SOMBOR INDEX OF LINE AND TOTAL GRAPHS AND PERICONDENSED BENZENOID HYDROCARBONS

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ABSTRACT

Gutman proposed a new alternative interpretation of vertex-degree-based topological index, called Sombor index. It is defined via the term $\sqrt{\text{deg}(u)^2 + \text{deg}(v)^2}$. In this paper, we determine the explicit expressions of Sombor index for line and total graphs and several pericondensed benzenoid hydrocarbons.

Keywords: Sombor Index, Chemical Indicator, Pericondensed Benzenoid, Hydrocarbons

1. INTRODUCTION

In the mathematical and chemical literature, several dozens of vertex-degree-based graph invariants have been introduced and extensively studied in Pal et al. (2019), Todeschini and Consonni (2009). For a graph $G$, let $e(G)$, $\sigma(G)$ and $\Delta(G)$ and $\text{deg}_G(u)$ denote the size, the minimum degree and the maximum degree and
the degree of the vertex \( u \), respectively. The line graph \( L(G) \) is the graph whose vertex set is the edges of \( G \), two vertices \( a \) and \( b \) of \( L(G) \) being adjacent if and only if corresponding edges in \( G \) are adjacent. The total graph \( T(G) \) of a graph is the graph whose vertex set is with two vertices of being adjacent if and only if the corresponding elements of are either adjacent or incident.

Recently, Gutman (2021) introduced a new index defined as

\[
SO = SO(G) = \sum_{uv \in E(G)} \sqrt{deg_G(u)^2 + deg_G(v)^2}
\]

called Sombor index.

The distance Gutman (2021) between the d-point \((x, y)\) and the origin of the coordinate system is the degree-radius (or d-radius) of the edge \( e_v \), denoted by \( r(x, y) \). Based on elementary geometry (Using Euclidean metrics), we have

\[
r(x, y) = \sqrt{x^2 + y^2}
\]

In Gutman (2021), Gutman presented a novel approach to the vertex-degree-based topological indices of (molecular) graphs. The upper and lower bounds of Sombor index for general trees and graphs are given, and some basic properties of the Sombor index are established. Cruza et al. (2021) characterized the graphs extremal with respect to the Sombor index over the following sets: (connected) chemical graphs, chemical trees, and hexagonal systems. Das and Gutman Das and Gutman (2022) presented bounds on SO index of trees in terms of order, independence number, and number of pendent vertices, and characterize the extremal cases. The mathematical relations between the Sombor index and some other well-known degree-based descriptors was investigated in Wang et al. (2022).

In 2015, Su and Xu (2015) studied the general sum-connectivity index and co-index of line graph of subdivision graphs. In 2021, Demirci et al. (2021) obtained the explicit expressions for the Omega index of line and total graphs. In Section 2, the Sombor index of \( L(G) \) and \( T(G) \) are determined, respectively.

Klavˇzar et al. (1997) determined the explicit expressions of Wiener index for several pericondensed benzenoid hydrocarbons. We also determine the explicit expressions of Sombor index for several pericondensed benzenoid hydrocarbons in Section 3.

2. RESULTS FOR LINE AND TOTAL GRAPHS

From the definitions, the following observation is immediate.

**Observation 1.** Let \( G \) be a graph, \( v, u_1, u_2 \in V(G) \), and \( u_1v, u_2v \in E(G) \). Then

\[
d_{L(G)}(u_1v) = d_G(v) + d_G(u_1) - 2 \quad \text{and} \quad d_{L(G)}(u_2v) = d_G(v) + d_G(u_2) - 2.
\]

**Theorem 2.1.** Let \( G \) be a connected graph of order \( n \), with maximum degree \( \Delta \) and minimum degree \( \delta \) \((\delta \geq 2)\). Then
\[ \sqrt{2n\delta(\delta - 1)^2} \leq SO(L(G)) \leq \sqrt{2n\Delta(\Delta - 1)^2}, \]

with equality if and only if \( G \) is a regular graph.

Proof. From the definition of Sombor index, we have

\[
SO(L(G)) = \sum_{(u,v) \in E} \sqrt{d^2_L(u,v) + d^2_L(u_2,v)} \\
= \sum_{u \in V(G), d(v) \geq 2 \forall u_1, u_2 \in N(v), u_1 \neq u_2} \sum \sqrt{(d(v) + d(u_1) - 2)^2 + (d(v) + d(u_2) - 2)^2}.
\]

Since \( 2 \leq \delta \leq d(v), d(u_1), d(u_2) \leq \Delta \), it follows that

\[
\sqrt{(d(v) + d(u_1) - 2)^2 + (d(v) + d(u_2) - 2)^2} \leq \sqrt{2d^2(v) + 2(\Delta - 2)^2 + 4d(v)d(\Delta - 2)} \\
\leq \sqrt{2\Delta + 2(\Delta - 2)^2} \\
= 2\sqrt{2}(\Delta - 1),
\]

with equality if and only if \( d(v) = d(u_1) = d(u_2) = \Delta \).

For any vertex \( v \in V(G) \), let \( N_v \) denote the set of vertices associated with \( v \).

Since \( |N(v)| = d(v) \) and \( |\{(u_1, u_2) | u_1, u_2 \in N(v), u_1 \neq u_2\}| = \binom{d(v)}{2} = \frac{d(v)(d(v)-1)}{2} \), it follows that

\[
SO(G) \leq \frac{n\Delta(\Delta - 1)}{2} \times 2\sqrt{2}(\Delta - 1) = \sqrt{2n\Delta(\Delta - 1)^2}.
\]

Similarly, to Theorem 2.1, we can give a lower bound of \( L(G) \) without its proof.

**Observation 2.** Let \( G \) be a graph, \( u \in V(G) \), \( uv \in E(G) \). Then \( d_{T(G)}(v) = 2d_G(v) \) and \( d_{T(G)}(uv) = d_G(v) + d_G(u) \).

**Theorem 2.2.** Let \( G \) be a connected graph of order \( n \) with \( m \) edges such that its maximum and minimum degrees are \( \Delta \) and \( \delta \), respectively. Then

\[
\sqrt{2\delta(2m + n\delta + n\delta^2)} \leq SO(T(G)) \leq \sqrt{2\Delta(2m + n\Delta + n\Delta^2)},
\]

with equality if and only if \( G \) is a regular graph.

Proof. Let

\[
I_1 = \sum_{u \in V(G)} \sqrt{(2d(u))^2 + (2d(v))^2}, \\
I_2 = \sum_{v \in V(G), d(v) \geq 2 \forall u_1, u_2 \in N(v), u_1 \neq u_2} \sum \sqrt{(d(u_1) + d(v))^2 + (d(u_2) + d(v))^2}, \\
I_3 = \sum_{v \in V(G), u \in N(v)} \sum \sqrt{(2d(u))^2 + (d(v))^2}.
\]
From the definition of Sombor index, we have

\[ SO(T(G)) = I_1 + I_2 + I_3. \]

Since \( \delta \leq d(u), d(v) \leq \Delta \), it follows that

\[ 2 \sqrt{2} m \delta \leq I_1 \leq 2 \sqrt{2} m \Delta. \]

For any vertex \( v \in V(G) \), since \( |N(v)| = d(v) \) and

\[ |\{(u_1, u_2) | u_1, u_2 \in N(v), u_1 \neq u_2\}| = \left( \frac{d(v)}{2} \right) = \frac{d(v)(d(v)-1)}{2}, \]

it follows that

\[ \sqrt{2} n \delta^2 (\delta - 1) \leq I_2 \leq \sqrt{2} n \Delta^2 (\Delta - 1), \]
\[ 2 \sqrt{2} n \delta^2 \leq I_3 \leq \sqrt{2} n \Delta^2, \]

and hence

\[ \sqrt{2} \delta (2m + n\delta + n\delta^2) \leq SO(T(G)) \leq \sqrt{2} \Delta (2m + n\Delta + n\Delta^2), \]

with equality if and only if \( G \) is a regular graph.

3. RESULTS FOR PERICONDENSED BENZENOID HYDROCARBONS

In this section, we determine the explicit exact values for Sombor index of several pericondensed benzenoid hydrocarbons.

3.1. PARALLELOGRAM BENZENOID SYSTEM

For \( n \geq 1 \) and \( 1 \leq k \leq n \), let \( P(n, k) \) be the parallelogram benzenoid system. The definition of \( P(n, k) \) should be clear from the example \( P(7, 4) \) shown in Figure 1, Klavžar et al. (1997).

Figure 1

![Figure 1 Parallelogram Benzenoid System](image)
**Theorem 3.1.** Let $n, k$ be two integers with $n \geq 1$ and $1 \leq k \leq n$. Let $P(n, k)$ be the parallelogram benzenoid system. Then

$$SO(P(n, k)) = 6\sqrt{8} + (4n + 4k - 8)\sqrt{13} + (3nk - 2n - 2k + 1)\sqrt{18}.$$

Proof. For $P(n, k)$, we have $E = (2k + 2)(n + 1) - 2$. From the definition of Sombor index, we have

$$SO(P(n,k)) = \sum_{v_i, v_j \in E(P(n,k))} \sqrt{\deg_{P(n,k)}(v_i)^2 + \deg_{P(n,k)}(v_j)^2}$$

$$= 6r(2,2) + (4n + 4k - 8)r(2,3) + (3nk - 2n - 2k + 1)r(3,3)$$

$$= 6\sqrt{8} + (4n + 4k - 8)\sqrt{13} + (3nk - 2n - 2k + 1)\sqrt{18}.$$

**3.2. TRAPEZIUM BENZENOID SYSTEM**

For $n \geq 1$ and $1 \leq k \leq n$, let $T(n, k)$ be the trapezium benzenoid system. The definition of $T(n, k)$ should be clear from the example $T(9,5)$ shown in Figure 2, Klavzar (1997).

**Figure 2**

![Trapezium Benzenoid System $T(9,5)$](image)

**Theorem 3.2.** Let $n, k$ be two integers with $n \geq 1$ and $1 \leq k \leq n$. Let $T(n, k)$ be the trapezium benzenoid system. Then

$$SO(T(n,k)) = 6\sqrt{8} + (4n + 2k - 6)\sqrt{13} + \left(3nk - \frac{3}{2}k^2 + \frac{1}{2}k - 2n\right)\sqrt{18}.$$

Proof. For $T(n, k)$, we have $E = (k + 1)(2n + 1) - k(k - 1)$, and hence
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\begin{equation}
SO(T(n,k)) = \sum_{v_i \in E_T(n,k)} \sqrt{deg_{T(n,k)}(v_i)^2 + deg_{T(n,k)}(v_j)^2}
\end{equation}

\begin{align*}
&= 6r(2,2) + (4n + 2k - 6)r(2,3) + \left[\sum_{i=1}^{k} (n - m) + 2\sum_{h=1}^{k-1} (n - h)\right]r(3,3) \\
&= 6r(2,2) + (4n + 2k - 6)r(2,3) + \left[\frac{k(2n - k - 1)}{2} + (k - 1)(2n - k)\right]r(3,3) \\
&= 6r(2,2) + (4n + 2k - 6)r(2,3) + \left[3nk - \frac{3}{2}k^2 + \frac{1}{2}k - 2n\right]r(3,3) \\
&= 6\sqrt{8} + (4n + 2k - 6)\sqrt{13} + \left[3nk - \frac{3}{2}k^2 + \frac{1}{2}k - 2n\right]\sqrt{18}.
\end{align*}

3.3. PARALLELOGRAM-LIKE BENZENOID SYSTEMS

For \( n \geq 1 \) and \( 1 \leq k \leq n \), let \( P_1(n,k) \) be the parallelogram-like benzenoid system of type 1. The definition of \( P_1(n,k) \) should be clear from the example \( P_1(7,3) \) shown in Figure 3, Klav\'zar (1997).

**Theorem 3.3.** Let \( n, k \) be two integers with \( n \geq 1 \) and \( 1 \leq k \leq n \). Let \( P_1(n,k) \) be the parallelogram-like benzenoid system of type 1. Then

\begin{equation}
SO(P_1(n,k)) = (2k + 4)\sqrt{8} + (4n + 4k - 4)\sqrt{13} + (6nk - 2n - 2k - 1)\sqrt{18}.
\end{equation}

**Proof.** From the definition of Sombor index, we have

\begin{align*}
SO(P_1(n,k)) &= \sum_{v_i \in E_{P_1(n,k)}} \sqrt{deg_{P_1(n,k)}(v_i)^2 + deg_{P_1(n,k)}(v_j)^2} \\
&= (2k + 4)r(2,2) + (4n + 4k - 4)r(2,3) + (6nk - 2n - 2k - 1)r(3,3) \\
&= (2k + 4)\sqrt{8} + (4n + 4k - 4)\sqrt{13} + (6nk - 2n - 2k - 1)\sqrt{18}.
\end{align*}
For \( n \geq 1 \) and \( 1 \leq k \leq n \), let \( P_2(n, k) \) be the parallelogram-like benzenoid system of type 2. The definition of \( P_2(n, k) \) should be clear from the example \( P_2(7,4) \) shown in Figure 3, Klav’zar (1997).

**Theorem 3.4.** Let \( n, k \) be two integers with \( n \geq 1 \) and \( 1 \leq k \leq n \). Let \( P_2(n, k) \) be the parallelogram-like benzenoid system of type 2. Then

\[
SO(P_2(n,k)) = (2k + 4)\sqrt{8} + (4n + 4k - 8)\sqrt{13} + (6nk - 5n - 5k + 4)\sqrt{18}.
\]

**Figure 4**

\[\text{Figure 4 Parallelogram-Like Benzenoid System of } P_2(7, 4)\]

**Proof.** From the definition of Sombor index, we have

\[
SO(P_2(n,k)) = \sum_{v_j \in E(P_2(n,k))} \sqrt{\text{deg}_{P_2}(n,k)(v_j)^2 + \text{deg}_{P_2}(n,k)(v_j)^2}
\]

\[
= (2k + 4)r(2,2) + (4n + 4k - 8)r(2,3) + (6nk - 5n - 5k + 4)r(3,3)
\]

\[
= (2k + 4)\sqrt{8} + (4n + 4k - 8)\sqrt{13} + (6nk - 5n - 5k + 4)\sqrt{18}.
\]

For \( n \geq 1 \) and \( 1 \leq k \leq n + 1 \), let \( P_3(n, k) \) be the parallelogram-like benzenoid system of type 3. The definition of \( P_3(n, k) \) should be clear from the example \( P_3(4,3) \) shown in Figure 5, Klav’zar (1997).

**Theorem 3.5.** Let \( n, k \) be two integers with \( n \geq 1 \) and \( 1 \leq k \leq n \). Let \( P_3(n, k) \) be the parallelogram-like benzenoid system of type 3. Then

\[
SO(P_3(n,k)) = (2k + 2)\sqrt{8} + (4n + 4k - 4)\sqrt{13} + (6nk - 5n + k - 4)\sqrt{18}.
\]
Proof. From the definition of Sombor index, we have

\[ SO(P_3(n,k)) = \sum_{v_j \in E(P_3(n,k))} \sqrt{\deg_{P_3(n,k)}(v_j)^2 + \deg_{P_3(n,k)}(v_j)^2} \]

\[ = (2k + 2)r(2,2) + (4n + 4k - 4)r(2,3) + (6nk - 5n + k - 4)r(3,3) \]

\[ = (2k + 2)\sqrt{8} + (4n + 4k - 4)\sqrt{13} + (6nk - 5n + k - 4)\sqrt{18}. \]

### 3.4. BITRAPEZIUM BENZENOID SYSTEM

For \( n \geq 1 \), \( 1 \leq k_1 \leq n - 1 \), \( 1 \leq k_2 \leq n - 1 \), and \( k_1 + k_2 \leq n \), let \( BT(n, k_1, k_2) \) be the bitrapezium benzenoid system. The definition of \( BT(n, k_1, k_2) \) should be clear from the example \( BT(6,2,3) \) shown in Figure 6, Klavzar (1997).

**Theorem 3.6.** Let \( n, k_1, k_2 \) be three integers with \( n \geq 1 \) and \( 0 \leq k_1 \leq n - 1 \), \( 0 \leq k_2 \leq n - 1 \) and \( k_1 + k_2 \leq n \). Let \( BT(n, k_1, k_2) \) be a bitrapezium benzenoid system. Then

\[ SO(BT(n, k_1, k_2)) = 6\sqrt{8} + (4n + 2k_1 + 2k_2 - 4)\sqrt{13} \]

\[ + \left( 3n(k_1 + k_2) - \frac{3}{2}(k_1^2 + k_2^2) - \frac{5}{2}(k_1 + k_2) + n - 1 \right)\sqrt{18}. \]
Proof. From the definition of Sombor index, we have

\[
\text{SO}(\text{BT}(n, k_1, k_2)) = \sum_{v_i \in E(\text{BT}(n, k_1, k_2))} \sqrt{\text{deg}_{\text{BT}(n, k_1, k_2)}(v_i)^2 + \text{deg}_{\text{BT}(n, k_1, k_2)}(v_j)^2} \\
= 6r(2, 2) + 2(2n + k_1 + k_2 - 2)r(2, 3) + \left(\sum_{n=1}^{k_1+1} (n-m)\right) \\
+ \sum_{h=1}^{k_1} (n-h) + 2\sum_{i=1}^{k_1} (n-i) + 2\sum_{j=1}^{k_2} (n-j) - (n-1)r(3,3) \\
= 6r(2, 2) + 2(2n + k_1 + k_2 - 2)r(2, 3) + \left(\frac{(k_1+1)(2n-k_1-2)}{2}\right) \\
+ \frac{(k_2+1)(2n-k_2-2)}{2} + k_1(2n-k_1-1) + k_2(2n-k_2-1) - (n-1)r(3,3) \\
= 6\sqrt{8} + (4n + 2k_1 + 2k_2 - 4)\sqrt{13} \\
+ \left(3n(k_1 + k_2) - \frac{3}{2}(k_1^2 + k_2^2) - \frac{5}{2}(k_1 + k_2) + n-1\right)\sqrt{18}.
\]

3.5. GENERAL BENZENOID SYSTEM

For \( n \geq 1, 1 \leq k_1 \leq k_2 \leq n, 1 \leq k_3 \leq k_4 \leq n, \) and \( k_1 + k_2 = k_3 + k_4 \), let \( GB(n, k_1, k_2, k_3, k_4) \) be the bitrapezium benzenoid system. The definition of \( GB(n, k_1, k_2, k_3, k_4) \) should be clear from the example \( GB(7,3,4,5,2) \) shown in Figure 7, Klavžar (1997).
Theorem 3.7. Let \( n, k_1, k_2, k_3, k_4 \) be five integers with \( n \geq 1, 0 \leq k_1 \leq k_3 \leq n \), \( 0 \leq k_4 \leq k_2 \leq n \) and \( k_1 + k_2 = k_3 + k_4 \). Let \( GB(n, k_1, k_2, k_3, k_4) \) be a general benzenoid system. Then

\[
SO(GB(n, k_1, k_2, k_3, k_4)) = 6\sqrt{8} + (4n + 6k_1 + 4k_2 - 2k_4 - 2)\sqrt{13} + \left( (3k_1 + 3k_2 + 1)n + \frac{3}{2}k_1^2 - \frac{3}{2}k_4^2 + 3k_1k_2 - \frac{3}{2}k_1 - 2k_2 - \frac{1}{2}k_4 - 3 \right)\sqrt{18}.
\]

Proof. From the definition of Sombor index, we have

\[
SO(GB(n, k_1, k_2, k_3, k_4)) = \sum_{v, v' \in E(GB(n, k_1, k_2, k_3, k_4))} \sqrt{\text{deg}_{GB(n, k_1, k_2, k_3, k_4)}(v)^2 + \text{deg}_{GB(n, k_1, k_2, k_3, k_4)}(v')^2} \\
= 6r(2, 2) + (4n + 6k_1 + 4k_2 - 2k_4 - 2)r(2, 3) + \left( \sum_{m=1}^{k_1+1} (n + m) + \sum_{k=0}^{k_1-1} (n + k_1 - h) + 2 \sum_{i=0}^{k_2} (n + i) + 2 \sum_{j=0}^{k_2} (n + k_1 - j) \\
+ 3nk_2 - 3nk_4 + 3k_1k_2 - 3k_1k_4 + 2k_2 - 2k_4 \right)r(3, 3) \\
= 6r(2, 2) + (4n + 6k_1 + 4k_2 - 2k_4 - 2)r(2, 3) + \left( (3k_1 + 3k_2 + 1)n + \frac{3}{2}k_1^2 - \frac{3}{2}k_4^2 + 3k_1k_2 - \frac{3}{2}k_1 - 2k_2 - \frac{1}{2}k_4 - 3 \right)r(3, 3) \\
= 6\sqrt{8} + (4n + 6k_1 + 4k_2 - 2k_4 - 2)\sqrt{13} + \left( (3k_1 + 3k_2 + 1)n + \frac{3}{2}k_1^2 - \frac{3}{2}k_4^2 + 3k_1k_2 - \frac{3}{2}k_1 - 2k_2 - \frac{1}{2}k_4 - 3 \right)\sqrt{18}.
\]
3.6. L-POLYGONAL CHAIN $PC_n$

Let $P_{1,n}$, $P_{n}$ A polygonal chain of $n$ cycles (polygons) is obtained from a sequence of cycles, $O_1, O_2, \ldots, O_n$, by adding a bridge to each pair of consecutive cycles. If all such cycles are $l$-cycles, then this polygonal chain is called an $l$-polygonal chain of length $n$ and denoted by $PC_n$. The cycle $O_i$ will be called the $i$-th polygon of $PC_n$. Note that, there are many ways to add a bridge between two consecutive cycles. So $PC_n$ may not be unique when $n \geq 3$. But $PC_n$ is unique when $n = 1, 2$. The definition of $PC_n$ should be clear from the shown in Figure 8, Wei and Shiu (2019).

Figure 8

\[ \text{Figure 8 L-Polygonal Chain } PC_n \]

**Theorem 3.8.** Let $PC_n$ be an $l$-polygonal chain (of length $n$). Then

\[
SO(PC_n) = [4(l - 2) + k(2l - 8) + (n - k - 2)(2l - 3) + (3n - 3)]\sqrt{2} + [4 + 4k + 2(n - k - 2)\sqrt{13}].
\]

**Proof.** From the definition of Sombor index, we have

\[
SO(PC_n) = \sum_{v \in PC_n} \sqrt{\deg_{PC}(v)^2 + \deg_{PC}(v)^2} = 2(l - 2)\sqrt{2^2 + 2^2 + 4\sqrt{2^2 + 3^2} + k[\sqrt{(l - 4)^2 + 2^2 + 4\sqrt{2^2 + 3^2}]} + (n - k - 2)\sqrt{(l - 3)\sqrt{2^2 + 2^2 + 2\sqrt{2^2 + 3^2} + \sqrt{3^2 + 3^2} + (n - 1)\sqrt{3^2 + 3^2}}} + [4(l - 2) + k(2l - 8) + (n - k - 2)(2l - 3) + (3n - 3)]\sqrt{2} + [4 + 4k + 2(n - k - 2)\sqrt{13}].
\]

3.7. TITANIA NANOTUBES $T_1(m, n)$

Titania nanotubes are comprehensively studied in materials science. The $TiO_2$ sheets with a thickness of a few atomic layers were found to be remarkably stable. Let $T_1(m, n)$ be the $m$ rows and $n$ columns of the titanium nanotubes. The definition of $T_1(5,3)$ should be clear from the shown in Figure 9, Imran et al. (2021).

**Theorem 3.9.** Let $T_1(m, n)$ denote the graph of titanium nanotubes with $m$ rows and $n$ columns. Then
Proof. From the definition of Sombor index, we have

\[ SO(T_i(m,n)) = 5(4n - 1) + (13m - 10)\sqrt{2} + (24n - 6)\sqrt{5} + 2\sqrt{13} + (8mn - 2m - 4n + 1)\sqrt{29} + (12mn - 16n - 3m + 4)\sqrt{34}. \]

CONFLICT OF INTERESTS
None.

ACKNOWLEDGMENTS
None.

REFERENCES


