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δ-Sombor Index and its Exponential for Certain Nanotubes

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Abstract: Gutman considered a class of novel topological invariants of which the Sombor index was introduced. In this study, we introduce the δ-Sombor index, δ-Sombor exponential of a molecular graph. Furthermore we compute the δ-Sombor index and its corresponding exponential for certain nanotubes.

Keywords: Sombor index, δ-Sombor index, δ-Sombor exponential, nanotube.

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C09

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 branch of Mathematical Chemistry, which has an important affect 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. Let $\delta(G)$ denote the minimum degree among the vertices of G. We refer [3] for undefined notations and terminologies.

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

$$ASO(G)=\sqrt{\left(d_G(u)-\frac{2m}{n}\right)^2+\left(d_G(v)-\frac{2m}{n}\right)^2}$$

where $|V(G)| = n$ and $|E(G)| = m$.

Motivated by the definition of average Sombor index and its applications, we now put forward the δ-Sombor index of a molecular graph G and defined as

$$\delta S(G)=\sum_{uv\in E(G)}\sqrt{\left(d_G(u)-\delta(G)+1\right)^2+\left(d_G(v)-\delta(G)+1\right)^2}.$$

Let $\delta_u = d_G(u)-\delta(G)+1.$ Then we write

$$\delta S(G)=\sum_{uv\in E(G)}\sqrt{\delta_u^2+\delta_v^2}.$$

Considering the δ-Sombor index, we define the δ-Sombor exponential of a graph G as

$$\delta S(G,x)=\sum_{uv\in E(G)}x^{\sqrt{\delta_u^2+\delta_v^2}}.$$

In Chemical Graph Theory, some Sombor indices were introduced and studied in [5, 6, 7, 8]. Recently, some new topological indices and their polynomials were studied in [9, 10, 11]. In this paper, we obtain some results on the δ-Sombor index and its corresponding exponential for some nanotubes.

2. Results for $HC_5C_7[p, q]$ Nanotubes

In this section, we focus on the family of nanotubes, denoted by $HC_5C_7[p,q]$, in which p is the number of heptagons in the first row and q rows of pentagons repeated alternately. Let G be the graph of a nanotube $HC_5C_7[p,q]$.

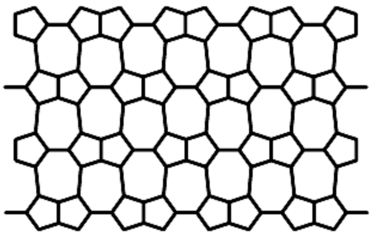

Figure 1: 2-*D* lattice of nanotube HC_5C_7 [8, 4]

The 2-D lattice of nanotube $HC_5C_7[p, q]$ is shown in Figure 1.. By calculation, we obtain that G has $4pq$ vertices and $6pq - p$ edges. The graph G has two types of edges based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_1| = 4p$.
$E_2 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_2| = 6pq - 5p$.

Clearly $\delta(G)=2$. Therefore $\delta_u = d_G(u) - \delta(G) + 1 = d_G(u) - 1$. Thus there are two types of δ-edges as given in Table 1.

δ_u , δ_v \ $uv \in E(G)$	(1, 2)	(2, 2)
Number of edges	$4p$	$6pq - 5p$

Table 1: δ-edge partition of $HC_5C_7[p, q]$

Theorem 1. Let G be the graph of a nanotube $HC_5C_7[p, q]$. Then

(i) $\delta S\left(HC_5C_7[p,q]\right)=12\sqrt{2}pq+\left(4\sqrt{5}-10\sqrt{2}\right)p.$

(ii) $\delta S\left(HC_5C_7[p,q],x\right)=4px^{\sqrt{5}}+\left(6pq-5p\right)x^{2\sqrt{2}}.$

Proof: From definitions and by using Table 1, we deduce

(i) $$\delta S\left(HC_5C_7[p,q]\right)=\sum_{uv\in E(G)}\sqrt{\delta_u^2+\delta_v^2}=\left(1^2+2^2\right)^{\frac{1}{2}}4p+\left(2^2+2^2\right)^{\frac{1}{2}}(6pq-5p)$$
$$=12\sqrt{2}pq+\left(4\sqrt{5}-10\sqrt{2}\right)p.$$

(ii) $$\delta S\left(HC_5C_7[p,q],x\right)=\sum_{uv\in E(G)}x^{\sqrt{\delta_u^2+\delta_v^2}}=4px^{\left(1^2+2^2\right)^{\frac{1}{2}}}+(6pq-5p)x^{\left(2^2+2^2\right)^{\frac{1}{2}}}$$
$$=4px^{\sqrt{5}}+(6pq-5p)x^{2\sqrt{2}}.$$

3. Results for $SC_5C_7[p,q]$ nanotubes

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

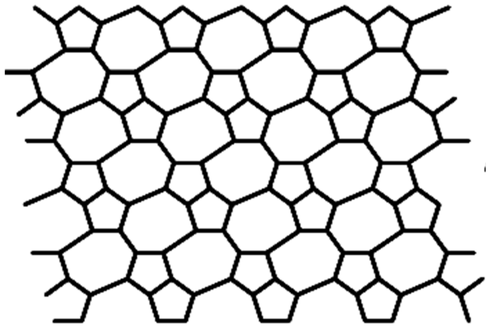

Figure 2: 2-*D* lattice of nanotube $SC_5C_7[p,q]$

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, we get that G has three types of edges based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_1| = q$.
$E_2 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_2| = 6q$.
$E_2 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_3| = 6pq - p–7q$.

Clearly $\delta(G)$=2. Thus $\delta_u = d_G(u) - \delta(G) + 1 = d_G(u) - 1$. There are three types of δ-edges as given in Table 2.

δ_u , $\delta_v \setminus uv \in E(G)$	(1, 1)	(1, 2)	(2, 2)
Number of edges	q	$6q$	$6pq - p - 7q$

Table 2: δ-edge partition of $SC_5C_7[p, q]$

Theorem 2. Let G be the graph of a nanotube $SC_5C_7[p, q]$. Then

(i) $\delta S\left(SC_5C_7[p,q]\right)=12\sqrt{2}pq-2\sqrt{2}p+\left(6\sqrt{5}-13\sqrt{2}\right)q.$

(ii) $\delta S\left(SC_5C_7[p,q],x\right)=qx^{\sqrt{2}}+6qx^{\sqrt{5}}+(6pq-p-7q)x^{2\sqrt{2}}.$

Proof: From definitions and by using Table 2, we derive

(i) $\delta S\left(SC_5C_7\left[p,q\right]\right)=\sum_{uv\in E(G)}\sqrt{\delta_u^2+\delta_v^2}$

$=\left(1^2+1^2\right)^{\frac{1}{2}}q+\left(1^2+2^2\right)^{\frac{1}{2}}6q+\left(2^2+2^2\right)^{\frac{1}{2}}\left(6pq-p-7q\right).$

$=12\sqrt{2}pq-2\sqrt{2}p+\left(6\sqrt{5}-13\sqrt{2}\right)q.$

(ii) $\delta S\left(SC_5C_7\left[p,q\right],x\right)=\sum_{uv\in E(G)}x^{\sqrt{\delta_u^2+\delta_v^2}}$

$=qx^{\left(1^2+1^2\right)^{\frac{1}{2}}}+6qx^{\left(1^2+2^2\right)^{\frac{1}{2}}}+\left(6pq-p-7p\right)x^{\left(2^2+2^2\right)^{\frac{1}{2}}}$

$=qx^{\sqrt{2}}+6qx^{\sqrt{5}}+\left(6pq-p-7q\right)x^{2\sqrt{2}}.$

4. Results for $KTUC_4C_8(S)$ nanotubes

In this section, we focus on the graph structure of a family of $TUC_4C_8(S)$ nanotubes. The 2-*D* lattice of $TUC_4C_8(S)$ is denoted by $KTUC_4C_8[p,q]$, where p is the number of columns and q is the number of rows. The graph of $KTUC_4C_8[p,q]$ is shown in Figure 3.

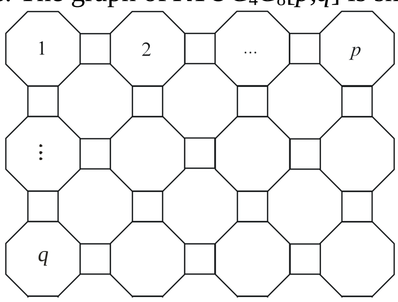

Figure 3: The graph of $KTUC_4C_8[p,q]$ nanotube

Let G be the graph of a nanotube $KTUC_4C_8[p,q]$. By calculation, we obtain that G has $12pq - 2p - 2q$ edges. The graph G has three types of edges based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_1| = 2p + 2q + 4$.

$E_2 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_2| = 4p + 4q - 8$.

$E_3 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_3| = 12pq - 8p - 8q + 4$.

Clearly $\delta(G)=2$. Thus $\delta_u = d_G(u) - \delta(G) + 1 = d_G(u) - 1$. Therefore there are three types of δ-edges as given in Table 3.

$\delta_u, \delta_v \backslash uv \in E(G)$	(1, 1)	(1, 2)	(2, 2)
Number of edges	$2p+2q+4$	$4p+4q-8$	$12pq - 8p - 8q+4$

Table 3: δ-edge partition of $KTUC_4C_8[p, q]$

Theorem 3. Let G be the graph of a nanotube $KTUC_4C_8[p,q]$. Then

(i) $\delta S\left(KTUC_4C_8\left[p,q\right]\right)=24\sqrt{2}pq+\left(4\sqrt{5}-14\sqrt{2}\right)q+12\sqrt{2}-8\sqrt{5}.$

(ii) $\delta S\left(\mathrm{G},x\right)=\left(2p+2q+4\right)x^{\sqrt{2}}+\left(4p+4q-8\right)x^{\sqrt{5}}+\left(12pq-8p-8q+4\right)x^{2\sqrt{2}}.$

Proof: From definitions and by using Table 3, we obtain

(i) $\delta S\left(KTUC_4C_8\left[p,q\right]\right)=\sum_{uv\in E(G)}\sqrt{\delta_u^2+\delta_v^2}$

$=\left(1^2+1^2\right)^{\frac{1}{2}}\left(2p+2q+4\right)+\left(1^2+2^2\right)^{\frac{1}{2}}\left(4p+4q-8\right)+\left(2^2+2^2\right)^{\frac{1}{2}}\left(12pq-8p-8q-4\right).$

$=24\sqrt{2}pq+\left(4\sqrt{5}-14\sqrt{2}\right)p+\left(4\sqrt{5}-14\sqrt{2}\right)q+12\sqrt{2}-8\sqrt{5}.$

(ii) $\delta S\left(KTUC_5C_7\left[p,q\right],x\right)=\sum_{uv\in E(G)}x^{\sqrt{\delta_u^2+\delta_v^2}}$

$=\left(2p+2q+4\right)x^{\left(1^2+1^2\right)^{\frac{1}{2}}}+\left(4p+4q-8\right)x^{\left(1^2+2^2\right)^{\frac{1}{2}}}+\left(12pq-8p-8q+4\right)x^{\left(2^2+2^2\right)^{\frac{1}{2}}}.$

$=\left(2p+2q+4\right)x^{\sqrt{2}}+\left(4p+4q-8\right)x^{\sqrt{5}}+\left(12pq-8p-8q+4\right)x^{2\sqrt{2}}.$

5. Results for *GTUC₄C₈(S)* nanotubes

In this section, we focus on the graph structure of family of $TUC_4C_8(S)$ nanotubes. The 2-dimensional lattice of $TUC_4C_8(S)$ is denoted by $G=GTUC_4C_8[p,q]$ where p is the number of columns and q is the number of rows. The graph of $GTUC_4C_8[p,q]$ is depicted in Figure 4.

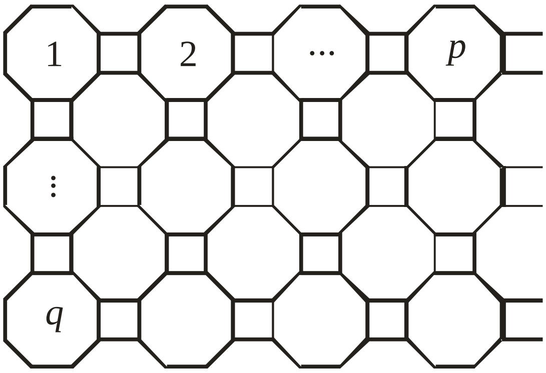

Figure 4: The graph of $GTUC_4C_8[p, q]$ nanotube

Let G be the molecular graph of $GTUC_4C_8[p,q]$ nanotube. By calculation, we obtain that G has $12pq - 2p$ edges. Also by calculation, we obtain that G has three types of edges based on the degree of end vertices of each edge as follows:

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

$E_2 = \{uv \in E(G) \mid d_G(u) =2, d_G(v) = 3\}$, $|E_2| = 4p$.

$E_3 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_3| = 12pq - 8p$.

Clearly we have $\delta(G)=2$. Hence $\delta_u = d_G(u) - \delta(G)+1= d_G(u) -1$. Thus there are three types of δ-edges as given in Table 4.

$\delta_u, \delta_v \backslash uv \in E(G)$	(1, 1)	(1, 2)	(2, 2)
Number of edges	$2p$	$4p$	$12pq - 8p$

Table 4: δ-edge partition of G

Theorem 4. Let G be the graph of $GTUC_4C_8[p,q]$. Then

(i) $\delta S\left(GTUC_4C_8\left[p,q\right]\right)=24\sqrt{2}pq+\left(4\sqrt{5}-14\sqrt{2}\right)p.$

(ii) $\delta S\left(GTUC_4C_8[p,q],x\right)=2px^{\sqrt{2}}+4px^{\sqrt{5}}+(12pq-8p)x^{2\sqrt{2}}$.

Proof: From definitions and by using Table 4, we have

(i) $\delta S\left(GTUC_4C_8[p,q]\right)=\sum_{uv\in E(G)}\sqrt{\delta_u^2+\delta_v^2}$

$=(1^2+1^2)^{\frac{1}{2}}2p+(1^2+2^2)^{\frac{1}{2}}4p+(2^2+2^2)^{\frac{1}{2}}(12pq-8p)=24\sqrt{2}pq+\left(4\sqrt{5}-14\sqrt{2}\right)p.$

(ii) $\delta S\left(GTUC_5C_7[p,q],x\right)=\sum_{uv\in E(G)}x^{\sqrt{\delta_u^2+\delta_v^2}}$

$=2px^{(1^2+1^2)^{\frac{1}{2}}}+4px^{(1^2+2^2)^{\frac{1}{2}}}+(12pq-8p)x^{(2^2+2^2)^{\frac{1}{2}}}=2px^{\sqrt{2}}+4px^{\sqrt{5}}+(12pq-8p)x^{2\sqrt{2}}.$

6. Some remarks

Clearly if $\delta(G)$=1, then $\delta S(G)$ is the Sombor index $SO(G)$. If $\delta(G)$=2, then $\delta S(G)$ is the reduced Sombor index $RSO(G)$.

7. Conclusion

In this study, we have introduced the δ-Sombor index and δ-Sombor exponential of a molecular graph. Furthermore we have computed the δ-Sombor index and its exponential for four families of nanotubes.

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