descriptors of molecular topology, was introduced in 1947 by Wiener1 as the half-sum of all topological distances in the hydrogen-depleted graph representing the skeleton of the molecule. Here, we denote by d(u,v), the topological distance between vertices u and v of the graph G, which is the length of a minimum path between these vertices. We encourage the readers to consult two survey articles by Dobrynin and his co-authors2,3 and references therein for background material and historical aspect of Wiener index.

Diudea4-10 was the first scientist who investigated the mathematical properties of nanostructures. He and his team studied several nanostructures by computing their topological indices and designed a package named TopoCluj11 for computing topological indices of the molecular graphs of nanostructures.

Khadikar and co-authors12-15 defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. It is defined as PI(G) = \( \sum_{e=uv}[m_u(e) + m_v(e)] \), where \( m_u(e) \) is the number of edges of G lying closer to u than to v and \( m_v(e) \) is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted.

The Szeged index is another topological index introduced by Ivan Gutman.16-18 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) = \( \sum_{e=uv} |n_u(e) - n_v(e)| \). It may be noted that vertices equidistance from u and v are not taken into account. The edge Szeged index of G is defined similarly by \( Sz_e(G) = \sum_{e=uv} |m_u(e) - m_v(e)| \).19

Recently, the first author of this paper continued the pioneering work of Diudea and his team to compute PI and Szeged indices of some classes of nanostructures.20-25 We also encourage the reader to consult papers by Iranmanesh26-28 and Taeri29,30 for more information on this subject. Our notation is standard and taken from literature.31-34

Results and discussion

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. In this section we compute PI and Szeged indices of a nanostar dendrimer NS[\( n \)], (Fig. 1). Using a simple calculation, one can show that IV(NS[\( n \)]) = 120.2^6 – 108 and IE(NS[\( n \)]) = 140.2^8 – 127. We begin by computing \( n_u(e) \) and \( n_v(e) \) for the edges \( e = E_j \),...
For e = uv = E_i^j, 1 ≤ i ≤ n, 1 ≤ j ≤ 2^{i+1} then by an inductive argument n_u(e) = 30(2^n - 1).

We now consider edges of the hexagons K_1 and K_4, (Fig. 3). One can see that for an arbitrary edge e = uv of this type, n_u(e) = 3. On the other hand, for edges of the hexagons K_2 and K_3, n_u(e) = 30(2^n - 1) + 3 = 30.2^n - 15. Also, for two edges e_1 = u_1v_1 and e_4 = u_3v_4, n_u(e_1) = n_u(e_4) = 6 and for two other edges e_2 = u_2v_3 and e_3 = u_3v_3, n_u(e_2) = n_u(e_3) = 30(2^{n-1}) + 15 = 30.2^{n-1} - 15.

Using these calculations, we have:
**Theorem 1:** The Szeged index of the dendrimer NS[n] is computed as follows:

\[ \text{Sz}(\text{NS}[n]) = -284400.4^n + 187200.n.4^n - 75600.n.2^n + 415944.2^n - 131184. \]

**Proof:** By our calculations given above, we have:

\[
\text{Sz}(\text{NS}[n]) = \sum_{e=uv} n_u(e)n_v(e) = 9(5.2^{n+2} - 18)^2 + 180 \sum_{i=1}^{n} 2^{i+1} \times (5.2^{n+2} - 5.2^{n-i+1} - 13)(2^{n-i+1} - 1) + 216(10.2^n - 9)^2 + 36(20.2^n - 19)(20.2^n - 17) + 4 \sum_{i=1}^{n} 2^{i+1}(60.2^n - 39)(120.2^n - 60.2^{n-i} - 69) + 2 \sum_{i=1}^{n} 2^{i+1}(30.2^n - 15)(120.2^n - 30.2^{n-i} - 93) + 144(2^n - 1)(120.2^n - 111) + 12 \sum_{i=1}^{n} 2^{i+1}(30.2^n - 27)(120.2^n - 30.2^{n-i} - 81) + 48(2^{n-1})(120.2^n - 114) + 2 \sum_{i=1}^{n} 2^{i+1}(30.2^n - 24)(120.2^n - 30.2^{n-i} - 84) \]

Now consider Fig. 3, for edges \( e = uv \) of the hexagons \( K_1 \) and \( K_4 \), \( m_u(e) = 2 \) and for edges \( e = uv \) of hexagons \( K_2 \) and \( K_3 \), \( m_u(e) = 34.(2^{n-i} - 1) + (2^{n-i+1} - 2) + 2 = 36.2^n - 34. \)

Finally, for two edges \( e_1 = u_1v_1 \) and \( e_2 = u_2v_2 \), \( m_u(e_1) = m_u(e_2) = 6 \) and for two edges \( e_2 = u_2v_2 \) and \( e_3 = u_3v_3 \), \( m_u(e_2) = m_u(e_3) = 34.(2^{n-i} - 1) + (2^{n-i+1} - 2) + 6 = 36.2^n - 30. \)

Therefore:

**Theorem 2:** The PI index of the nanostar dendrimer NS[n] is computed as follows:

\[ \text{PI}(\text{NS}[n]) = 19600.4^n - 35820.2^n + 16364. \]

**Proof:** By our calculations given above, we have:

\[ \text{PI}(\text{NS}[n]) = \sum_{e=uv} [m_u(e) + m_v(e)] = (120(2^n - 1) + 12)(140.2^n - 129) + (20(2^n - 1) + 1)(140.2^n - 128) = 19600.4^n - 35820.2^n + 16364, \]

which proves the theorem.

We are now ready to compute the edge Szeged index of a nanostar dendrimer.

**Theorem 3:** The edge Szeged index of the nanostar dendrimer NS[n] is computed as follows:

\[ \text{Sz}_e(\text{NS}[n]) = -426332.4^n + 259280.n.4^n - 102752.n.2^n + 632456.2^n - 205872. \]

**Proof:** By calculations before Theorem 2, one can see that

\[ \text{Sz}_e(\text{NS}[n]) = \sum_{e=uv} [m_u(e)m_v(e)] = (70.2^n - 64)^2 + \sum_{i=1}^{n} 2^{i+1}(35.2^{n-i} - 36) \times (140.2^n - 35.2^{n-i} - 92) + 8(35.2^n - 33)(105.2^n - 96) + 4(70.2^n - 68)(70.2^n - 61) + 4 \sum_{i=1}^{n} 2^{i+1}(70.2^n - 47)(140.2^n - 70.2^{n-i} - 82) + 2 \sum_{i=1}^{n} 2^{i+1}(36.2^{n-i} - 20)(140.2^n - 36.2^{n-i} - 109) + 96(2^n - 1)(140.2^n - 131) + 12 \sum_{i=1}^{n} 2^{i+1}(36.2^{n-i} - 34)(140.2^n - 36.2^{n-i} - 95) + 48(2^n - 1)(140.2^n - 134) + 2 \sum_{i=1}^{n} 2^{i+1}(36.2^{n-i} - 30)(140.2^n - 36.2^{n-i} - 98) = 426332.4^n + 259280.n.4^n - 102752.n.2^n + 632456.2^n - 205872, \]

proving our theorem.
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References