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Computing of Szeged Index in Nanotrees Dendrimer T $^{\kappa,\eta}$ [n]

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Abstract

A dendrimer nanostar is a synthesized molecule built up from branched unit called monomers. Dendrimers are a new class of polymeric materials. They are highly branched, monodisperse macromolecules. The structure of these materials has a great impact on their physical and chemical properties. As a result of their unique behavior dendrimers are suitable for a wide range of biomedical and industrial applications. The paper gives a concise review of dendrimers' physico-chemical properties and their possible use in various areas of research, technology and treatment. In ecological studies, topological indices are defined to test the ecological and chemical characteristics, such as oxidation, melting point, boiling point, toxicity, and other biological activity. As a basic molecular structure, dendrimers widely appeared in chemical, biology, pharmacy, medicine, and material engineering. To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Assume that $M_{ev}(e \mid G)$ is the number of vertices of G lying closer to u and $M_{ev}(e \mid G)$ is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as

$$SZ(G) = \sum_{e=uv\in E(G)} M_{eu}(e \mid G) M_{ev}(e \mid G)$$

Keywords: Dendrimer; Szeged Index; Topological Index; Nanostar; Graph Theory

Introduction

Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A topological index is a numerical value associated with the chemical constitution of a certain chemical compound aiming to correlate various physical and chemical properties, or some biological activity in it. Carbon nanostructures have found many potential industrial applications such as energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes, just to name a few. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices. The nanotrees dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. Carbon nanotubes are molecular-scale tubes of graphitic carbon with outstanding properties. They are among the stiffest and strongest fibers known and have remarkable electronic properties and many other unique characteristics. For these reasons, they have attracted huge academic and industrial interest, with thousands of papers on nanotubes being published every year, though commercial applications have been rather slowly developing, primarily because of the high production costs of better quality nanotubes. Dendrimer chemistry, as other specialised research fields, has its own terms and abbreviations. Furthermore, a more brief structural nomenclature is applied to describe the different chemical events taking place at the dendrimer surface. In the following section a number of terms and abbreviations common in dendrimer chemistry will be explained, and a brief structural nomenclature will be introduced. Hyperbranched polymers is a term describing a major class of polymers mostly achieved by incoherent polymerisation of ABn (n≥2) monomers, often utilising one-pot reactions. Dendrimers having a well-defined finite structure belongs to a special case of hyperbranched polymers (Figure 1).

A major part of the current research in mathematical chemistry, chemical graph theory, and quantitative structure-activity relationship studies involves investigations of topological indices. Topological indices (TI) are numerical graph invariants that quantitatively characterize molecular structure.

Let G be a simple molecular graph without directed and multiple edges and without loops, the sets of vertices and edges of which are denoted by V (G) and E(G), respectively. A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index. Its numerous chemical applications were reported and its mathematical properties are well understood [1-9].

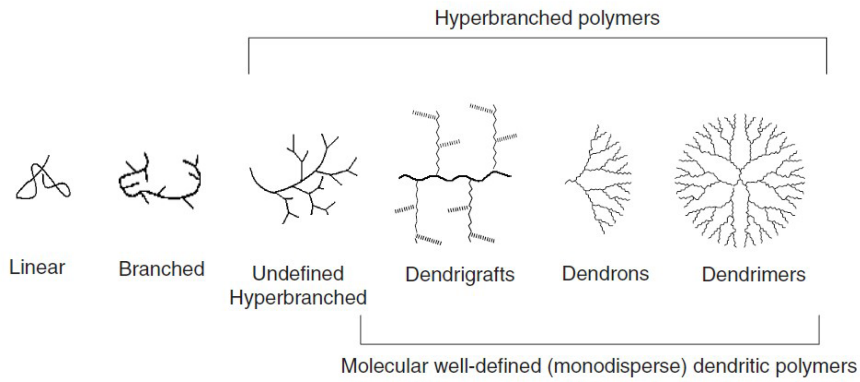

Figure1: Evolution of polymers towards dendritic structure

The problem of distances in a graph continues to attract the attention of scientists both theoretically and practically. In 1947, Harold Wiener introduced his path number as the total distance between all carbon atoms for correlating with the thermodynamic properties of alkanes. Its numerous chemical applications were reported and its mathematical properties are well understood. The Szeged index is another topological index introduced by Ivan Gutman. To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Assume that Meu(e | G) is the number of vertices of G lying closer to u and Mev (e | G) is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as

$$SZ(G) = \sum_{e=uv\in E(G)} M_{eu}(e|G)M_{ev}(e|G)$$

Note that vertices equidistant from u and v are not taken into account.

Main Result

In this section, the behavior of a Nanotree T is investigated under one new topological Szeged index. We prove that

$$=\frac{8}{3}\left(2^{2n+3}\right)+2^{n+3}+\frac{1}{3}\left(2^{2n-2\kappa+4}-2^{2n-2\eta+3}\right)-\frac{1}{3}\left(2^{n-2\kappa+4}+2^{n+2\eta+5}\right)+2^{\kappa+2}+\frac{1}{3}\left(2^{2\eta+4}\right)-\frac{28}{3}.$$

$$Where \quad k=[(n+1)/2], \eta=[n/2].$$

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. As we mentioned before, the oldest and most thoroughly examined such invariant is the Wiener index. Another, newly introduced invariant of the same kind is the Szeged index Sz. A few basic properties of Sz were established and some of its chemical applications reported [1-8,12,13].

In this section, we compute the Szeged index of a Nano tree. To do this, we first compute the value of $M_{eu}(e|G)M_{ev}(e|G)$ for all edges e∈E(G).

Lemma 1

We have $\forall n\in N, |V(G)| = 2^{n+2}-3$

Proof. Indeed, $|V(G)| = 4(2^n-1)+1 = 2^{n+2}-3.$

Lemma 2

Assume that $e_{2j-1} = uv$. Then

$$M_{e_{2j-1}u}(e_{2j-1}|G)M_{e_{2j-1}v}(e_{2j-1}|G) = 2^{2n-2j+4}-2^{2n-4j+4}-2^{n-2j+3}-2^{n+2}+2^{n-2j+2}+2$$

where $1\le j\le \kappa.$

Proof. Consider Figures. 4(i), (ii), (iv), (vi), 2 &3 (a) and (c). then we have:

$$M_{e_{2j-1}v}\left(e_{2j-1}|G\right) = 2^{n-2j+2}-1$$

and

$$M_{e_{2j-1}u}\left(e_{2j-1}|G\right) = (2^{n+2}-3) - M_{e_{2j-1}v}\left(e_{2j-1}|G\right) = 2^{n+2}-2^{n-2j+2}-2$$

then

$$M_{e_{2j-1}u}(e_{2j-1}|G)M_{e_{2j-1}v}(e_{2j-1}|G) = 2^{2n-2j+4}-2^{2n-4j+4}-2^{n-2j+3}-2^{n+2}+2^{n-2j+2}+2$$

which proves the lemma.

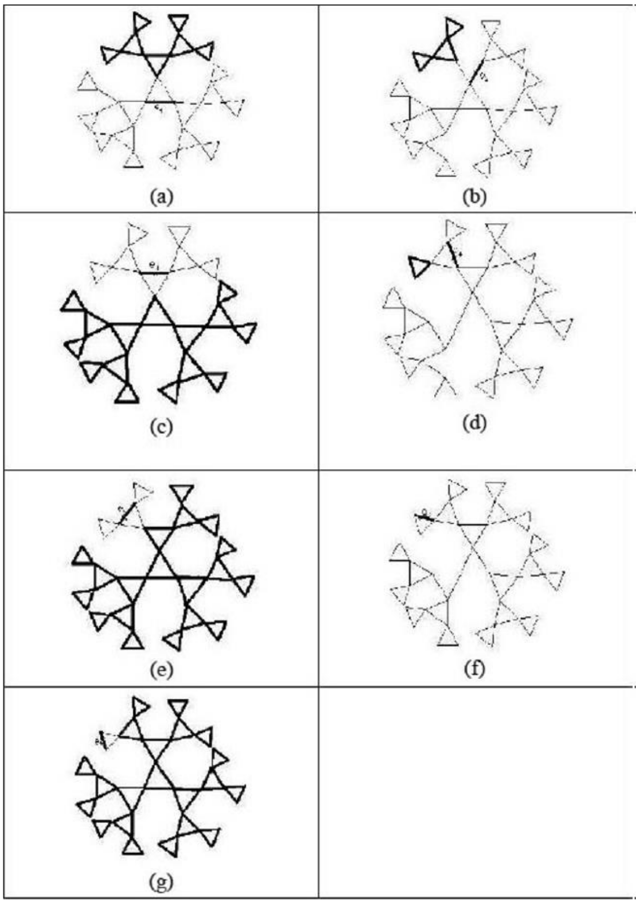

Figure 2: Seven cases of parallel edges with a fixed edge in T[4]

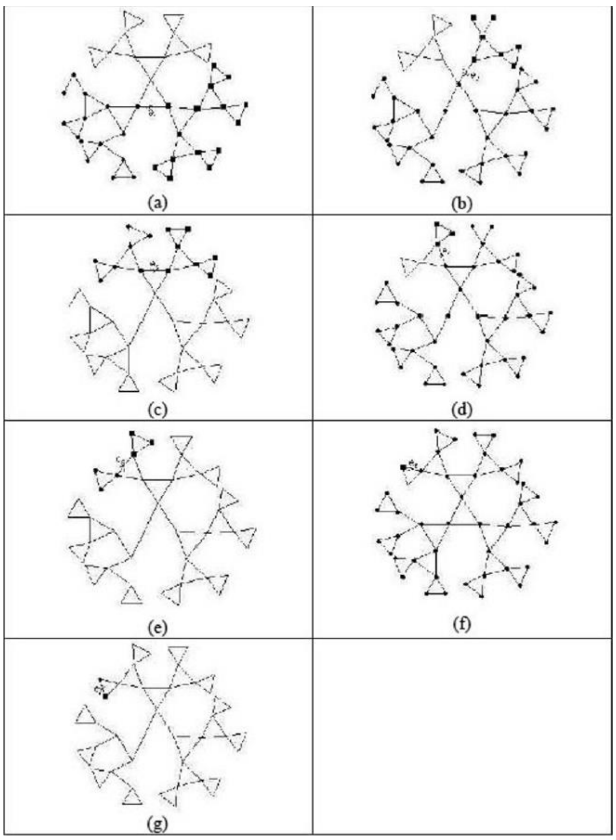

Figure 3: Seven cases of parallel vertices with a fixed edge in T[4]

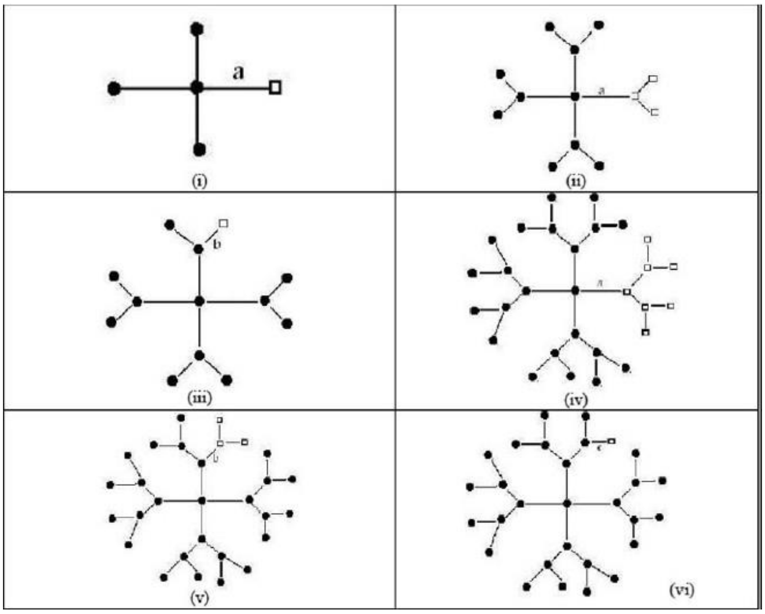

Figure 4: Six cases of codistant vertices of fixed edges of T[1], T[2], T[3]

Lemma3

Assume that $e_{2j} = uv$. Then

$$M_{e_{2j}u}(e_{2j} \mid G) M_{e_{2j}v}(e_{2j} \mid G) = 2^{2n-2j+2} - 2^{2n-4j+2} - 2^{n-2j+2} - 2^{n+2} + 2^{n-2j+1} + 2$$

Where $1 \le j \le \eta$.

Proof. Consider Figs. 4(iii), (v), and 2&3 (b). Then we have

$$M_{e_{2j-1}v}\left(e_{2j-1} \mid G\right) = 2^{n-2j+2} - 1$$

and

$$M_{e_{2j-1}u}\left(e_{2j-1} \mid G\right) = (2^{n+2} - 3) - M_{e_{2j-1}v}\left(e_{2j-1} \mid G\right) = 2^{n+2} - 2^{n-2j+2} - 2$$

then

$$M_{e_{2j}u}(e_{2j} \mid G) M_{e_{2j}v}(e_{2j} \mid G) = 2^{2n-2j+2} - 2^{2n-4j+2} - 2^{n-2j+2} - 2^{n+2} + 2^{n-2j+1} + 2$$

which proves the lemma.

now we are ready to state our second main result.

Theorem 2.1: *The Szeged index dendrimer is computed of a nano as follows:*

$$Sz(T) = 8/3(2^{2n+3}) + 2^{2n+3} + 1/3(2^{2n-2k+4} - 2^{2n-2\eta+3}) - 1/3\left(2^{n+2k+4} + 2^{n+2\eta+5}\right)$$

$$+2^{k+2} + 1/3(2^{2\eta+4}) - 28/3,$$

$$Where \quad k = [(n+1)/2], \eta = [n/2].$$

Proof. The proof is straightforward and follows from Lemmas 2.17–2.19:

$$Sz\ (T) = \sum_{e=uv \in E(G)} M_{eu}\left(e \mid G\right) M_{ev}\left(e \mid G\right)$$

$$2^{2j}\left[M_{e_{2j-1}u}\left(e_{2j-1} \mid G\right) M_{e_{2j-1}v}\left(e_{2j-1} \mid G\right)\right] + 2^{2j+1}\left[M_{e_{2j}u}\left(e_{2j} \mid G\right) M_{e_{2j}v}\left(e_{2j} \mid G\right)\right]$$

$$\sum_{j=1}^{\kappa} 2^{2j}[2^{2n-2j+4} - 2^{2n-4j+4} - 2^{n-2j+3} - 2^{n+2} + 2^{n-2j+2} + 2]$$

$$+\sum_{j=1}^{\eta} 2^{2j+1}[2^{2n-2j+2} - 2^{2n-4j+2} - 2^{n-2j+2} - 2^{n+2} + 2^{n-2j+1} + 2]$$

$$=[2^{2n+4}-\frac{2^{2n+4}}{3}+\frac{2^{2n-2\kappa+4}}{3}-2^{n+3}+\frac{2^{n+4}}{3}-\frac{2^{n+2\kappa+4}}{3}+2^{n+2}-\frac{12}{3}+2^{\kappa+2}]$$

$$+[2^{2n+3}-\frac{2^{2n+3}}{3}-\frac{2^{n-2\eta+3}}{3}-2^{n+3}+\frac{2^{n+5}}{3}-\frac{2^{n+2\eta+5}}{3}+2^{n+2}-\frac{16}{3}+\frac{2^{2\eta+4}}{3}]$$

$$=\frac{8}{3}\left(2^{2n+3}\right)+2^{n+3}+\frac{1}{3}\left(2^{2n-2\kappa+4}-2^{2n-2\eta+3}\right)-\frac{1}{3}\left(2^{n-2\kappa+4}+2^{n+2\eta+5}\right)+2^{\kappa+2}+\frac{1}{3}\left(2^{2\eta+4}\right)-\frac{28}{3}.$$

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