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Research Article

Computing the Narumi–Katayama Index and Modified Narumi–Katayama Index of Some Families of Dendrimers and Tetrathiafulvalene

Islam Goli Farkoush,[1] Mehdi Alaeiyan,[2] Mohammad Reza Farahani,[2] and Mohammad Maghasedi[1]

[1]*Department of Mathematics, Karaj Branch, Islamic Azad University, Karaj, Iran*
[2]*Department of Mathematics, Iran University of Science and Technology, Narmak, Tehran 16844, Iran*

Correspondence should be addressed to Mehdi Alaeiyan; alaeiyan@iust.ac.ir

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A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In mathematical chemistry, a particular attention is given to degree-based graph invariant. The Narumi–Katayama index and its modified Narumi–Katayama index of a graph G denoted by NK (G) and $\mathrm{NK}^*(G)$ are equal to the product of the degrees of the vertices of G. In this paper, we calculate the Narumi–Katayama Index and modified Narumi–Katayama index for some families of dendrimers.

1. Introduction

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of a molecular graph represents an atom of the molecule and its edges to the bonds between atoms. Chemical Graph Theory has an important effect on the development of Chemical Sciences.

In Chemical Science, the multiplicative connectivity indices are used in the analysis of drug molecular structures which are helpful to find out the biological and chemical characteristics of drugs.

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. In chemistry, biochemistry, and nanotechnology, different topological indices are used for modeling physicochemical, pharmacologic, toxicologic, biological, and other properties of chemical compounds. As a result of their unique behavior, dendrimers are suitable for a wide range of biomedical and industrial applications [1].

A molecular graph $G=(V, E)$ with the vertex set $V(G)$ and the edge set $E(G)$ is a graph whose vertices denote atoms and edges denote bonds between the atoms of any underlying chemical structure. The degree of a vertex v of G denoted by $d_G(v)$ is the number of edges that are incident to it (for simplicity, $d_G(v) = d_v$). A topological index Top (G) of graph G is a number with the property, so Top $(H) =$ Top (G) means a graph H is isomorphic with a graph G. The idea of topological list originated from work done by Wiener [2]. In [3], Narumi and Katayama considered the product of d_v over all degrees of vertices in G as "simple topological index." Then, the papers, mostly used the name "Narumi–Katayama index" for this index. So, we use from it in this paper, too. In [4–6], authors studied some properties of Narumi–Katayama indices as follows:

$$\mathrm{NK}(G) = \prod_{u\in V(G)} d_u, \quad (1)$$

and the modified of Narumi–Katayama indices as follows:

$$\mathrm{NK}^*(G) = \prod_{u\in V(G)} d_{u^{d_u}}. \quad (2)$$

Several articles contributed to determining the topological indices of some families of dendrimer structures and nanostar dendrimers (see [7–15]), porphyrin dendrimers (see [16]), and EThyleneAmidoAmine dendrimers (see [17, 18]).

In this paper, we compute the Narumi–Katayama index and modified Narumi–Katayama index for some families of dendrimers like PD_1 $[n]$ be PAMAM dendrimers with n growth of stages and $n \in N$. For example, the graph PD_2 $[3]$ is shown in Figure 1. Another kind of dendrimers, namely, tetrathiafulvalene dendrimer (see Figures 2 and 3), is denoted by TD_2 $[n]$, $n \in N \cup \{0\}$. In Figure 3, we can see the graph TD_2 $[0]$ and TD_2 $[2]$.

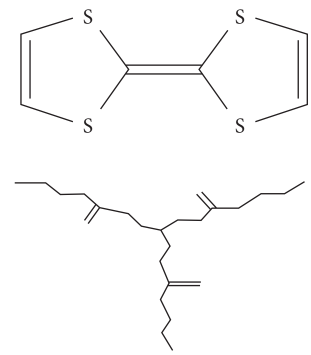

FIGURE 1: Tetrathiafulvalene $(H_2C_2S_2C)_2$ and the core of PD_1 $[0]$.

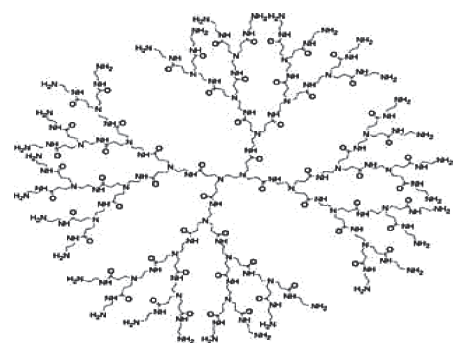

FIGURE 2: PAMAM dendrimers with 3 growth stages PD_2 $[3]$ [18].

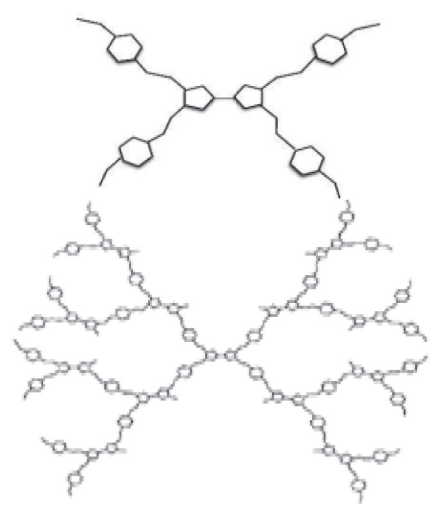

FIGURE 3: Tetrathiafulvalene dendrimer with 2 growth stages TD_2 $[0]$ and TD_2 $[2]$ [19–21].

2. Main Results

In this section, we shall compute the Narumi–Katayama indices and modified Narumi–Katayama index of some families of dendrimers, PD_1 $[n]$, PD_2 $[n]$, and TD_2 $[n]$.

Theorem 1. *Let PD_1 $[n]$ be PAMAM dendrimers with n growth of stages where $n \in N \cup \{0\}$. Then, the Narumi–Katayama index and modified Narumi–Katayama index of PD_1 $[n]$ are given by*

(i) $NK(PD_1[n]) = 2^{30\times 2^n - 15} \times 3^{9\times 2^n - 5}$.

(ii) $NK^*(PD_1[n]) = 2^{60\times 2^n - 30} \times 3^{27\times 2^n - 15}$.

Proof. Let TD_1 $[n] = G_n$ where $n \in N \cup \{0\}$. The number of vertices and edges in G_n is $48 \times 2^n - 23$ and $48 \times 2^n - 24$, respectively. The vertex set $V(G_n)$ can be divided into three vertex partitions based on degrees of vertices as V_1, V_2, and V_3, where $V_i = \{u \mid u \in V(G_n), \deg(u) = i\}$; $1 \le i \le 3$. It is easy to see that $|V_1(G_n)| = 9 \times 2^n - 3$; moreover, we have

$$\begin{cases} V_1(G_n) + 2V_2(G_n) + 3V_3(G_n) = 2E(G_n) \\ V_1(G_n) + V_2(G_n) + V_3(G_n) = V(G_n) \end{cases}. \quad (3)$$

Therefore, by solving the above system of equations, the number of vertices in $V_2(G_n)$ and $V_3(G_n)$ is $30 \times 2^n - 15$ and $9 \times 2^n - 5$. Now, by using (1) and (2), we have

$$\text{(i)} \quad \begin{aligned} NK(G_n) &= \prod_{u \in V(G_n)} du \\ &= \prod_{u_1 \in V_1(G_n)} du_1 \times \prod_{u_2 \in V_2(G_n)} du_2 \times \prod_{u_3 \in V_3(G_n)} du_3 \\ &= 1^{|V_1(G_n)|} \times 2^{|V_2(G_n)|} \times 3^{|V_3(G_n)|} \\ &= 1^1 \times 2^{30\times 2^n - 15} \times 3^{9\times 2^n - 5} \\ &= 2^{30\times 2^n - 15} \times 3^{9\times 2^n - 5}. \end{aligned}$$

$$\text{(ii)} \quad \begin{aligned} NK^*(G_n) &= \prod_{u \in V(G_n)} du^{du} \\ &= \prod_{u_1 \in V_1(G_n)} du_1^{du_1} \times \prod_{u_2 \in V_2(G_n)} du_2^{du_2} \times \prod_{u_3 \in V_3(G_n)} du_3^{du_3} \\ &= 1^{1^{|V_1(G_n)|}} \times 2^{2^{|V_2(G_n)|}} \times 3^{3^{|V_3(G_n)|}} \\ &= 2^{2^{30\times 2^n - 15}} \times 3^{3^{9\times 2^n - 5}} \\ &= 2^{60\times 2^n - 30} \times 3^{27\times 2^n - 15}. \end{aligned}$$

□

Theorem 2. *Let PD_2 $[n]$ be PAMAM dendrimers with n growth of stages and $n \in N$. Then, the Narumi–Katayama index and its modified of PD_2 $[n]$ are given by*

(i) $NK(PD_2[n]) = 2^{40\times 2^n - 4} \times 3^{12\times 2^n + 20}$.

(ii) $NK^*(PD_2[n]) = 2^{80\times 2^n - 8} \times 3^{36\times 2^n + 60}$.

Proof. This is similar to the proofs of Theorem 1. □

Theorem 3. *Let TD_2 $[n]$ be tetrathiafulvalene dendrimer with n growth of stages and $n \in N \cup \{0\}$. Then, the Narumi–Katayama index and its modified of TD_2 $[n]$ are given by*

(i) $NK(TD_2[n]) = 2^{76\times 2^n - 44} \times 3^{40\times 2^n - 26}$.

(ii) $NK^*(TD_2[n]) = 2^{152\times 2^n - 88} \times 3^{120\times 2^n - 78}$.

Proof. This is similar to the proofs of Theorems 1 and 2. □

Example 1. Consider tetrathiafulvalene dendrimer $TD_2[0] = G_0$ where $n \in N \cup \{0\}$ is shown in Figure 3. Theorem 3, $|V(G_0)| = 50$ and $|E(G_0)| = 55$. The vertex partitions $V_1(G_0), V_2(G_0)$, and $V_3(G_0)$ contain, respectively, 4, 32, and 14 vertices. Then,

$$\text{(i)}\quad \begin{aligned} \mathrm{NK}(G_0) &= \prod_{u\in V(G_0)} \mathrm{d}u \\ &= \prod_{u_1\in V_1(G_0)} \mathrm{d}u_1 \times \prod_{u_2\in V_2(G_0)} \mathrm{d}u_2 \times \prod_{u_3\in V_3(G_0)} \mathrm{d}u_3 \\ &= 1^{|V_1(G_0)|} \times 2^{|V_2(G_0)|} \times 3^{|V_3(G_0)|} \\ &= 2^{32} \times 3^{14}. \end{aligned}$$

$$\text{(ii)}\quad \begin{aligned} \mathrm{NK}^*(G_0) &= \prod_{u\in V(G_0)} \mathrm{d}u^{\mathrm{d}u} \\ &= \prod_{u_1\in V_1(G_0)} \mathrm{d}u_1^{\mathrm{d}u_1} \times \prod_{u_2\in V_2(G_0)} \mathrm{d}u_2^{\mathrm{d}u_2} \times \prod_{u_3\in V_3(G_0)} \mathrm{d}u_3^{\mathrm{d}u_3} \\ &= 1^{1^{|V_1(G_0)|}} 2^{2^{|V_2(G_0)|}} \times 3^{3^{|V_3(G_0)|}} \\ &= 2^{64} \times 3^{42}. \end{aligned}$$

3. Conclusions

In this paper, we determined the Narumi–Katayama index and modified Narumi–Katayama index for some families of dendrimers, namely, PAMAM and tetrathiafulvalene dendrimer. In the future, we are interested to study and compute topological indices of various families of dendrimers or nanostructures, in general.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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