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Neighborhood Elliptic Sombor and Modified Neighborhood Elliptic Sombor Indices of Certain Nanostructures

V. R. Kulli[1,*]

[1]*Department of Mathematics, Gulbarga University, Kalaburgi, Karnataka, India*

Abstract

In this study, we introduce the neighborhood elliptic Sombor and modified neighborhood elliptic Sombor indices and their corresponding exponentials of a graph. Furthermore, we compute these newly defined neighborhood elliptic Sombor indices and their corresponding exponentials for certain nanostructures of chemical importance like nanocones and dendrimers.

Keywords: neighborhood elliptic Sombor index; modified neighborhood elliptic Sombor index; nanocones; dendrimers.

2020 Mathematics Subject Classification: 05C07, 05C09, 05C92.

1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. Let $\delta(G)$ denote the minimum degree among the vertices of G. We refer [1] for undefined notations and terminologies. A graph index is a numerical parameter mathematically derived from the graph structure. Several graph indices have been considered in Theoretical Chemistry and many graph indices were defined by using vertex degree concept [2]. The Zagreb, Sombor, Nirmala, Dharwad, Gourava indices are the most degree based graph indices in Chemical Graph Theory, see [3–20]. Graph indices have their applications in various disciplines in Science and Technology [21,22]. The elliptic Sombor index [23] of a graph G is defined as

$$ESO(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)) \sqrt{d_G(u)^2 + d_G(v)^2}$$

Recently, some elliptic indices were studied in [24–28]. The neighborhood elliptic Sombor index of a molecular graph G is defined as

$$NESO(G) = \sum_{uv \in E(G)} (S_G(u) + S_G(v)) \sqrt{S_G(u)^2 + S_G(v)^2}$$

*Corresponding author (vrkulli@gmail.com)

Considering the neighborhood elliptic Sombor index, we introduce the neighborhood elliptic Sombor exponential of a graph G and defined it as

$$NESO\left(G,x\right)=\sum_{uv\in E(G)}x^{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}$$

We define the modified neighborhood elliptic Sombor index of a graph G as

$$^{m}NESO\left(G\right)=\sum_{uv\in E(G)}\frac{1}{\left(S_G\left(u\right)+S_G\left(v\right)\right)\sqrt{S_G\left(u\right)^2+S_G\left(v\right)^2}}$$

Considering the modified neighborhood elliptic Sombor index, we introduce the modified neighborhood elliptic Sombor exponential of a graph G and defined it as

$$^{m}NESO\left(G,x\right)=\sum_{uv\in E(G)}x^{\frac{1}{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}}$$

Recently, some neighborhood indices were studied in [29–35]. In this work, we determine the neighborhood elliptic Sombor and modified neighborhood elliptic Sombor indices and their exponentials for certain families of nanocones and dendrimers.

2. Results For Nanocones $C_n[k]$

In this section, we consider nanocones $C_n[k]$. The molecular structure of C_4 [2] is shown in Figure 1.

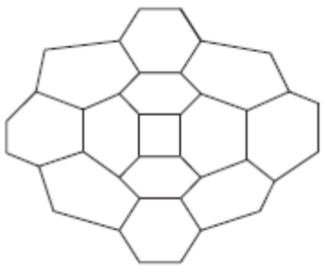

Figure 1: The molecular structure of C_4 [2]

Let G be the molecular structure of $C_n[k]$. By calculation, G has $n(k+1)^2$ vertices and $\frac{n}{2}\left(k+1\right)\left(3k+2\right)$ edges. Also by calculation, we obtain that G has five types of edges based on $S_G(u)$ and $S_G(v)$ the degrees of end vertices of each edge as given in Table 1.

$S_G(u), S_G(v)\backslash uv \in E(G)$	Number of edges
(5, 5)	n
(5, 7)	$2n$
(6, 7)	$2(k-1)n$
(7, 9)	nk
(9, 9)	$\frac{nk}{2}\left(3k-1\right)$

Table 1: Edge partition of $C_n[k]$ based on $S_G(u), S_G(v)$

In the following theorem, we compute the neighborhood elliptic Sombor index and its exponential of $C_n[k]$.

Theorem 2.1. *Let $C_n[k]$ be the family of nanocones. Then*

(i) $NESO(G) = \left(243\sqrt{2}\right)nk^2 + \left(26\sqrt{85} + 16\sqrt{130} - 81\sqrt{2}\right)nk + \left(50\sqrt{2} + 24\sqrt{74} - 26\sqrt{85}\right)n.$

(ii) $NESO(G,x) = nx^{50\sqrt{2}} + 2nx^{12\sqrt{74}} + 2(k-1)nx^{13\sqrt{85}} + nkx^{16\sqrt{130}} + \frac{nk}{2}(3k-1)x^{162\sqrt{2}}.$

Proof. Let G be the molecular graph of $C_n[k]$. By using the definitions and Table 1, we deduce

(i)
$$\begin{aligned} NESO(G) &= \sum_{uv\in E(G)} (S_G(u) + S_G(v))\sqrt{S_G(u)^2 + S_G(v)^2} \\ &= (5+5)\sqrt{5^2+5^2}n + (5+7)\sqrt{5^2+7^2}2n + (6+7)\sqrt{6^2+7^2}2(k-1)n \\ &+ (7+9)\sqrt{7^2+9^2}nk + (9+9)\sqrt{9^2+9^2}\frac{nk}{2}(3k-1). \end{aligned}$$

After simplification, we get the desired result.

(ii)
$$\begin{aligned} NESO(G,x) &= \sum_{uv\in E(G)} x^{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}} \\ &= nx^{(5+5)\sqrt{5^2+5^2}} + 2nx^{(5+7)\sqrt{5^2+7^2}} + 2(k-1)nx^{(6+7)\sqrt{6^2+7^2}} \\ &+ nkx^{(7+9)\sqrt{7^2+9^2}} + \frac{nk}{2}(3k-1)x^{(9+9)\sqrt{9^2+9^2}} \\ &= nx^{50\sqrt{2}} + 2nx^{12\sqrt{74}} + 2(k-1)nx^{13\sqrt{85}} + nkx^{16\sqrt{130}} + \frac{nk}{2}(3k-1)x^{162\sqrt{2}}. \end{aligned}$$

□

In the following theorem, we compute the modified neighborhood elliptic Sombor index and its exponential of $C_n[k]$.

Theorem 2.2. *Let $C_n[k]$ be the family of nanocones. Then*

(i) ${}^mNESO(G) = \left(\frac{1}{50\sqrt{2}} + \frac{2}{12\sqrt{74}} - \frac{2}{13\sqrt{85}}\right)n + \left(\frac{2}{13\sqrt{85}} + \frac{1}{16\sqrt{130}} - \frac{1}{324\sqrt{2}}\right)nk + \frac{3}{324\sqrt{2}}nk^2.$

(ii) ${}^mNESO(G,x) = nx^{\frac{1}{50\sqrt{2}}} + 2nx^{\frac{1}{12\sqrt{74}}} + 2(k-1)nx^{\frac{1}{13\sqrt{85}}} + nkx^{\frac{1}{16\sqrt{130}}} + \frac{nk}{2}(3k-1)x^{\frac{1}{162\sqrt{2}}}.$

Proof. Let G be the molecular graph of $C_n[k]$. By using the definitions and Table 1, we deduce

(i)
$$\begin{aligned} {}^mNESO(G) &= \sum_{uv\in E(G)} \frac{1}{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}} \\ &= \frac{n}{(5+5)\sqrt{5^2+5^2}} + \frac{2n}{(5+7)\sqrt{5^2+7^2}} + \frac{2(k-1)n}{(6+7)\sqrt{6^2+7^2}} \\ &+ \frac{nk}{(7+9)\sqrt{7^2+9^2}} + \frac{1}{(9+9)\sqrt{9^2+9^2}}\frac{nk}{2}(3k-1) \\ &= \frac{n}{50\sqrt{2}} + \frac{2n}{12\sqrt{74}} + \frac{2(k-1)n}{13\sqrt{85}} + \frac{nk}{16\sqrt{130}} + \frac{1}{162\sqrt{2}}\frac{nk}{2}(3k-1). \end{aligned}$$

After simplification, we get the desired result.

(ii) $$^{m}NESO\left(G,x\right)=\sum_{uv\in E(G)}x^{\frac{1}{\left(S_G(u)+S_G(v)\right)\sqrt{S_G(u)^2+S_G(v)^2}}}$$

$$=nx^{\frac{1}{(5+5)\sqrt{5^2+5^2}}}+2nx^{\frac{1}{(5+7)\sqrt{5^2+7^2}}}+2\left(k-1\right)nx^{\frac{1}{(6+7)\sqrt{6^2+7^2}}}$$

$$+nkx^{\frac{1}{(7+9)\sqrt{7^2+9^2}}}+\frac{nk}{2}\left(3k-1\right)x^{\frac{1}{(9+9)\sqrt{9^2+9^2}}}.$$

After simplification, we obtain the desired result.

□

3. Results for $NS_2[n]$ Dendrimers

In this section, we focus on the class of $NS_2[n]$ dendrimers with $n \geq 1$. The graph of $NS_2[3]$ is shown in Figure 2.

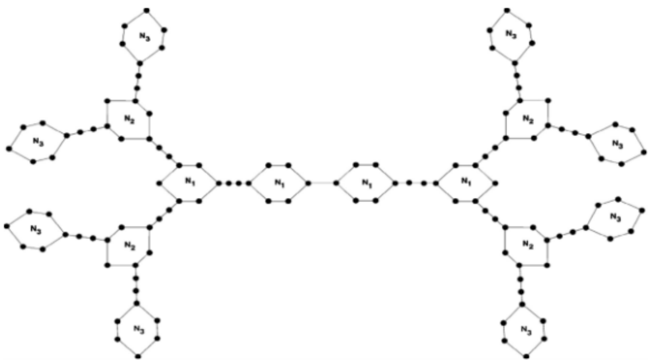

Figure 2: The graph of $NS_2[3]$

Let G be the graph of $NS_2[n]$. By calculation, G has $16 \times 2^n - 4$ vertices and $18 \times 2^n - 5$ edges. Also by calculation, we obtain that G has seven types of edges based on $S_G(u)$, $S_G(v)$ the degrees of end vertices of each edge as given in Table 2.

$S_G(u), S_G(v)\backslash uv \in E(G)$	(4, 4)	(5, 4)	(5, 5)	(5, 6)	(7, 7)	(5, 7)	(6, 6)
Number of edges	2×2^n	2×2^n	2×2^n +2	6×2^n	1	4	$6 \times 2^n - 12$

Table 2: Edge partition of $NS_2[n]$ based on $S_G(u)$ and $S_G(v)$

In the following theorem, we compute the neighborhood elliptic Sombor index and its exponential of $NS_2[n]$.

Theorem 3.1. *Let $NS_2[n]$ be the family of dendrimers. Then*

(i) $NESO(G) = \left(596\sqrt{2} + 18\sqrt{41} + 66\sqrt{61}\right) 2^n + 112\sqrt{2} + 48\sqrt{74}.$

(ii) $NESO(G, x) = 2 \times 2^n x^{32\sqrt{2}} + 2 \times 2^n x^{9\sqrt{41}} + (2 \times 2^n + 2)x^{50\sqrt{2}} + 6 \times 2^n x^{11\sqrt{61}} + 1x^{98\sqrt{2}} + 4x^{12\sqrt{74}} + (6 \times 2^n - 12)x^{72\sqrt{2}}.$

Proof. Let G be the molecular graph of $NS_2[n]$. By using the definitions and Table 2, we deduce

(i) $$NESO(G) = \sum_{uv \in E(G)} (S_G(u) + S_G(v)) \sqrt{S_G(u)^2 + S_G(v)^2}$$
$$= (4+4)\sqrt{4^2+4^2} 2 \times 2^n + (5+4)\sqrt{5^2+4^2} 2 \times 2^n + (5+5)\sqrt{5^2+5^2}(2 \times 2^n + 2)$$
$$+ (5+6)\sqrt{5^2+6^2} 6 \times 2^n + (7+7)\sqrt{7^2+7^2} 1 + (5+7)\sqrt{5^2+7^2} 4$$
$$+ (6+6)\sqrt{6^2+6^2}(6 \times 2^n - 12).$$

After simplification, we obtain the desired result.

(ii) $$NESO(G,x) = \sum_{uv \in E(G)} x^{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}$$
$$= 2 \times 2^n x^{(4+4)\sqrt{4^2+4^2}} + 2 \times 2^n x^{(5+4)\sqrt{5^2+4^2}} + (2 \times 2^n + 2) x^{(5+5)\sqrt{5^2+5^2}}$$
$$+ 6 \times 2^n x^{(5+6)\sqrt{5^2+6^2}} + 1 x^{(7+7)\sqrt{7^2+7^2}} + 4 x^{(5+7)\sqrt{5^2+7^2}}$$
$$+ (6 \times 2^n - 12) x^{(6+6)\sqrt{6^2+6^2}}.$$

After simplification, we obtain the desired result.

□

In the following theorem, we compute the modified neighborhood elliptic Sombor index and its exponential of $NS_2[n]$.

Theorem 3.2. *Let $NS_2[n]$ be the family of dendrimers. Then*

(i) $${}^{m}NESO(G) = \left(\frac{1}{16\sqrt{2}} + \frac{1}{25\sqrt{2}} + \frac{1}{12\sqrt{2}} + \frac{2}{9\sqrt{41}} + \frac{6}{11\sqrt{61}}\right) 2^n + \frac{1}{25\sqrt{2}} + \frac{1}{98\sqrt{2}} - \frac{1}{6\sqrt{2}} + \frac{1}{3\sqrt{74}}.$$

(ii) $${}^{m}NESO(G,x) = 2 \times 2^n x^{\frac{1}{32\sqrt{2}}} + 2 \times 2^n x^{\frac{1}{9\sqrt{41}}} + (2 \times 2^n + 2) x^{\frac{1}{50\sqrt{2}}} + 6 \times 2^n x^{\frac{1}{11\sqrt{61}}} + 1 x^{\frac{1}{98\sqrt{2}}} + 4 x^{\frac{1}{12\sqrt{74}}} + (6 \times 2^n - 12) x^{\frac{1}{72\sqrt{2}}}.$$

Proof. Let G be the molecular graph of $NS_2[n]$. By using the definitions and Table 2, we deduce

(i) $${}^{m}NESO(G) = \sum_{uv \in E(G)} \frac{1}{(S_G(u) + S_G(v)) \sqrt{S_G(u)^2 + S_G(v)^2}}$$
$$= \frac{2 \times 2^n}{(4+4)\sqrt{4^2+4^2}} + \frac{2 \times 2^n}{(5+4)\sqrt{5^2+4^2}} + \frac{2 \times 2^n + 2}{(5+5)\sqrt{5^2+5^2}} + \frac{6 \times 2^n}{(5+6)\sqrt{5^2+6^2}}$$
$$+ \frac{1}{(7+7)\sqrt{7^2+7^2}} + \frac{4}{(5+7)\sqrt{5^2+7^2}} + \frac{6 \times 2^n - 12}{(6+6)\sqrt{6^2+6^2}}.$$

After simplification, we obtain the desired result.

(ii) $${}^{m}NESO(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}}$$
$$= 2 \times 2^n x^{\frac{1}{(4+4)\sqrt{4^2+4^2}}} + 2 \times 2^n x^{\frac{1}{(5+4)\sqrt{5^2+4^2}}} + (2 \times 2^n + 2) x^{\frac{1}{(5+5)\sqrt{5^2+5^2}}} + 6 \times 2^n x^{\frac{1}{(5+6)\sqrt{5^2+6^2}}}$$
$$+ 1 x^{\frac{1}{(7+7)\sqrt{7^2+7^2}}} + 4 x^{\frac{1}{(5+7)\sqrt{5^2+7^2}}} + (6 \times 2^n - 12) x^{\frac{1}{(6+6)\sqrt{6^2+6^2}}}.$$

After simplification, we obtain the desired result.

□

$S_G(u), S_G(v)\backslash uv \in E(G)$	(4, 4)	(5, 4)	(5, 7)	(6, 7)	(7, 7)
Number of edges	3×2^n	3×2^n	3×2^n	$9 \times 2^n - 12$	$3 \times 2^n - 3$

Table 3: Edge partition of $NS_3[n]$ based on $S_G(u)$ and $S_G(v)$

4. Results for $NS_3[N]$ Dendrimers

In this section, we focus on another type of dendrimers $NS_3[n]$ with $n \geq 1$. The molecular structure of $NS_3[2]$ is presented in Figure 3.

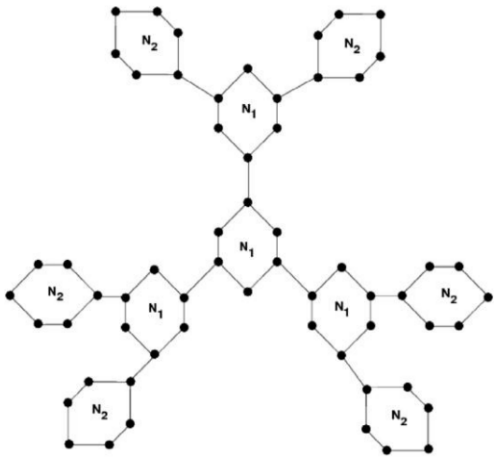

Figure 3: The structure of $NS_3[2]$

Let G be the molecular graph of $NS_3[n]$. By calculation, we obtain that G has $18 \times 2^n - 12$ vertices and $21 \times 2^n - 15$ edges. Also by calculation, we get that G has five types of edges based on $S_G(u)$ and $S_G(v)$ the degrees of end vertices of each edge as given in Table 3.

In the following theorem, we compute the neighborhood elliptic Sombor index and its exponential of $NS_3[n]$.

Theorem 4.1. *Let $NS_3[n]$ be the family of dendrimers. Then*

(i) $NESO(G) = \left(390\sqrt{2} + 27\sqrt{41} + 36\sqrt{74} + 117\sqrt{85}\right) 2^n - 294\sqrt{2} - 156\sqrt{85}.$

(ii) $NESO(G, x) = 3 \times 2^n x^{32\sqrt{2}} + 3 \times 2^n x^{9\sqrt{41}} + +3 \times 2^n x^{12\sqrt{74}} + (9 \times 2^n - 12)x^{13\sqrt{85}} + (3 \times 2^n - 3)x^{98\sqrt{2}}.$

Proof. Let G be the molecular graph of $NS_3[n]$. By using the definitions and Table 3, we deduce

(i) $$NESO(G) = \sum_{uv \in E(G)} (S_G(u) + S_G(v)) \sqrt{S_G(u)^2 + S_G(v)^2}$$
$$= (4+4)\sqrt{4^2+4^2}3 \times 2^n + (5+4)\sqrt{5^2+4^2}3 \times 2^n + (5+7)\sqrt{5^2+7^2}3 \times 2^n$$
$$+ (6+7)\sqrt{6^2+7^2}(9 \times 2^n - 12) + (7+7)\sqrt{7^2+7^2}(3 \times 2^n - 3).$$

After simplification, we obtain the desired result.

(ii) $NESO(G,x) = \sum_{uv \in E(G)} x^{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}$

$$= 3 \times 2^n x^{(4+4)\sqrt{4^2+4^2}} + 3 \times 2^n x^{(5+4)\sqrt{5^2+4^2}} + 3 \times 2^n x^{(5+7)\sqrt{5^2+7^2}}$$
$$+ (9 \times 2^n - 12) x^{(6+7)\sqrt{6^2+7^2}} + (3 \times 2^n - 3) x^{(7+7)\sqrt{7^2+7^2}}.$$

After simplification, we obtain the desired result.

□

In the following theorem, we compute the modified neighborhood elliptic Sombor index and its exponential of $NS_3[n]$.

Theorem 4.2. *Let $NS_3[n]$ be the family of dendrimers. Then*

(i) $^mNESO(G) = \left(\frac{3}{32\sqrt{2}} + \frac{3}{9\sqrt{41}} + \frac{3}{12\sqrt{74}} + \frac{9}{13\sqrt{85}} + \frac{3}{98\sqrt{2}}\right) 2^n - \frac{3}{98\sqrt{2}} - \frac{12}{13\sqrt{85}}.$

(ii) $^mNESO(G,x) = 3 \times 2^n x^{\frac{1}{32\sqrt{2}}} + 3 \times 2^n x^{\frac{1}{9\sqrt{41}}} + 3 \times 2^n x^{\frac{1}{12\sqrt{74}}} + (9 \times 2^n - 12) x^{\frac{1}{13\sqrt{85}}} + (3 \times 2^n - 3) x^{\frac{1}{98\sqrt{2}}}.$

Proof. Let G be the molecular graph of $NS_3[n]$. By using the definitions and Table 3, we deduce

(i) $^mNESO(G) = \sum_{uv \in E(G)} \frac{1}{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}$

$$= \frac{3 \times 2^n}{(4+4)\sqrt{4^2+4^2}} + \frac{3 \times 2^n}{(5+4)\sqrt{5^2+4^2}} + \frac{3 \times 2^n}{(5+7)\sqrt{5^2+7^2}}$$
$$+ \frac{9 \times 2^n - 12}{(6+7)\sqrt{6^2+7^2}} + \frac{3 \times 2^n - 3}{(7+7)\sqrt{7^2+7^2}}.$$

After simplification, we obtain the desired result.

(ii) $^mNESO(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{(S_G(u)+S_G(v))\sqrt{S_G(u)^2+S_G(v)^2}}}$

$$= 3 \times 2^n x^{\frac{1}{(4+4)\sqrt{4^2+4^2}}} + 3 \times 2^n x^{\frac{1}{(5+4)\sqrt{5^2+4^2}}} + 3 \times 2^n x^{\frac{1}{(5+7)\sqrt{5^2+7^2}}}$$
$$+ (9 \times 2^n - 12) x^{\frac{1}{(6+7)\sqrt{6^2+7^2}}} + (3 \times 2^n - 3) x^{\frac{1}{(7+7)\sqrt{7^2+7^2}}}.$$

After simplification, we obtain the desired result.

□

5. Conclusion

In this work, we have determined the neighborhood elliptic Sombor and modified neighborhood elliptic Sombor indices and their exponentials for certain families of nanocones and dendrimers.

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