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Research Article

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Eccentric Related Indices of an Infinite Class of Nanostar Dendrimers (II)

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ABSTRACT

Considerable studies indicate that there is a strong internal link existing between the characteristics of chemical compounds and drugs and their molecular structures. The boiling point and melting point could be one of the most typical examples among the chemical compounds and drugs. Some researchers found the effectiveness of the topological indices defined on the molecular structure and make use of the structure to get a better understanding for the physical features, chemical reactivity, and biological activity. As a result, serving as the essential component of the chemical experiment, the research of topological indices on chemical structure of chemical materials and drugs laid a theoretical foundation for the manufacturing of drugs and chemical materials. In this paper, in terms of molecular structural analysis, we determine some eccentric related indices of an infinite class of nanostar dendrimers which is denoted by G_n .

Keywords: Theoretical chemistry, eccentricity, nanostar dendrimer

INTRODUCTION

Keeping the rapid pace with technology, these years also welcome the prosperous development in pharmaceutical techniques. Meanwhile, a great quantity of new nanomaterials, crystalline materials, and drugs come to the force every year. Numerous chemical experiments are needed to determine the chemical properties of the new emerging compounds and drugs. In other words, the chemical and pharmaceutical researchers may have more workload on the relevant experiments. However, thanks to the discovery of the strong internal link between topology molecular structures and their physical behaviors, chemical characteristics, and biological features, like melting point, boiling point, and toxicity of drugs.

The topological index of a molecule structure can be taken as a nonempirical numerical quantity which represents the molecular structure and its branching pattern. In this way, as a descriptor of the molecule under testing, the topological index is also considered as a score function which maps each molecular structure to a real number. In order to grasp the relationships between the molecular structure and the potential physicochemical characteristics, such as PI index, Zagreb index, harmonic index, Wiener index, and connectivity index, we can use some famous indices(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).

Theoretically, researchers tend to represent chemical compounds, materials, and drugs as (molecular) graphs. Each vertex stands for an atom of molecule structure and each edge corresponds to thecovalent 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. Then we can make an assumption that all the graphs here in the paper are simple graphs without loop and multiple edge. [11]provides the references for the notations and terminologies used but not clearly undefined in this paper.

There are several important eccentric related indices and polynomials introduced in chemical engineering.

- The second multiplicative Zagreb index, $\prod_2^*(G) = \prod_{uv \in E(G)} ec(u)ec(v)$.
- The third multiplicative Zagreb index, $\prod_3^*(G) = \prod_{uv \in E(G)} (ec(u)+ec(v))$.
- 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, $Zg_6(G,x) = \sum_{uv \in E(G)} x^{ec(u)ec(v)}$.

Nanostar dendrimers, a common chemical structure, see a wide applications in chemical, material and pharmaceutical engineering (see Ashrafiand 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).

Recent years have seen some considerable development in PI index, Zagreb index, Wiener index, hyper-Wiener index, and sum connectivity index of different kinds of nanostar dendrimers. However, the research on topological indices for nanostar dendrimers still wait for further developments. Moreover, nanostar dendrimers structures has wide applications in pharmaceutical field and medical science. As a result, the research on the eccentric related topological indices of special nanostar dendrimers molecular structure from a mathematical point of view has attracted lots of industrial and academic interests.

In this paper, as the continue study of Gao [19], we focus on the special infinite class of nanostar dendrimers G_n (here *n* is the step of growth) which is descripted as follows:

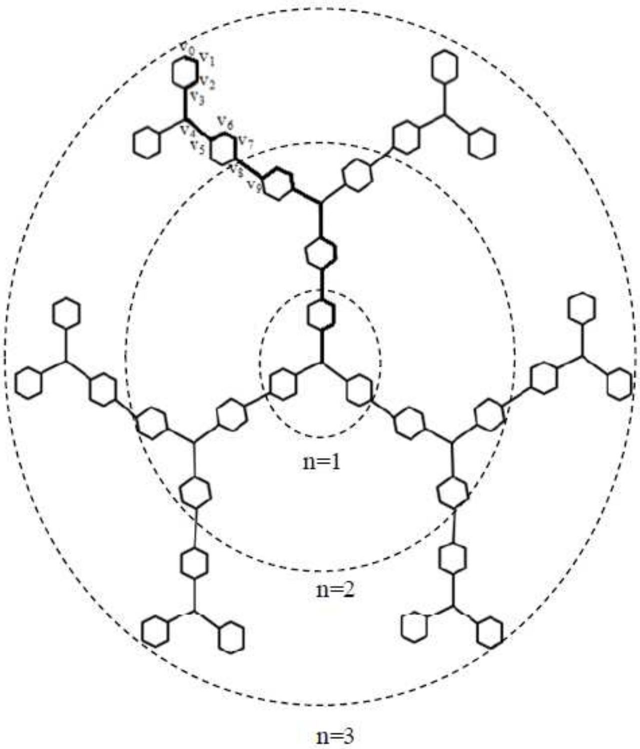

Figure 1. The structures of G_n

1. Main results and proofs

By the analysis of its molecular structure, we see that there are $3\times 2^{i-2}$ copy of G_1 in the *i*-th level of molecular graph G_n .Thus, in view of the definition of eccentric related indices, we get

$$\Pi_2^*(G_n)=\prod_{uv\in E(G_n)} ec(u)ec(v)$$

$$=\{\prod_{i=0}^{n-2}(\prod_{j=0}^{2}(36n-21-18i-2j)^4\prod_{j=3,5,6,7}(36n-21-18i-2j)^2\prod_{j=4,8}(36n-21-18i-2j))^{3\cdot 2^{n-i-2}}\}\times$$

$$\prod_{i=1}^{3}(18n-2i-1)^6\times(18n-9)^3,$$

$$\Pi_3^*(G_n)=\prod_{uv\in E(G_n)}(ec(u)+ec(v))$$

$$=\{\prod_{i=0}^{n-2}(\prod_{j=0}^{2}((18n-10-9i-j)(18n-11-9i-j))^4\prod_{j=3,5,6,7}((18n-10-9i-j)(18n-11-9i-j))^2\times$$

$$\prod_{j=4,8}(18n-10-9i-j)(18n-11-9i-j))^{3\cdot 2^{n-i-2}}\}\times\prod_{i=1}^{3}((9n-i)(9n-i-1))^6\times((9n-4)(9n-5))^3,$$

$$Zg_4(G_n)=\sum_{uv\in E(G_n)}(ec(u)+ec(v))$$

$$=\sum_{i=0}^{n-2}3\cdot 2^{n-i-2}(4\sum_{j=0}^{2}(36n-21-18i-2j)+2\sum_{j=3,5,6,7}(36n-21-18i-2j)+\sum_{j=4,8}(36n-21-18i-2j))$$

$$+6\sum_{i=1}^{3}(18n-2i-1)+3(18n-9),$$

$$Zg_6(G_n)=\sum_{uv\in E(G_n)}(ec(u)ec(v))$$

$$=\sum_{i=0}^{n-2}3\cdot 2^{n-i-2}(4\sum_{j=0}^{2}(18n-10-9i-j)(18n-11-9i-j)+2\sum_{j=3,5,6,7}(18n-10-9i-j)(18n-11-9i-j)$$

$$+\sum_{j=4,8}(18n-10-9i-j)(18n-11-9i-j))+6\sum_{i=1}^{3}(9n-i)(9n-i-1)+3(9n-4)(9n-5),$$

$$Zg_4(G_n,x)=\sum_{uv\in E(G_n)}x^{ec(u)+ec(v)}$$

$$=\sum_{i=0}^{n-2}3\cdot 2^{n-i-2}(4\sum_{j=0}^{2}x^{36n-21-18i-2j}+2\sum_{j=3,5,6,7}x^{36n-21-18i-2j}+\sum_{j=4,8}x^{36n-21-18i-2j})+6\sum_{i=1}^{3}x^{18n-2i-1}+3x^{18n-9},$$

$$Zg_6(G_n,x)=\sum_{uv\in E(G_n)}x^{ec(u)ec(v)}$$

$$=\sum_{i=0}^{n-2}3\cdot 2^{n-i-2}(4\sum_{j=0}^{2}x^{(18n-10-9i-j)(18n-11-9i-j)}+2\sum_{j=3,5,6,7}x^{(18n-10-9i-j)(18n-11-9i-j)}+\sum_{j=4,8}x^{(18n-10-9i-j)(18n-11-9i-j)})$$

$$+6\sum_{i=1}^{3}x^{(9n-i)(9n-i-1)}+3x^{(9n-4)(9n-5)}.$$

CONCLUSION

This paper reported the eccentric related indices of nanostar dendrimers by using the molecular graph structural analysis and mathematical derivation. The eccentric related indices are favored by many researchers from a variety of fields, because of its usefulness for analyzing the chemical procedure for chemical compounds. As a consequence, the theoretical results achieved in the paper have a promising prospects for the wide applications in chemical and pharmacy engineering.

REFERENCES

[1] LYan;YLi;WGao;JSLi,*J. Chem. Pharm. Res.*, **2014**, 6(3),477-481.
[2] L Yan; WGao; JS Li,*J.Comput.Theor.Nanos.*, **2015**, 12(10), 3940–3944.
[3] WGao, *J. Chem. Pharm. Res.*, **2015**, 7(4), 634-639.
[4] W Gao;MR Farahani,*J. Nanotechnology*, Volume 2016, Article ID 3129561, 6 pages, http://dx.doi.org/10.1155/2016/3129561.
[5] WGao; MRFarahani, *Appl. Math. Nonl. Sc.*, **2016**, 1 (1), 94-117.
[6] W Gao;WF Wang,*J. Chem.*, Volume **2014**, Article ID 906254, 8 pages, http://dx.doi.org/10.1155/2014/906254.
[7] W Gao; WF Wang, *Computational and Mathematical Methods in Medicine*, Volume 2015, Article ID 418106, 10 pages, http://dx.doi.org/10.1155/2015/418106.
[8] W Gao; WF Wang; MRFarahani, *J. Chem.*, **2016**, Article ID 3216327, 8 pages, http://dx.doi.org/10.1155/2016/3216327.
[9] MRFarahani; W Gao, *J. Chem. Pharm. Res.*, **2015**, 7(10), 535-539.
[10] MRFarahani; MK Jamil; M Imran,*Appl. Math.Nonl.*Sc., **2016**, 1 (1), 175-182.
[11] JABondy; USRMutry, Graph Theory,Spring, Berlin, **2008**, 1-40.
[12] AR Ashrafi; MMirzargar, *Indian J.Chem.*,**2008**, 47A, 538-541.
[13] MMirzargar, *MATCH Commun. Math.Comput. Chem.*, **2009**, 62,363-370.
[14] AR. Ashrafi;AKarbasioun, *Dig. J. Nanomater. Bios.*,**2009**, 4(4), 663-666.
[15] P Manuel; IRajasingh;MArockiaraj,*J. Comput. Theor.Nanos.*,**2014**, 11, 160-164.
[16] MRDarafsheh; MH Khalifeh, *ArsCombin.*, **2011**, 100, 289-298
[17] NDorosti; AIranmanesh; MV Diudea, *Optoelectron. Adv. Mat.*, ***20*10**, 4(3), 381-384.
[18] T Tada; D Nozaki; M Kondo; K Yoshizawa,*J. Phys. Chem. B*,**2003**, 107(51), 14204-14210.
[19] W Gao, *J. Chem. Pharm. Res.*, **2016**, 8(4),1187-1190.