Research Article

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

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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 $NK^*(G)$ 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:

$$NK(G) = \prod_{v \in V(G)} d_v, \tag{1}$$

and the modified of Narumi–Katayama indices as follows:

$$NK^*(G) = \prod_{v \in V(G)} d_{v^v}. \tag{2}$$
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 PD1 [n] be PAMAM dendrimers with n growth of stages and n ∈ N. For example, the graph PD2 [3] is shown in Figure 1. Another kind of dendrimers, namely, tetrathiafulvalene dendrimer (see Figures 2 and 3), is denoted by TD2 [n], n ∈ N∪ {0}. In Figure 3, we can see the graph TD2 [0] and TD2 [2].

2. Main Results

In this section, we shall compute the Narumi–Katayama indices and modified Narumi–Katayama index of some families of dendrimers, PD1 [n], PD2 [n], and TD2 [n].

Theorem 1. Let PD1 [n] be PAMAM dendrimers with n growth of stages where n ∈ N∪ {0}. Then, the Narumi–Katayama index and modified Narumi–Katayama index of PD1 [n] are given by

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

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

Proof. Let TD1[n] = G_n where n ∈ N∪ {0}. The number of vertices and edges in G_n is 48 × 2^n–23 and 48 × 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_1 = \{u | u ∈ V (G_n), deg(u) = i\}; 1 ≤ i ≤ 3. It is easy to see that |V_1(G_n)| = 9 × 2^n – 3; moreover, we have

\[
\begin{align*}
V_1(G_n) + 2V_2(G_n) + 3V_3(G_n) &= 2E(G_n) \\
V_1(G_n) + V_2(G_n) + V_3(G_n) &= V(G_n)
\end{align*}
\]

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

\[
NK(G_n) = \prod_{u \in V(G_n)} du = u_1V_1(G_n) \times u_2V_2(G_n) \times u_3V_3(G_n)
\]

\[
= 3^{30n^2-15} \times 3^{9n^2-5} \times 3^{27n^2-15}
\]

\[
NK^\star(G_n) = \prod_{u \in V(G_n)} du = u_1V_1(G_n) \times u_2V_2(G_n) \times u_3V_3(G_n)
\]

\[
= 2^{60n^2-30} \times 3^{27n^2-15}
\]

Theorem 2. Let PD2 [n] be PAMAM dendrimers with n growth of stages and n ∈ N. Then, the Narumi–Katayama index and its modified of PD2 [n] are given by

(i) \( NK(PD_2[n]) = 2^{90n^2-4} \times 3^{12n^2+20} \)

(ii) \( NK^\star(PD_2[n]) = 2^{80n^2-8} \times 3^{16n^2+60} \)

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

Theorem 3. Let TD2 [n] be tetrathiafulvalene dendrimer with n growth of stages and n ∈ N∪ {0}. Then, the Narumi–Katayama index and its modified of TD2 [n] are given by

(i) \( NK(TD_2[n]) = 2^{78n^2-44} \times 3^{40n^2-26} \)
\( (ii) \ NK^* (TD_2 [n]) = 2^{152x2^{−88}} \times 3^{120x2^{−78}}. \)

**Proof.** This is similar to the proofs of Theorems 1 and 2. \( \square \)

**Example 1.** Consider tetrahtiafulvalene dendrimer \( TD_2 [0] = G_0 \) where \( n \in N U \) \( [0] \) 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,

\[ NK(G_0) = \prod_{u \in V(G_0)} du \]

\[ (i) \ NK^* (G_0) = \prod_{u \in V(G_0)} du_1 \times \prod_{u \in V(G_0)} du_2 \times \prod_{u \in V(G_0)} du_3 \]

\[ = 1 |V_1 (G_0)| \times 2 |V_2 (G_0)| \times 3 |V_3 (G_0)| \]

\[ = 2^{32} \times 3^{14}. \]

**3. Conclusions**

In this paper, we determined the Narumi–Katayama index and modified Narumi–Katayama index for some families of dendrimers, namely, PAMAM and tetrahtiafulvalene 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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