Computing the Narumi-Katayama Indices and its Modified Version of Some Families of Dendrimers

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ABSTRACT

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 version 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 its Modified for some families of dendrimers.

KEYWORDS: Narumi-Katayama indices, Modified Narumi-Katayama indices, Dendrimer, Graph;

1 INTRODUCTION

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 awide 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 $d_G(v)=dv$. A topological list $Top(G)$ of graph G is a number with theproperty that, for each diagram H isomorphic to chart G, $Top(H) = Top(G)$. The idea of topological list originated from work done by Wiener [2]. In [3] Narumi and Katayama considered the product of dv overall degrees of vertices in G as "simple topological index". Then the papers, mostly used from the name "Narumi-Katayama index" for this index. So we use from it in this paper, too. In [4] authors studied some properties of Narumi-Katayama indices as follows:

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

And the modified of Narumi-Katayama indices as follows:

$$NK^*(G) = \prod_{u \in V(G)} {d_u}^{d_u} \, . \qquad (2)$$

Several articles contributed to determining the topologicalindices of some families of dendrimers; (see [5-10]). Among the dendrimers are PAMAMs, which are very popular in drug delivery. Figure 1 shows a dendrimer PAMAM with three generations. Many PAMAM dendrimers with altered levels are not immune-stimulating, are water-soluble, and contain mutable end amines that can attach to different guest or target molecules. The internal cavity of PAMAM dendrimers can host metal or guest molecules due to its unique structure, which contains triple amine and amide bonds.

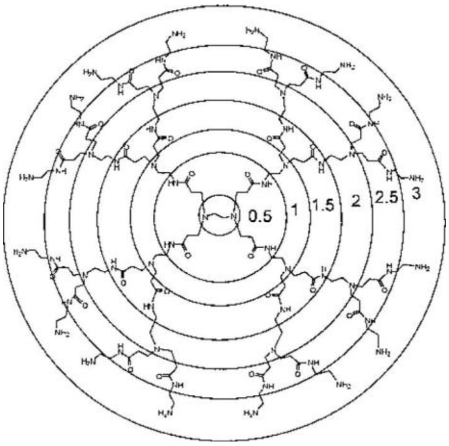

Figure 1. PAMAM dendrimer of generations Gn with growth stages $PD_1[3]$.

In this paper, we compute the Narumi-Katayama index and its modified for some families of dendrimers like $PD_1[n]$ be PAMAM dendrimers with n growth stages and $n \in \mathbb{N} \cup \{0\}$. The core of $PD_1[0]$ is shown in Figure 2, $PD_2[n]$ be PAMAM dendrimers with n growth of stages and $n \in \mathbb{N}$. For example the graph $PD_2[3]$ is shown in Figure 3. Another kind of dendrimers, namely tetrathiafulvalene dendrimer, denoted by $TD_2[n]$, $n \in \mathbb{N} \cup \{0\}$. In Figure 4 we can see the graph $TD_2[0]$, $TD_2[2]$.

2 MAIN RESULTS

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

Theorem 2.1.1. Let $PD_1[n]$ be PAMAM dendrimers with n growth of stages where $n \in \mathbb{N} \cup \{0\}$. Then the Narumi-Katayama indices and its modified 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 $PD_1[n]=G_n$ where $n\in \mathbb{N}\cup\{0\}$. The number of vertices and edges in G_n are $48\times 2^n-23$ 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, 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

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

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

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

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

□

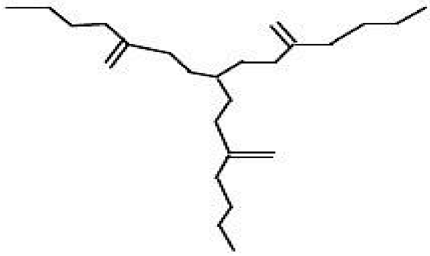

Figure 2. The core of $PD_1[0]$

Theorem 2.1.2. Let $PD_2[n]$ be PAMAM dendrimers with n growth of stages and $n \in \mathbb{N}$. Then the Narumi-Katayama indices 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. Let $PD_2[n] = G_n$ where $n \in \mathbb{N}$. The number of vertices and edges in G_n are $64\times 2^n - 28$ and $64\times 2^n - 29$. The vertex set $V(G_n)$ is divided into three vertex partitions based on degrees of vertices as $V(G_n) = \bigcup_{i=1}^{3} V_i$ where $V_i = \{u / u \in V(G_n), d_u = i; 1 \le i \le 3\}$.
It is easy to see that $|V_1(G_n)| = 12\times 2^n - 4$, moreover we have

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

Therefore, by solving the above equation, the number of vertices in $V_2(G_n)$ and $V_3(G_n)$ are $40\times 2^n - 44$ and $12\times 2^n + 20$. Now by using (1) and (2), we have

$$\begin{aligned} i)NK(G_n) &= \prod_{u\in V(G_n)} d_u \\ &= \prod_{u_1\in V_1(G_n)} d_{u_1} \times \prod_{u_2\in V_2(G_n)} d_{u_2} \times \prod_{u_3\in V_3(G_n)} d_{u_3} \\ &= 1^{|V_1(G_n)|} \times 2^{|V_2(G_n)|} \times 3^{|V_3(G_n)|} \\ &= 1^1 \times 2^{40\times 2^n-44} \times 3^{12\times 2^n+20} \\ &= 2^{40\times 2^n-44} \times 3^{12\times 2^n+20}. \end{aligned}$$

$$ii) NK^*(G_n) = \prod_{u \in V(G_n)} {d_u}^{d_u}$$

$$= \prod_{u_1 \in V_1(G_n)} {d_{u_1}}^{d_{u_1}} \times \prod_{u_2 \in V_2(G_n)} {d_{u_2}}^{d_{u_2}} \times \prod_{u_3 \in V_3(G_n)} {d_{u_3}}^{d_{u_3}}$$

$$= \left(1^1\right)^{|V_1(G_n)|} \times \left(2^2\right)^{|V_2(G_n)|} \times \left(3^3\right)^{|V_3(G_n)|}$$

$$= \left(2^2\right)^{40\times 2^n - 44} \times \left(3^3\right)^{12\times 2^n + 20}$$

$$= 2^{80\times 2^n - 88} \times 3^{36\times 2^n + 60}.$$

□

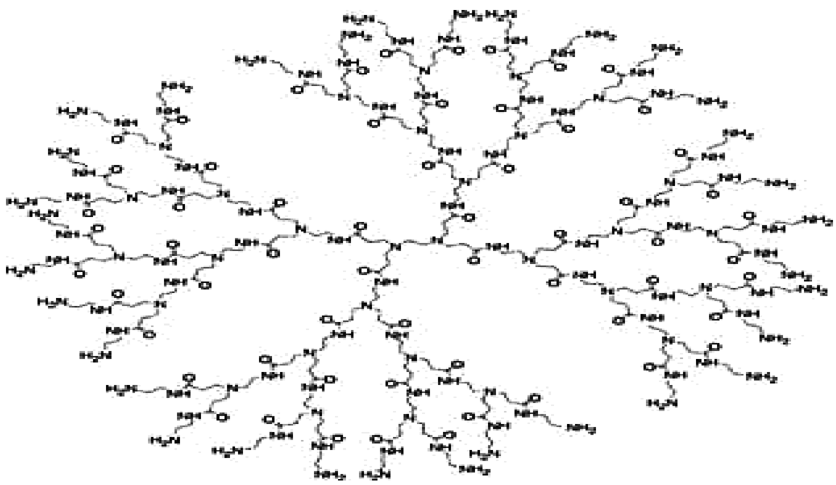

Figure 3. PAMAM dendrimers with 3-growth stages $PD_2[3]$

Theorem 2.1.3. Let $TD_2[n]$ be tetrathiafulvalene dendrimer with n growth of stages and $n \in \mathbb{N} \cup \{0\}$. Then the Narumi-Katayama indices 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. Similar to the proofs of theorem 2-1-1, 2-1-2.

□

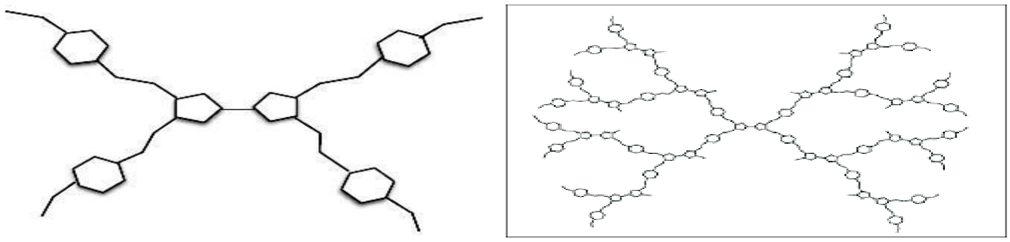

Figure 4. Tetrathiafulvalene dendrimer with 2-growth stages $TD_2[0], TD_2[2]$

Example 2.1.3. Consider tetrathiafulvalene dendrimer $TD_2[0]=G_0$ where $n \in \mathbb{N} \cup \{0\}$, is shown in Figure 3. By theorem 2.1.3, $|V(G_0)|=50$ and $|E(G_0)|=55$. The vertex partitions $V_1(G_0), V_2(G_0)$ and $V_3(G_0)$ contains respectively 4,32 and 14 vertices. Then

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

$$
\begin{aligned}
ii)\, NK^*(G_0) &= \prod_{u\in V(G_0)} d_u^{\,d_u} \\
&= \prod_{u_1\in V_1(G_0)} d_{u_1}^{\,d_{u_1}} \times \prod_{u_2\in V_2(G_0)} d_{u_2}^{\,d_{u_2}} \times \prod_{u_3\in V_3(G_0)} d_{u_3}^{\,d_{u_3}} \\
&= \left(1^1\right)^{|V_1(G_0)|} \times \left(2^2\right)^{|V_2(G_0)|} \times \left(3^3\right)^{|V_3(G_0)|} \\
&= 2^{64} \times 3^{42}.
\end{aligned}
$$

3 CONCLUSION

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

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