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Neighborhood Sombor Index of Some Nanostructues

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Abstract: *In Chemical Graph Theory, several degree based topological indices were introduced and studied since 1972. Recently, Gutman considered a class of novel graph invariants of which the Sombor index was defined. In this paper, we introduce some new Sombor indices: the second, third, fourth and neighborhood (or fifth) Sombor indices of a graph. Furthermore, we compute the Sombor and neighborhood Sombor indices and their exponentials of some important nanostructures which appeared in nanoscience.*

Keywords: *nanoscience, Sombor index, neighborhood Sombor index, neighborhood Sombor exponential, dendrimer.*

Mathematics Subject Classification: 05*C*05, 05*C*12, 05*C*35.

I. Introduction

In Chemical Graph Theory, concerning the definition of the topological index on the molecular graph and concerning chemical properties of drugs can be studied by the topological index calculation, see [1]. Several degree based indices of a graph have been appeared in the literature, see [2, 3, 4, 5] and have found some applications, especially in QSPR/QSAR study, see [6, 7].

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 $S_G(u)$ be the sum of the degrees of all vertices adjacent to vertex u. For undefined term and notation, we refer the book [8].

The Sombor index of a graph G was introduced by Gutman in [9] and defined it as

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

Considering the Sombor index, Kulli introduced the Sombor exponential [10] of a graph G, defined as

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

Motivated by the previous research in Sombor index and its applications, we now introduce the second, third and fourth Sombor indices of the molecular graph as follows:

The second Sombor index of a molecular graph G is defined as

$$SO_2(G)=\sum_{uv\in E(G)}\sqrt{n_u^2+n_v^2}$$

where the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The third Sombor index of a molecular graph G is defined as

$$SO_3(G)=\sum_{uv\in E(G)}\sqrt{m_u^2+m_v^2}$$

where the number m_u of edges of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The fourth Sombor index of a molecular graph G is defined as

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$$SO_4(G)=\sum_{uv\in E(G)}\sqrt{\varepsilon(u)^2+\varepsilon(v)^2}$$

where the number $\varepsilon(u)$ is the eccentricity of vertex u.

The neighborhood Sombor index of a molecular graph G is defined as

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

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

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

Recently some Sombor and Sombor type indices were studied, for example, in [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24] and some neighborhood indices were studied, for example, in [25, 26, 27, 28, 29, 30, 31, 32].

In this paper, we compute the Sombor index, Sombor exponential, neighborhood Sombor index, neighborhood Sombor exponential of some important nanostructures such as dominating oxide networks, regular triangulate oxide networks, H-Naphtalenic nanotubes and nanocones.

II. RESULTS FOR DOMINATING OXIDE NETWORKS *DOX*(*n*)

In this section, we consider the graph of a dominating oxide network $DOX(n)$, see Figure 1.

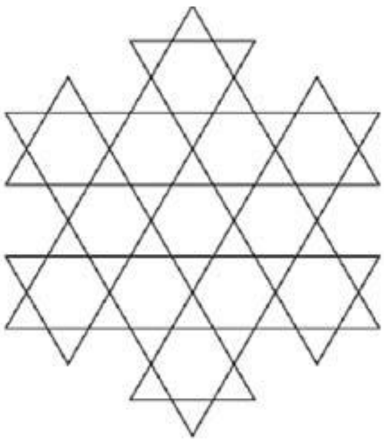

Figure 1

Let G be the graph of $DOX(n)$. By calculation, we obtain that G has $54n^2-54n+18$ edges. Also by calculation, there are two types of edges in G based on the degrees of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_1| = 24n-12$.

$E_2 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}$, $|E_2| = 54n^2-78n+30$.

The partition of the edges with respect to their sum degree of end vertices of dominating oxide networks is given in Table 1.

(S_u, S_v)	(8, 12)	(8, 14)	(12, 12)	(12, 14)	(14, 16)	(16, 16)
Number of edges	$12n$	$12n-12$	6	$12n-12$	$24n-24$	$54n^2-114n+60$

Table 1 . Edge partition of *DOX*(*n*) based on $S_G(u)$, $S_G(v)$

In the following theorem, we compute the Sombor index and its exponential of $DOX(n)$.

Theorem 1. Let $DOX(n)$ be the family of dominating oxide networks. Then

(i) $SO(DOX(n))=216\sqrt{2}n^2+(48\sqrt{5}-312\sqrt{2})n-24\sqrt{5}+120\sqrt{2}.$

(ii) $SO\left(DOX\left(n\right),x\right)=(24n-12)x^{2\sqrt{5}}+\left(54n^{2}-78n+30\right)x^{4\sqrt{2}}.$

Proof: Let G be the molecular graph of *DOX*(n). By using the definitions and cardinalities of the edge partition of *DOX(n)*, we deduce

(i) $$SO\left(DOX\left(n\right)\right)=\sum_{uv\in E(G)}\sqrt{d_G(u)^2+d_G(v)^2}$$

$$=\left(2^2+4^2\right)^{\frac{1}{2}}(24n-12)+\left(4^2+4^2\right)^{\frac{1}{2}}(54n^2-78n+30).$$

After simplification, we get the desired result.

(ii) $$SO\left(DOX\left(n\right),x\right)=\sum_{uv\in E(G)}x^{\sqrt{d_G(u)^2+d_G(v)^2}}$$

$$=(24n-12)x^{\left(2^2+4^2\right)^{\frac{1}{2}}}+(54n^2-78n+30)x^{\left(4^2+4^2\right)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

In the following theorem, we compute the neighborhood Sombor index and its exponential of *DOX*(n).

Theorem 2. Let *DOX*(n) be the family of dominating oxide networks. Then

(i) $NSO\left(DOX\left(n\right)\right)=864\sqrt{2}n^2+\left(48\sqrt{13}+24\sqrt{65}+24\sqrt{85}+48\sqrt{113}-1824\sqrt{2}\right)n$
$-24\sqrt{65}+24\sqrt{18}-24\sqrt{85}-48\sqrt{113}+960\sqrt{2}.$

(ii) $NSO\left(DOX\left(n\right),x\right)=12nx^{4\sqrt{13}}+(12n-12)x^{2\sqrt{65}}+6x^{4\sqrt{18}}+(12n-12)x^{2\sqrt{85}}$
$+(24n-24)x^{2\sqrt{113}}+\left(54n^2-114n+60\right)x^{16\sqrt{2}}.$

Proof: Let G be the molecular graph of *DOX*(n). By using the definitions and Table 1, we deduce

(i) $$NSO\left(DOX\left(n\right)\right)=\sum_{uv\in E(G)}\sqrt{S_G(u)^2+S_G(v)^2}$$

$$=\left(8^2+12^2\right)^{\frac{1}{2}}12n+\left(8^2+14^2\right)^{\frac{1}{2}}(12n-12)+\left(12^2+12^2\right)^{\frac{1}{2}}6+\left(12^2+14^2\right)^{\frac{1}{2}}(12n-12)$$
$$+\left(14^2+16^2\right)^{\frac{1}{2}}(24n-24)+\left(16^2+16^2\right)^{\frac{1}{2}}(54n^2-114n+60).$$

After simplification, we get the desired result.

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

$$=12nx^{\left(8^2+12^2\right)^{\frac{1}{2}}}+(12n-12)x^{\left(8^2+14^2\right)^{\frac{1}{2}}}+6x^{\left(12^2+12^2\right)^{\frac{1}{2}}}+(12n-12)x^{\left(12^2+14^2\right)^{\frac{1}{2}}}$$
$$+(24n-24)x^{\left(14^2+16^2\right)^{\frac{1}{2}}}+(54n-114n+60)x^{\left(16^2+16^2\right)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

III. RESULTS FOR REGULAR TRIANGULATE OXIDE NETWORKS *RTOX*(n)

In this section, we consider a family of regular triangulate oxide networks which is denoted by *RTOX*(n) , $n\geq 3$. The graph of RTOX(5) is shown in Figure 2.

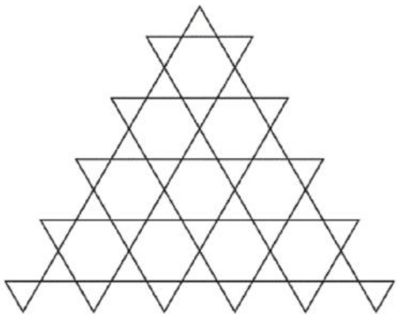

Figure 2

Let G be the graph of *RTOX(n)*. By calculation, we obtain that G has $3n^2+6n$ edges. Also by calculation, there are three types of edges in G based on the degrees of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_1| = 2$.
$E_2 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_2| = 6n$.
$E_3 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}$, $|E_4| = 3n^2-2$.

The partition of the edges with respect to their sum degree of end vertices of regular triangulate oxide networks is given in Table 2.

(S_u, S_v)	(6,6)	(6,12)	(8,12)	(8,14)	(12,12)	(12,14)	(14,14)	(14,16)	(16, 16)
Number of edges	2	4	4	$6n-8$	1	6	$6n-9$	$6n-12$	$3n^2-12n+12$

Table 2. Edge partition of *RTOX*(*n*) based on $S_G(u)$, $S_G(v)$

In the following theorem, we compute the Sombor index and its exponential of *RTOX*(*n*).

Theorem 3. Let *RTOX*(*n*) be the family of regular triangulate oxide networks. Then

(i) $SO(RTOX(n)) = 12\sqrt{2}n^2 + 12\sqrt{5}n - 4\sqrt{2}$.

(ii) $SO(RTOX(n), x) = 2x^{2\sqrt{2}} + 6nx^{2\sqrt{5}} + (3n^2-2)x^{4\sqrt{2}}$.

Proof: Let G be the molecular graph of *RTOX*(*n*). By using the definitions and cardinalities of the edge partition of *RTOX(n)*, we deduce

(i)
$$SO(RTOX(n)) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$
$$= (2^2+2^2)^{\frac{1}{2}} 2 + (2^2+4^2)^{\frac{1}{2}} 6n + (4^2+4^2)^{\frac{1}{2}} (3n^2-2).$$

After simplification, we get the desired result.

(ii)
$$SO(RTOX(n), x) = \sum_{uv \in E(G)} x^{\sqrt{d_G(u)^2 + d_G(v)^2}}$$
$$= 2x^{(2^2+2^2)^{\frac{1}{2}}} + 6nx^{(2^2+4^2)^{\frac{1}{2}}} + (3n^2-2)x^{(4^2+4^2)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

In the following theorem, we compute the neighborhood Sombor index and its exponential of *RTOX*(*n*).

Theorem 4. Let *RTOX*(*n*) be the family of regular triangulate oxide networks. Then

(i) $NSO(RTOX(n)) = 48\sqrt{2}n^2 + \left(12\sqrt{65} + 12\sqrt{98} + 12\sqrt{113} - 192\sqrt{2}\right)n$
$+204\sqrt{2} + 24\sqrt{5} + 16\sqrt{13} - 16\sqrt{65} + 4\sqrt{18} + 12\sqrt{85} - 18\sqrt{98} - 24\sqrt{113}.$

(ii) $NSO(RTOX(n), x) = 2x^{6\sqrt{2}} + 4x^{6\sqrt{5}} + 4x^{4\sqrt{13}} + (6n-8)x^{2\sqrt{65}} + x^{4\sqrt{18}} + 6x^{2\sqrt{85}}$
$+(6n-9)x^{2\sqrt{98}} + (6n-12)x^{2\sqrt{113}} + \left(3n^2-12n+12\right)x^{16\sqrt{2}}.$

Proof: Let G be the molecular graph of $RTOX(n)$. By using the definitions and Table 2, we deduce

(i) $$NSO(RTOX(n)) = \sum_{uv\in E(G)} \sqrt{S_G(u)^2 + S_G(v)^2}$$

$$= (6^2+6^2)^{\frac{1}{2}} 2 + (6^2+12^2)^{\frac{1}{2}} 4 + (8^2+12^2)^{\frac{1}{2}} 4 + (8^2+14^2)^{\frac{1}{2}} (6n-8) + (12^2+12^2)^{\frac{1}{2}} + (12^2+14^2)^{\frac{1}{2}} 6$$

$$+ (14^2+14^2)^{\frac{1}{2}} (6n-9) + (14^2+16^2)^{\frac{1}{2}} (6n-12) + (16^2+16^2)^{\frac{1}{2}} (3n^2-12n+12).$$

After simplification, we get the desired result.

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

$$= 2x^{(6^2+6^2)^{\frac{1}{2}}} + 4x^{(6^2+12^2)^{\frac{1}{2}}} + 4x^{(8^2+12^2)^{\frac{1}{2}}} + (6n-8)x^{(8^2+14^2)^{\frac{1}{2}}} + x^{(12^2+12^2)^{\frac{1}{2}}} + 6x^{(12^2+14^2)^{\frac{1}{2}}}$$

$$+(6n-9)x^{(14^2+14^2)^{\frac{1}{2}}} + (6n-12)x^{(14^2+16^2)^{\frac{1}{2}}} + (3n^2-12n-12)x^{(16^2+16^2)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

IV. Results for H-Naphtalenic Nanotubes

In this section we consider a family of H-Naphtalenic nanotubes. This nanotube is a trivalent decoration having a sequence of C_6, C_6, C_4, C_6, C_6, C_4, … in the first row and a sequence of C_6, C_8, C_6, C_8, … in other row. This nanotube is denoted by $NHPX[m, n]$, where m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as shown in Figure 3.

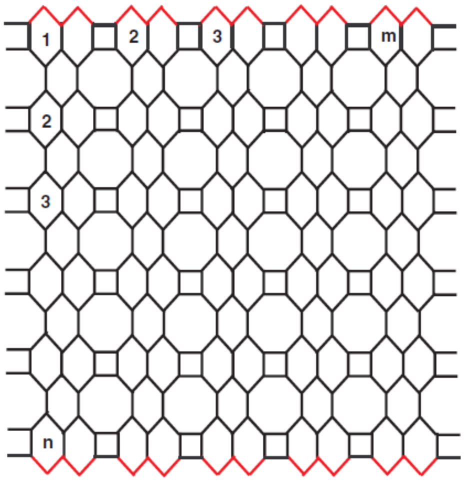

Figure 3

Let G be a graph of a nanotube $NHPX$ $[m, n]$. By calculation, G has $10mn$ vertices and $15mn – 2m$ edges. We obtain that G has two types of edges based on the degrees of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_1| = 8m$.

$E_2 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_2| = 15mn – 10m$.

The partition of the edges with respect to their sum degree of end vertices of H-Naphtalenic nanotubes is given in Table 3.

(S_u, S_v)	(6, 7)	(6, 8)	(8, 8)	(7, 9)	(8, 9)	(9, 9)
Number of edges	$4m$	$4m$	$2m$	$2m$	$4m$	$15mn– 18n$

Table 3. Edge partition of $NHPX[m, n]$ based on $S_G(u)$, $S_G(v)$

In the following theorem, we compute the Sombor index and its exponential of $NHPX[m, n]$.

Theorem 5. Let $NHPX[m, n]$ be the family of H-Naphtalenic nanotubes Then

(i) $SO\left(NHPX\left[m,\ n\right]\right)=45\sqrt{2}mn+\left(8\sqrt{13}-30\sqrt{2}\right)m.$

(ii) $SO\left(NHPX\left[m,\ n\right],x\right)=8mx^{\sqrt{13}}+(15mn-10m)\,x^{3\sqrt{2}}.$

Proof: Let G be the molecular graph of $NHPX[m, n]$. By using the definitions and cardinalities of the edge partition of $NHPX[m, n]$, we deduce

(i) $$SO\left(NHPX\left[m,\ n\right]\right)=\sum_{uv\in E(G)}\sqrt{d_G(u)^2+d_G(v)^2}$$

$$=\left(2^2+3^2\right)^{\frac{1}{2}}8m+\left(3^2+3^2\right)^{\frac{1}{2}}(15mn-10m)$$

After simplification, we get the desired result.

(ii) $$SO\left(NHPX\left[m,\ n\right],x\right)=\sum_{uv\in E(G)}x^{\sqrt{d_G(u)^2+d_G(v)^2}}$$

$$=8mx^{(2^2+3^2)^{\frac{1}{2}}}+(15mn-10m)x^{(3^2+3^2)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

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

Theorem 6 . Let $NHPX[m, n]$ be the family of H-Naphtalenic nanotubes. Then

(i) $NSO\left(NHPX\left[m,\ n\right]\right)=135\sqrt{2}mn+\left(4\sqrt{85}+40+2\sqrt{130}+4\sqrt{145}-146\sqrt{2}\right)m.$

(ii) $NSO\left(NHPX\left[m,\ n\right],x\right)=4mx^{\sqrt{85}}+4mx^{10}+2mx^{8\sqrt{2}}+2mx^{\sqrt{130}}+4mx^{\sqrt{145}}+(15mn-18m)x^{9\sqrt{2}}.$

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

(i) $$NSO\left(NHPX\left[m,\ n\right]\right)=\sum_{uv\in E(G)}\sqrt{S_G(u)^2+S_G(v)^2}$$

$$=\left(6^2+7^2\right)^{\frac{1}{2}}4m+\left(6^2+8^2\right)^{\frac{1}{2}}4m+\left(8^2+8^2\right)^{\frac{1}{2}}2m+\left(7^2+9^2\right)^{\frac{1}{2}}2m$$
$$+\left(8^2+9^2\right)^{\frac{1}{2}}4m+\left(9^2+9^2\right)^{\frac{1}{2}}(15mn-18m).$$

After simplification, we get the desired result.

(ii) $$NSO\left(NHPX\left[m,\ n\right],x\right)=\sum_{uv\in E(G)}x^{\sqrt{S_G(u)^2+S_G(v)^2}}$$

$$=4mx^{(6^2+7^2)^{\frac{1}{2}}}+4mx^{(6^2+8^2)^{\frac{1}{2}}}+2mx^{(8^2+8^2)^{\frac{1}{2}}}+2mx^{(7^2+9^2)^{\frac{1}{2}}}+4mx^{(8^2+9^2)^{\frac{1}{2}}}+(15mn-18)x^{(9^2+9^2)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

V. RESULTS FOR NANOCONES $C_n[k]$

In this section, we consider nanocones $C_n[k]$. The molecular structure of $C_2[4]$ is shown in Figure 4.

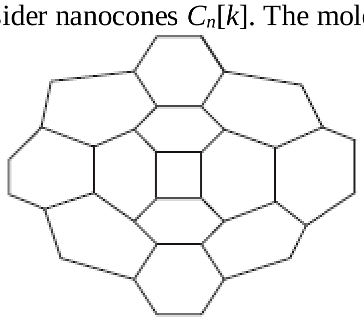

Figure 4

Let G be the molecular structure of $C_n[k]$. By calculation, G has $n(k+1)^2$ vertices and $\frac{3}{2}nk^2+\frac{5}{2}nk+n$ edges. . We obtain that G has three types of edges based on the degrees of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_1| = n$.
$E_2 = \{uv \in E(G) \mid d_G(u) =2, d_G(v) = 3\}$, $|E_2| = 2nk$.
$E_3 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_2| = \frac{3}{2}nk^2+\frac{1}{2}nk$.

Also by calculation, we obtain that G has five types of edges based on $S_G(u)$ and $S_G(v)$ the degree of end vertices of each edge as given in Table 4.

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

Table 4 . Edge partition of $C_n[k]$ based on $S_G(u)$, $S_G(v)$

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

Theorem 7. Let $C_n[k]$ be the family of nanocones. Then

(i) $SO(C_n[k])=\frac{9}{\sqrt{2}}nk^2+\left(\sqrt{13}+\frac{3}{\sqrt{2}}nk\right)nk+2\sqrt{2}n.$

(ii) $SO(C_n[k],x)=nx^{2\sqrt{2}}+nkx^{\sqrt{13}}+\left(\frac{3}{2}nk^2+\frac{1}{2}nk\right)x^{3\sqrt{2}}.$

Proof: Let G be the molecular graph of $C_n[k]$. By using the definitions and cardinalities of the edge partition of $C_n[k]$, we deduce

(i) $$SO(C_n[k])=\sum_{uv\in E(G)}\sqrt{d_G(u)^2+d_G(v)^2}$$

$$=(2^2+2^2)^{\frac{1}{2}}n+(2^2+3^2)^{\frac{1}{2}}nk+(3^2+3^2)^{\frac{1}{2}}\left(\frac{3}{2}nk^2+\frac{1}{2}nk\right).$$

After simplification, we get the desired result.

(ii) $$SO(C_n[k],x)=\sum_{uv\in E(G)}x^{\sqrt{d_G(u)^2+d_G(v)^2}}$$

$$=nx^{(2^2+2^2)^{\frac{1}{2}}}+nkx^{(2^2+3^2)^{\frac{1}{2}}}+\left(\frac{3}{2}nk^2+\frac{1}{2}nk\right)x^{(3^2+3^2)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

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

Theorem 8. Let $C_n[k]$ be the family of nanocones. Then

(i) $NSO(C_n[k])=\frac{27}{\sqrt{2}}nk^2+\left(2\sqrt{85}+\sqrt{130}-\frac{9}{\sqrt{2}}\right)nk+\left(5\sqrt{2}+2\sqrt{74}-2\sqrt{85}\right)n.$

(ii) $NSO(C_n[k],x)=nx^{5\sqrt{2}}+2nx^{5\sqrt{74}}+2(k-1)nx^{\sqrt{85}}+nkx^{\sqrt{130}}+\frac{nk}{2}(3k-1)x^{9\sqrt{2}}.$

Proof: Let G be the molecular graph of $C_n[k]$. By using the definitions and Table 4, we deduce

(i) $$NSO\left(C_n[k]\right)=\sum_{uv\in E(G)}\sqrt{S_G(u)^2+S_G(v)^2}$$

$$=\left(5^2+5^2\right)^{\frac{1}{2}}n+\left(5^2+7^2\right)^{\frac{1}{2}}2n+\left(6^2+7^2\right)^{\frac{1}{2}}2(k-1)n+\left(7^2+9^2\right)^{\frac{1}{2}}nk+\left(9^2+9^2\right)^{\frac{1}{2}}\frac{nk}{2}(3k-1).$$

After simplification, we get the desired result.

(ii) $$NSO\left(C_n[k],x\right)=\sum_{uv\in E(G)}x^{\sqrt{S_G(u)^2+S_G(v)^2}}$$

$$=nx^{\left(5^2+5^2\right)^{\frac{1}{2}}}+2nx^{\left(5^2+7^2\right)^{\frac{1}{2}}}+2(k-1)nx^{\left(6^2+7^2\right)^{\frac{1}{2}}}+nkx^{\left(7^2+9^2\right)^{\frac{1}{2}}}+\frac{nk}{2}(3k-1)x^{\left(9^2+9^2\right)^{\frac{1}{2}}}.$$

After simplification, we obtain the desired result.

Conclusion

In this study, we have introduced some new Sombor indices: the second, third, fourth and neighborhood Sombor indices of a graph. Furthermore, we have computed the Sombor and neighborhood Sombor indices and their exponentials of some important nanostructures such as dominating oxide networks, regular triangulate oxide networks, H-Naphtalenic nanotubes and nanocones.

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