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Research Article

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Eccentric Related Indices of an Infinite Class of Nanostar Dendrimers

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ABSTRACT

Clear indication has it in numerous studies that a strong inherent relationship exists between the chemical characteristics of chemical compounds and drugs (e.g., boiling point and melting point) and their molecular structures. There are several topological indices are defined on these chemical molecular structures and they can help researchers better understand the physical features, chemical reactivity, and biological activity. The study of the topological indices on chemical structure of chemical materials and drugs, therefore, will make the chemical experiments complete. It will also provide a theoretical basis for the manufacturing of drugs and chemical materials. In this paper, by means of molecular structural analysis, we report several eccentric related indices of an infinite class of nanostar dendrimers.

Keywords: Theoretical chemistry, eccentricity, nanostar dendrimer

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INTRODUCTION

As technology develops rapidly, recent years have witnessed that chemical and pharmaceutical techniques have been rapidly evolved, and thus a large number of new nanomaterials, crystalline materials, and drugs emerge every year. To determine the chemical properties of such a large number of new compounds and new drugs requires a large amount of chemical experiments, thereby greatly increasing the workload of the chemical and pharmaceutical researchers. It is fortunate to see that the chemical based experiments found that strong connection between topology molecular structures and their physical behaviors, chemical characteristics, and biological features exists, such as melting point, boiling point, and toxicity of drugs.

We can consider the topological index of a molecule structure as a nonempirical numerical quantity which quantitates the molecular structure and its branching pattern. From this perspective, we can regard topological index as a score function which maps each molecular structure to a real number and used as a descriptor of the molecule under testing. several famous indices are applied in chemical engineering (e.g., QSPR/QSAR study) for grasping the relationships between the molecular structure and the potential physicochemical characteristics, such as PI index, Zagreb index, harmonic index, Wiener index, and connectivity index(see Yan et al. [1-2], Gao [3], Gao and Farahani [4-5], Gao and Wang [6-7], Gao et al. [7], Farahani and Gao [9], Farahani et al. [10] for more details).

In theoretical chemistry setting, we usually express chemical compounds, materials, and drugs as (molecular) graphs in which each vertex represents an atom of molecule structure and each edge implies covalent bounds between two atoms. Let $G = (V(G), E(G))$ be a (molecular) graph with vertex set $V(G)$ and edge set $E(G)$, respectively. It is assumed that all the graphs considered in this paper are simple graphs, that is, no loop and multiple edge. The notations and terminologies used but not clearly undefined in this paper can be found in [11].

Let $ec(v)$ be the eccentricity of vertex *v* which defined as the largest distance between *v* and any other vertex *u* of *G*. There are several important eccentric related indices and polynomials introduced in chemical engineering.

- The fifth atom bond connectivity index, $ABC_5(G) = \sum_{uv \in E(G)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}$.
- The second multiplicative Zagreb index, $\Pi_2^*(G) = \prod_{uv \in E(G)} ec(u)ec(v)$.
- The third multiplicative Zagreb index, $\Pi_3^*(G) = \prod_{uv \in E(G)} (ec(u)+ec(v))$.
- The fourth Zagreb index, $Zg_4(G) = \sum_{uv \in E(G)} (ec(u)+ec(v))$.
- The sixth Zagreb index, $Zg_6(G) = \sum_{uv \in E(G)} ec(u)ec(v)$.
- The fourth Zagreb polynomial, $Zg_4(G,x) = \sum_{uv \in E(G)} x^{ec(u)+ec(v)}$.
- The sixth Zagreb polynomial, $Zg_6(G,x) = \sum_{uv \in E(G)} x^{ec(u)ec(v)}$.

As a common appeared chemical structure, nanostar dendrimers are widely used chemical, material and pharmaceutical engineering (seeAshrafiand Mirzargar [12], Mirzargar [13], Ashrafi and Karbasioun [14], Manuel et al. [15], Darafsheh and Khalifeh [16], Dorosti et al. [17]and Tada et al. [18] for more details).

Although several advances have been made in PI index, Zagreb index, Wiener index, hyper-Wiener index, and sum connectivity index of different kinds of nanostar dendrimers, the study of eccentric related topological indices for nanostar dendrimers has been largely limited. In addition, nanostar dendrimers structures is widely used in pharmaceutical field and medical science. Rely on these reasons, industrial interest and tremendous academic interest have been attracted to research the eccentric relatedtopological indices of specialnanostar dendrimers molecular structure from a mathematical point of view.

In this paper, we focus on the special infinite class of nanostar dendrimers $D[n]$ (here *n* is the step of growth) which is descripted as follows:

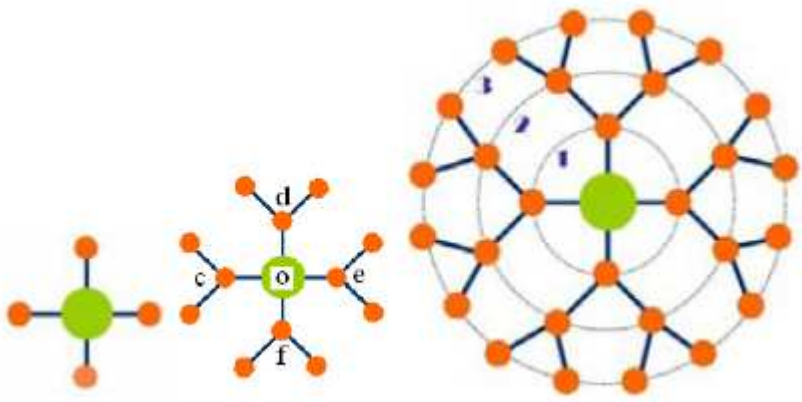

Figure 1. The structures of $D[1]$, $D[2]$ and $D[3]$.

1. Main results and proofs

By the analysis of its molecular structure, we see that the edge set of $D[n]$ can be divided into *n*parts:

- E_1: $ec(u)$ =*n* and $ec(v)$ =*n*+1;
- E_2: $ec(u)$ =*n*+1 and $ec(v)$ =*n*+2;
- ……
- E_i: $ec(u) = n+i-1$ and $ec(v) = n+i$;

- ……
- E_n: $ec(u)$=2n-1 and $ec(v)$=2n.

Furthermore, we have $|E_1|=4$, $|E_2|=8$,..., $|E_i|=2^{i+1}$,..., and $|E_n|=2^{n+1}$. Thus, in view of the definition of eccentric related indices, we get

$$ABC_5(D[n])=\sum_{uv\in E(D[n])}\sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}=\sum_{i=1}^{n}\sum_{uv\in E_i}\sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}=\sum_{i=1}^{n}2^{i+1}\sqrt{\frac{2n+2i-3}{(n+i-1)(n+i)}},$$

$$\Pi_2^*(D[n])=\prod_{uv\in E(D[n])}ec(u)ec(v)=\prod_{i=1}^{n}\prod_{uv\in E_i}ec(u)ec(v)=\prod_{i=1}^{n}((n+i-1)(n+i))^{2^{i+1}},$$

$$\Pi_3^*(D[n])=\prod_{uv\in E(D[n])}(ec(u)+ec(v))=\prod_{i=1}^{n}\prod_{uv\in E_i}(ec(u)+ec(v))=\prod_{i=1}^{n}(2n+2i-1)^{2^{i+1}},$$

$$Zg_4(D[n])=\sum_{uv\in E(D[n])}(ec(u)+ec(v))=\sum_{i=1}^{n}\sum_{uv\in E_i}(ec(u)+ec(v))=\sum_{i=1}^{n}2^{i+1}(2n+2i-1),$$

$$Zg_6(D[n])=\sum_{uv\in E(D[n])}(ec(u)ec(v))=\sum_{i=1}^{n}\sum_{uv\in E_i}(ec(u)ec(v))=\sum_{i=1}^{n}2^{i+1}(n+i-1)(n+i),$$

$$Zg_4(D[n],x)=\sum_{uv\in E(D[n])}x^{ec(u)+ec(v)}=\sum_{i=1}^{n}\sum_{uv\in E_i}x^{ec(u)+ec(v)}=\sum_{i=1}^{n}2^{i+1}x^{2n+2i-1},$$

$$Zg_6(D[n],x)=\sum_{uv\in E(D[n])}x^{ec(u)ec(v)}=\sum_{i=1}^{n}\sum_{uv\in E_i}x^{ec(u)ec(v)}=\sum_{i=1}^{n}2^{i+1}x^{(n+i-1)(n+i)}.$$

CONCLUSION

In our article, by virtue of the molecular graph structural analysis and mathematical derivation, the eccentric related indices of nanostar dendrimers are mainly reported. As researchers are using the eccentric related indices in a wider range when analyzing the chemical procedure for chemical compounds, it is illustrated that the theoretical conclusion obtained in this article have promising prospects of the application for the chemical and pharmacy engineering.

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