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Sombor Indices of Two Families of Dendrimer Nanostars

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Abstract. In this paper, we compute the Sombor index, modified Sombor index and their corresponding exponentials, first and second (*a*, *b*)-*KA* indices and their polynomials of certain dendrimer nanostars.

Keywords: Sombor index, modified Sombor index, (*a*, *b*)-*KA* indices, dendrimer

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*09

1. Introduction

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical Graph Theory is a branch of Mathematical Chemistry, which has an important effect on the development of the Chemical Sciences. A topological index is a numerical parameter mathematically derived from the graph structure. Several such topological indices have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR study see [1, 2].

Let $G = (V(G), E(G))$ be a finite, simple connected graph. Let $d_G(u)$ be the degree of a vertex u in G. We refer [3] for undefined notations and terminologies.

The Sombor index was introduced by Gutman in [4], defined it as

$$SO(G) = \sqrt{d_G(u)^2 + d_G(v)^2}.$$

Recently, some Sombor indices were studied in [5, 6, 7].

The Sombor exponential of a graph G was defined by Kulli in [8] as

$$SO(G,x) = \sum_{uv \in E(G)} x^{\sqrt{d_G(u)^2 + d_G(v)^2}}.$$

In [9], Kulli et al. introduced the modified Sombor index of a graph G and it is defined as

$$^{m}SO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}}$$

We define the modified Sombor exponential of a graph G as

$$^{m}SO(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}}}.$$

The first and second (a, b)-KA indices of a molecular graph G were defined by Kulli in [10] as

$$KA_{a,b}^{1}(G)=\sum_{uv\in E(G)}\left[d_G(u)^a+d_G(v)^a\right]^b, \qquad KA_{a,b}^{2}(G)=\sum_{uv\in E(G)}\left[d_G(u)^a\cdot d_G(v)^a\right]^b.$$

Considering the first and second (a, b)-KA indices, we define the first and second (a, b)-KA polynomials of a graph G as

$$KA_{a,b}^{1}(G,x)=\sum_{uv\in E(G)}x^{\left[d_G(u)^a+d_G(v)^a\right]^b}, \qquad KA_{a,b}^{2}(G,x)=\sum_{uv\in E(G)}x^{\left[d_G(u)^a d_G(v)^a\right]^b}.$$

Recently, some (a,b)-KA indices were studied, for example, see [11, 12, 13, 14, 15, 16]. In this paper, we determine the Sombor index, modified Sombor index, Sombor exponential, modified Sombor exponential, (a,b)-KA indices and their corresponding polynomials of certain dendrimer nanostars.

2. Results for dendrimer nanostars $D_1[n]$

In this section, we consider a family of dendrimer nanostar with n growth stages, denoted by $D_1[n]$. The molecular graph of $D_1[4]$ is shown in Figure 1.

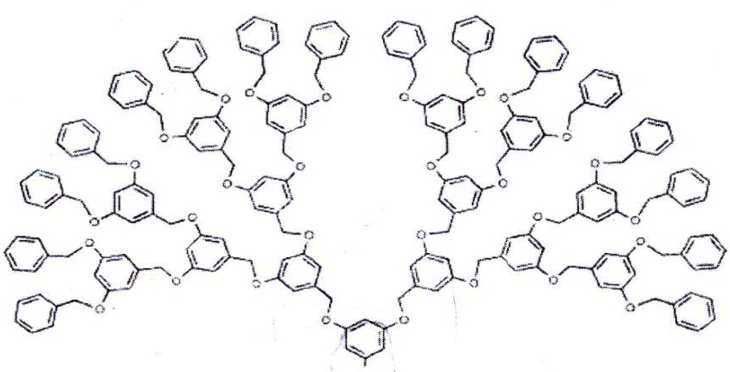

Figure 1: The molecular graph of $D_1[4]$

Let G be the molecular graph of $D_1[n]$. Clearly, the vertices of a dendrimer nanostar $D_1[n]$ are either of degree 1, 2 or 3, see Figure 1. By calculation, we obtain that G has $2^{n+4} - 9$ vertices and $18 \times 2^n - 11$ edges. We partition the edge set of $D_1[n]$ into three sets as follows:

$E_{13} = \{uv \in E(G) \mid d_G(u)=1, d_G(v)=3\}$, $|E_{13}| = 1$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v)=2\}$, $|E_{22}| = 6\times2^n - 2$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 12\times2^n - 10$.

Theorem 1. The first (a, b)-KA index of $D_1[n]$ is

$$KA_{a,b}^{1}(D_1[n])=(1^a+3^a)^b+(2\times2^a)^b(6\times2^n-2)+(2^a+3^a)^b(12\times2^n-10).$$

Proof: By definition and cardinalities of the edge partitions of $D_1[n]$, we have

$$KA^1_{a,b}(D_1[n]) = \sum_{uv\in E(G)} \left[d_G(u)^a + d_G(v)^a\right]^b$$
$$= (1^a+3^a)^b + (2^a+2^a)^b(6\times 2^n-2) + (2^a+3^a)^b(12\times 2^n-10)$$
$$= (1^a+3^a)^b + (2\times 2^a)^b(6\times 2^n-2) + (2^a+3^a)^b(12\times 2^n-10).$$

From Theorem 1, we obtain the following results.

Corollary 1.1. The Sombor index of $D_1[n]$ is

$$SO(D_1[n]) = (12\sqrt{2}+12\sqrt{3})2^n + (\sqrt{10}-4\sqrt{2}-10\sqrt{13}).$$

Corollary 1.2. The modified Sombor index of $D_1[n]$ is

$$^{m}SO(D_1[n]) = \left(\frac{3}{\sqrt{2}}+\frac{12}{\sqrt{13}}\right)2^n + \left(\frac{1}{\sqrt{10}}-\frac{1}{\sqrt{2}}-\frac{10}{\sqrt{13}}\right).$$

Theorem 2. The second (a, b)-KA index of $D_1[n]$ is

$$KA^2_{a,b}(D_1[n]) = 3^{ab} + 2^{2ab}(6\times 2^n-2)^b + 6^{ab}(12\times 2^n-10).$$

Proof: From definition and by cardinalities of the edge partitions of $D_1[n]$, we have

$$KA^2_{a,b}(D_1[n]) = \sum_{uv\in E(G)} \left[d_G(u)^a \cdot d_G(v)^a\right]^b$$
$$= (1^a\times 3^a)^b + (2^a\times 2^a)^b(6\times 2^n-2)^b + (2^a\times 3^a)^b(12\times 2^n-10)$$
$$= 3^{ab} + 2^{2ab}(6\times 2^n-2)^b + 6^{ab}(12\times 2^n-10).$$

Theorem 3. The first (a, b)-KA polynomial of $D_1[n]$ is

$$KA^1_{a,b}(D_1[n],x) = x^{(1^a+3^a)^b} + (6\times 2^n-2)x^{(2^a+2^a)^b} + (12\times 2^n-10)x^{(2^a+3^a)^b}.$$

Proof: By definition and cardinalities of the edge partitions of $D_1[n]$, we have

$$KA^1_{a,b}(D_1[n]) = \sum_{uv\in E(G)} x^{\left[d_G(u)^a+d_G(v)^a\right]^b}$$
$$= x^{(1^a+3^a)^b} + (6\times 2^n-2)x^{(2^a+2^a)^b} + (12\times 2^n-10)x^{(2^a+3^a)^b}.$$

From Theorem 3, we obtain the following results.

Corollary 3.1. The Sombor exponential of $D_1[n]$ is

$$SO(D_1[n],x) = x^{\sqrt{10}} + (6\times 2^n-2)x^{2\sqrt{2}} + (12\times 2^n-10)x^{\sqrt{13}}.$$

Corollary 3.2. The modified Sombor exponential of $D_1[n]$ is

$$^{m}SO(D_1[n],x) = x^{\frac{1}{\sqrt{10}}} + (6\times 2^n-2)x^{\frac{1}{2\sqrt{2}}} + (12\times 2^n-10)x^{\frac{1}{\sqrt{13}}}.$$

Theorem 4. The second (a, b)-KA polynomial of $D_1[n]$ is

$$KA^2_{a,b}(D_1[n],x) = x^{3^{ab}} + (6\times 2^n-2)x^{2^{2ab}} + (12\times 2^n-10)x^{6^{ab}}.$$

Proof: By definition and cardinalities of the edge partitions of $D_1[n]$, we have

$$KA_{a,b}^{2}\left(D_1[n]\right)=\sum_{uv\in E(G)} x^{\left[d_G(u)^a d_G(v)^a\right]^b}$$
$$= x^{\left(1^a\times 3^a\right)^b}+\left(6\times 2^n-2\right)x^{\left(2^a\times 2^a\right)^b}+\left(12\times 2^n-10\right)x^{\left(2^a\times 3^a\right)^b}$$
$$= x^{3^{ab}}+\left(6\times 2^n-2\right)x^{2^{2ab}}+\left(12\times 2^n-10\right)x^{6^{ab}}.$$

3. Results for dendrimer nanostars $D_3[n]$

In this section, we consider a family of dendrimer nanostars with n growth stages, denoted by $D_3[n]$. The molecular structure of $D_3[n]$ with 3 growth stages is presented in Figure 2.

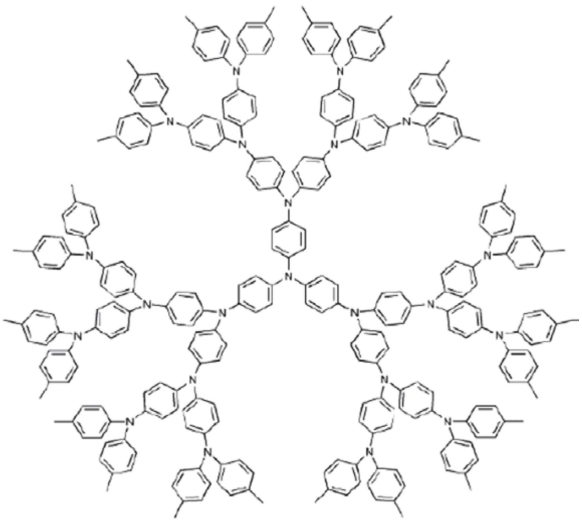

Figure 2: The molecular structure of $D_3[3]$

Let H be the graph of a dendrimer nanostar $D_3[n]$. Clearly, the vertices of a dendrimer nanostar $D_3[n]$ are either of degree 1, 2 or 3. By calculation, we obtain that H has $24 \times 2^n - 20$ vertices and $24 \times 2^{n+1} - 24$ edges. By calculation, we obtain that the edge set of $D_3[n]$ can be divided into four partitions as follows:

$E_{13} = \{uv \in E(H) \mid d_H(u)=1, d_H(v)=3\}$, $|E_{13}| = 3\times2^n$.
$E_{22} = \{uv \in E(H) \mid d_H(u) = d_H(v)=2\}$, $|E_{22}| = 12\times2^n - 6$.
$E_{23} = \{uv \in E(H) \mid d_H(u) = 2, d_H(v) = 3\}$, $|E_{23}| = 24\times2^n - 12$.
$E_{33} = \{uv \in E(H) \mid d_H(u) = d_H(v) = 3\}$, $|E_{33}| = 9\times2^n - 6$.

Theorem 5. The first (a, b)-KA index of $D_3[n]$ is

$$KA_{a,b}^{1}\left(D_3[n]\right)=\left(1^a+3^a\right)^b 3\times 2^n+\left(2^a+2^a\right)^b\left(12\times 2^n-6\right)+\left(2^a+3^a\right)^b\left(24\times 2^n-12\right)$$
$$+\left(3^a+3^a\right)^b\left(9\times 2^n-6\right).$$

Proof: By definition and cardinalities of the edge partitions of $D_3[n]$, we have

$$KA_{a,b}^{1}\left(D_3[n]\right)=\sum_{uv\in E(G)}\left[d_G(u)^a+d_G(v)^a\right]^b$$
$$=\left(1^a+3^a\right)^b 3\times 2^n+\left(2^a+2^a\right)^b\left(12\times 2^n-6\right)+\left(2^a+3^a\right)^b\left(24\times 2^n-12\right)$$
$$+\left(3^a+3^a\right)^b\left(9\times 2^n-6\right).$$

From Theorem 5, we obtain the following results.

Corollary 5.1. The Sombor index of $D_3[n]$ is

$$SO(D_3[n]) = (3\sqrt{10} + 51\sqrt{2} + 24\sqrt{13})2^n - (30\sqrt{2} + 12\sqrt{13}).$$

Corollary 5.2. The modified Sombor index of $D_3[n]$ is

$$^mSO(D_3[n]) = \left(\frac{3}{\sqrt{10}} + \frac{9}{\sqrt{2}} + \frac{24}{\sqrt{13}}\right)2^n - \left(\frac{5}{\sqrt{2}} + \frac{12}{\sqrt{13}}\right).$$

Theorem 6. The second (a, b)-KA index of $D_3[n]$ is

$$KA^2_{a,b}(D_3[n]) = 3^{ab}3\times 2^n + 2^{2ab}(12\times 2^n - 6)^b + 6^{ab}(24\times 2^n - 12) + 3^{2ab}(9\times 2^n - 6).$$

Proof: From definition and by cardinalities of the edge partitions of $D_3[n]$, we have

$$KA^2_{a,b}(D_1[n]) = \sum_{uv\in E(G)} \left[d_G(u)^a \cdot d_G(v)^a\right]^b$$

$$= (1^a\times 3^a)^b\, 3\times 2^n + (2^a\times 2^a)^b(12\times 2^n - 6)^b + (2^a\times 3^a)^b(24\times 2^n - 12)$$

$$+ (3^a\times 3^a)^b(9\times 2^n - 6)$$

$$= 3^{ab}3\times 2^n + 2^{2ab}(12\times 2^n - 6)^b + 6^{ab}(24\times 2^n - 12) + 3^{2ab}(9\times 2^n - 6).$$

Theorem 7. The first (a, b)-KA polynomial of $D_3[n]$ is

$$KA^1_{a,b}(D_3[n])$$

$$= 3\times 2^n x^{(1^a+3^a)^b} + (12\times 2^n - 6)x^{(2^a+2^a)^b} + (24\times 2^n - 12)x^{(2^a+3^a)^b} + (9\times 2^n - 6)x^{(3^a+3^a)^b}$$

Proof: By definition and cardinalities of the edge partitions of $D_3[n]$, we have

$$KA^1_{a,b}(D_3[n]) = \sum_{uv\in E(G)} x^{\left[d_G(u)^a + d_G(v)^a\right]^b}$$

$$= 3\times 2^n x^{(1^a+3^a)^b} + (12\times 2^n - 6)x^{(2^a+2^a)^b} + (24\times 2^n - 12)x^{(2^a+3^a)^b} + (9\times 2^n - 6)x^{(3^a+3^a)^b}.$$

From Theorem 7, we obtain the following results.

Corollary 7.1. The Sombor exponential of $D_3[n]$ is

$$SO(D_3[n], x) = 3\times 2^n x^{\sqrt{10}} + (12\times 2^n - 6)x^{2\sqrt{2}} + (24\times 2^n - 12)x^{\sqrt{13}} + (9\times 2^n - 6)x^{3\sqrt{2}}.$$

Corollary 7.2.The modified Sombor exponential of $D_3[n]$ is

$$^mSO(D_1[n], x) = 3\times 2^n x^{\frac{1}{\sqrt{10}}} + (12\times 2^n - 6)x^{\frac{1}{2\sqrt{2}}} + (24\times 2^n - 12)x^{\frac{1}{\sqrt{13}}} + (9\times 2^n - 6)x^{\frac{1}{3\sqrt{2}}}.$$

Theorem 8. The second (a, b)-KA polynomial of $D_3[n]$ is

$$KA^2_{a,b}(D_3[n], x) = 3\times 2^n x^{3^{ab}} + (12\times 2^n - 6)x^{2^{2ab}} + (24\times 2^n - 12)x^{6^{ab}} + (9\times 2^n - 6)x^{3^{2ab}}.$$

Proof: By definition and cardinalities of the edge partitions of $D_3[n]$, we have

$$KA^2_{a,b}(D_3[n]) = \sum_{uv\in E(G)} x^{\left[d_G(u)^a d_G(v)^a\right]^b}$$

$$= 3\times 2^n x^{(1^a\times 3^a)^b} + (12\times 2^n - 6)x^{(2^a\times 2^a)^b} + (24\times 2^n - 12)x^{(2^a\times 3^a)^b} + (9\times 2^n - 6)x^{(3^a\times 3^a)^b}$$

$$= 3\times 2^n x^{3^{ab}} + (12\times 2^n - 6)x^{2^{2ab}} + (24\times 2^n - 12)x^{6^{ab}} + (9\times 2^n - 6)x^{3^{2ab}}$$

4. Conclusion

In this study, we have determined the Sombor index, modified Sombor index, Sombor exponential, modified Sombor exponential of two families of dendrimer nanostars.

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