MULTIPLICATIVE SOMBOR INDICES OF CERTAIN NANOTUBES

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ABSTRACT

A topological index is a numeric quantity from structural graph of a molecule. In this paper, we introduce the multiplicative Sombor index, multiplicative modified Sombor index, multiplicative reduced Sombor index and multiplicative reduced modified Sombor index of a graph. Furthermore we compute these multiplicative Sombor indices for certain nanotubes.

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Keywords: multiplicative Sombor index, multiplicative modified Sombor index, multiplicative reduced Sombor index, nanotube.

1. INTRODUCTION

We consider only 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. For undefined term and notation, we refer the book [1].

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 affect on the development of the Chemical Sciences. Topological indices are useful for establishing correlation between the structure of a molecular compound and its physicochemical properties. Several topological indices [2] have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR study, see [3, 4, 5].

The Sombor index [6] was introduced and defined it as

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

The modified Sombor index was introduced by Kulli at al. in [7], defined as

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

Recently, some Sombor indices were studied in [8, 9, 10, 11, 12].

Inspired by work on Sombor indices, we introduce the multiplicative Sombor index, multiplicative modified Sombor index, general multiplicative first (a, b)-KA index of a graph as follows:

The multiplicative Sombor index of a graph G is defined as

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

The multiplicative modified Sombor index of a graph G is defined as

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

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The multiplicative first and second (a, b)-KA indices of a graph G were defined by Kulli in [13], as

$$KA_{a,b}^{1}II(G) = \prod_{uv \in E(G)} \left[d_{G}(u)^{a} + d_{G}(v)^{a} \right]^{b},$$

$$KA_{a,b}^{2}II(G) = \prod_{uv \in E(G)} \left[d_{G}(u)^{a} d_{G}(v)^{a} \right]^{b}.$$

Motivated by the definition of the reduced indices, we introduce the multiplicative reduced Sombor index, multiplicative reduced modified Sombor index, general multiplicative reduced first (a, b)-KA index of a graph as follows:

The multiplicative reduced Sombor index of a graph G is defined as

$$RSOII\left(G\right) = \prod_{uv \in E\left(G\right)} \sqrt{\left(d_{G}\left(u\right) - 1\right)^{2} + \left(d_{G}\left(v\right) - 1\right)^{2}}.$$

The multiplicative reduced modified Sombor index of a graph G is defined as

$${}^{m}RSOH(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{\left(d_{G}(u) - 1\right)^{2} + \left(d_{G}(v) - 1\right)^{2}}}.$$

The multiplicative reduced first and second (a, b)-KA indices of a graph G are defined as

$$RKA_{a,b}^{1}II(G) = \prod_{uv \in E(G)} \left[\left(d_{G}(u) - 1 \right)^{a} + \left(d_{G}(v) - 1 \right)^{a} \right]^{b},$$

$$RKA_{a,b}^{2}II(G) = \prod_{uv \in E(G)} \left[\left(d_{G}(u) - 1 \right)^{a} \left(d_{G}(v) - 1 \right)^{a} \right]^{b}.$$

Recently some reduced indices were studied in [14, 15, 16] and also some multiplicative indices were studied in [17, 18, 19, 20, 21, 22].

In this paper, we compute the multiplicative Sombor index, multiplicative modified Sombor index, multiplicative reduced Sombor index, multiplicative reduced modified Sombor index, multiplicative first (a, b)-KA index, multiplicative reduced first (a, b)-KA index of $HC_5C_7[p, q]$ and $SC_5C_7[p, q]$ nanotubes. For nanotubes, see [23].

2. Results For $HC_5C_7[p, q]$ NANOTUBES

In this section, we focus on $HC_5C_7[p, q]$ nanotubes in which p is the number of heptagons in the first row and q rows of pentagons repeated alternately. The 2-dimensional lattice of nanotube $HC_5C_7[8, 4]$ is shown in Figure 1.

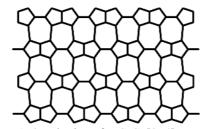


Figure-1: 2-*D* lattice of HC_5C_7 [8, 4] nanotube.

Let G be the graph of a nanotube $HC_5C_7[p, q]$. By calculation, G has 4pq vertices and 6pq - p edges. Also by calculation, there are two types of edges based on the degree of the vertices of each edge as given in Table 1.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 3)	(3, 3)
Number of edges	4 <i>p</i>	6pq – 5p

Table-1: Edge partition of *G*

In the following Theorem, we compute the general multiplicative first (a, b)-KA index of a nanotue $HC_5C_7[p, q]$.

Theorem 1: The general first (a, b)-KA index of $HC_5C_7[p, q]$ nanotubes is given by

$$KA_{ab}^{1}II(HC_{5}C_{7}[p,q]) = (2^{a} + 3^{a})^{4bp} \times (2 \times 3^{a})^{b(6pq-5p)}$$
.

Proof: Let $G = HC_5C_7[p, q]$. By definition and by using Table 1, we deduce

$$KA_{a,b}^{1}II\left(HC_{5}C_{7}\left[p,q\right]\right) = \prod_{uv \in E(G)} \left[d_{G}\left(u\right)^{a} + d_{G}\left(v\right)^{a}\right]^{b}$$
$$= \left(2^{a} + 3^{a}\right)^{b4p} \times \left(3^{a} + 3^{a}\right)^{b(6pq - 5p)}$$
$$= \left(2^{a} + 3^{a}\right)^{4bp} \times \left(2 \times 3^{a}\right)^{b(6pq - 5p)}.$$

Using Theorem 2, we establish the following results.

Corollary 1.1: The multiplicative Sombor index of $HC_5C_7[p, q]$ is

$$SOII(HC_5C_7[p,q]) = 13^{2p} \times (\sqrt{18})^{(6pq-5p)}$$

Corollary 1.2: The modified Sombor index of $HC_5C_7[p, q]$ is

^m SOII
$$\left(HC_5C_7\left[p,q\right]\right) = \left(\frac{1}{13}\right)^{2p} \times \left(\frac{1}{\sqrt{18}}\right)^{6pq-5p}$$
.

In the following Theorem, we determine the general multiplicative reduced first (a, b)-KA index of $HC_5C_7[p, q]$.

Theorem 2: The general reduced first (a, b)-KA index of $HC_5C_7[p, q]$ is given by

$$RKA_{ab}^{1}II(HC_{5}C_{7}[p,q]) = (1+2^{a})^{4pb} \times (2\times 2^{a})^{b(6pq-5p)}$$

Proof: Let $G = HC_5C_7[p, q]$. By definition and by using Table 1, we deduce

$$RKA_{a,b}^{1} II \left(HC_{5}C_{7}[p,q]\right) = \prod_{uv \in E(G)} \left[\left(d_{G}(u) - 1\right)^{a} + \left(d_{G}(v) - 1\right)^{a} \right]^{b}$$

$$= \left((2-1)^{a} + (3-1)^{a} \right)^{b \times 4p} \times \left((3-1)^{a} + (3-1)^{a} \right)^{b(6pq-5p)}$$

$$= \left(1 + 2^{a} \right)^{4pb} \times \left(2 \times 2^{a} \right)^{b(6pq-5p)}.$$

The following results are obtained from Theorem 2.

Corollary 2.1: The multiplicative reduced Sombor index of $HC_5C_7[p, q]$ is

$$RSOII(HC_5C_7[p,q]) = 5^{2p} \times (\sqrt{8})^{(6pq-5p)}$$
.

Corollary 2.2: The multiplicative reduced modified Sombor index of $HC_5C_7[p, q]$ is

^m SOII
$$\left(HC_5C_7[p,q]\right) = \left(\frac{1}{5}\right)^{2p} \times \left(\frac{1}{\sqrt{8}}\right)^{6pq-5p}$$
.

2. RESULTS FOR $SC_5C_7[p,q]$ NANOTUBES

In this section, we focus on $SC_5C_7[p, q]$ nanotubes, in which p is the number of heptagons in the first row and q rows of vertices and edges are repeated alternately. The 2-dimensional lattice of nanotube $SC_5C_7[8,4]$ is shown in Figure 2.

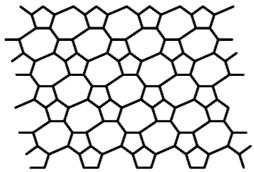


Figure-2: 2-*D* lattice of nanotube $SC_5C_7[8,4]$

Let G be the graph of $SC_5C_7[p, q]$. By calculation, we obtain that G has 4pq vertices and 6pq - p edges. Also by calculation, there are three types of edges based on the degree of end vertices of each edge as given in Table 2.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)
Number of edges	q	6q	6pq - p - 7q

Table-2: Edge partition of *G*

In the following theorem, we compute the general multiplicative first (a,b)-KA index of $SC_5C_7[p,q]$.

Theorem 3: The general multiplicative first (a, b)-KA index of $SC_5C_7[p, q]$ nanotubes is given by

$$KA_{ab}^{1}II(SC_{5}C_{7}[p,q]) = (2\times2^{a})^{bq} \times (2^{a}+3^{a})^{6bq} \times (2\times3^{a})^{b(6pq-p-7q)}$$

Proof: Let $G = SC_5C_7[p, q]$. By definition and Table 2, we deduce

$$KA_{a,b}^{1}II\left(SC_{5}C_{7}\left[p,q\right]\right) = \prod_{uv \in E(G)} \left[d_{G}\left(u\right)^{a} + d_{G}\left(v\right)^{a}\right]^{b}.$$

$$= \left(2^{a} + 2^{a}\right)^{bq} \times \left(2^{a} + 3^{a}\right)^{b6q} \times \left(3^{a} + 3^{a}\right)^{b(6pq - p - 7q)}$$

$$= \left(2 \times 2^{a}\right)^{bq} \times \left(2^{a} + 3^{a}\right)^{6bq} \times \left(2 \times 3^{a}\right)^{b(6pq - p - 7q)}.$$

From Theorem 3, the following results are established.

Corollary 3.1: The multiplicative Sombor index of $SC_5C_7[p, q]$ is

$$SOH(SC_5C_7[p,q]) = (\sqrt{8})^q \times (\sqrt{13})^{6q} \times (\sqrt{18})^{6pq-p-7q}$$
.

Corollary 3.2: The multiplicative modified Sombor index of $SC_5C_7[p, q]$ is

$$^{m}SOII(SC_{5}C_{7}[p,q]) = \left(\frac{1}{\sqrt{8}}\right)^{q} \times \left(\frac{1}{\sqrt{13}}\right)^{6q} \times \left(\frac{1}{\sqrt{18}}\right)^{6pq-p-7q}.$$

In the following theorem, we determine the general multiplicative reduced first (a, b)-KA index of $SC_3C_7[p, q]$.

Theorem 4: The general multiplicative reduced first (a, b)-KA index of $SC_5C_7[p, q]$ is given by

$$RKA_{a,b}^{1}II\left(SC_{5}C_{7}\left[p,q\right]\right)=2^{bq}\times\left(1+2^{a}\right)^{b6q}\times\left(2\times2^{a}\right)^{b(6pq-p-7q)}.$$

Proof: Let $G = SC_5C_7[p, q]$. By definition and using Table 2, we obtain

$$\begin{split} RKA_{a,b}^{1} II\left(SC_{5}C_{7}\left[p,q\right]\right) &= \prod_{uv \in E(G)} \left[\left(d_{G}\left(u\right)-1\right)^{a} + \left(d_{G}\left(v\right)-1\right)^{a}\right]^{b}. \\ &= \left[\left(2-1\right)^{a} + \left(2-1\right)^{a}\right]^{bq} \times \left[\left(2-1\right)^{a} + \left(3-1\right)^{a}\right]^{b6q} \times \left[\left(3-1\right)^{a} + \left(3-1\right)^{a}\right]^{b(6pq-p-7q)}. \\ &= 2^{bq} \times \left(1+2^{a}\right)^{b6q} \times \left(2\times 2^{a}\right)^{b(6pq-p-7q)}. \end{split}$$

From Theorem 4, we establish the following results.

Corollary 4.1: The multiplicative reduced Sombor index of $SC_5C_7[p, q]$ is

$$RSOII(SC_5C_7[p,q]) = (\sqrt{2})^q \times (5)^{3q} \times (\sqrt{8})^{6pq-p-7q}$$
.

Corollary 4.2: The multiplicative reduced modified Sombor index of $SC_5C_7[p, q]$ is

^m RSOII
$$\left(SC_5C_7[p,q]\right) = \left(\frac{1}{\sqrt{2}}\right)^q \times \left(\frac{1}{5}\right)^{3q} \times \left(\frac{1}{\sqrt{8}}\right)^{6pq-p-7q}$$
.

4. CONCLUSION

In this study, we have introduced the multiplicative Sombor index, multiplicative modified Sombor index, multiplicative reduced Sombor index, multiplicative reduced modified Sombor index, multiplicative first (a, b)-KA index, multiplicative reduced first (a, b)-KA index of a molecular graph. Also these multiplicative indices for HC_5C_7 [p, q] and $SC_5C_7[p, q]$ nanotubes are computed.

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