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Sombor Index and Elliptic Sombor Index of Benzenoid Systems

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Abstract

Let G be a graph with vertex set V and edge set E. A topological index has the form

$$TI = TI(G) = \sum_{uv \in E} f(d_G(u), d_G(v)),$$

where $f = f(x, y)$ is a pertinently chosen function which must be symmetric and real-valued for all x, y pertaining to vertex degrees of the graph G. Particularly interesting are the Sombor index and the elliptic Sombor index, defined by the functions $f(x, y) = \sqrt{x^2 + y^2}$ and $f(x, y) = (x + y)\sqrt{x^2 + y^2}$, respectively. Let $q = 2f(2, 3) - f(2, 2) - f(3, 3)$. In this paper, we characterize the extremal graphs that achieve the upper bounds of the topological index TI for benzenoid systems, where TI satisfies the conditions $0 < q < \frac{f(2,2)}{2}$ or $-\frac{f(2,2)}{4} < q < 0$, respectively. In addition, we provide a lower bound for the Sombor index on benzenoid systems.

1 Introduction

Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. As usual, we denote $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$. For each vertex $u \in V(G)$, we use $d_G(u)$ to denote the degree of u in G.

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A topological index has the form

$$TI = TI(G) = \sum_{uv \in E} f(d_G(u), d_G(v)), \tag{1}$$

where $f = f(x, y)$ is a pertinently chosen function which must be symmetric and real-valued for all x, y pertaining to vertex degrees of the graph G. Particularly interesting are the recently created elliptic Sombor index and Sombor index, which are defined by the functions $f(x, y) = (x + y)\sqrt{x^2 + y^2}$ and $f(x, y) = \sqrt{x^2 + y^2}$, respectively. For recent results on the Sombor index, we refer the reader to [3, 5, 8, 11, 16, 19]. Both topological indices were conceived based on geometric considerations and have demonstrated good predictive potential [6, 9, 18].

Benzenoid systems are finite, 2-connected plane graphs in which all interior regions are mutually congruent hexagons. They provide a natural graphical representation of benzenoid hydrocarbons, which are of great importance in chemistry. For notation and basic concepts on benzenoid systems, we refer the reader to [7].

Let $\mathcal{HS}_h$ be the set of benzenoid systems with $h \geq 2$ hexagons. For an edge of $H \in \mathcal{HS}_h$, connecting a vertex of degree i and a vertex of degree j, is called an (i, j)-edge. The number of such edges will be denoted by $m_{i,j}(H)$. An edge shared by two hexagons is called an *internal edge*, while an edge belonging to only one hexagon is called an *external edge*. We use $m_i(H)$ and $m_e(H)$ to denote the number of internal edges and external edges of H, respectively. The external edges form a cycle, which is referred to as the *perimeter* of the benzenoid system. The vertices of a benzenoid system lying on its perimeter are called *external vertices*, while the remaining vertices are referred to as *internal vertices*. We use $n_i(H)$ and $n_e(H)$ to denote the number of internal vertices and external vertices of H, respectively. Clearly, $m_e(H) = n_e(H)$.

In [10], Harary and Harborth proved that

$$0 \leq n_i(H) \leq 2h + 1 - \lceil \sqrt{12h - 3} \rceil. \tag{2}$$

The benzenoid system that attain the lower bound of (2) are called *cat-*

acondensed benzenoid system, a class that has been studied in [17]. The benzenoid system that attain the upper bound of (2) are called *anacondensed benzenoid system*. For results on anacondensed benzenoid system, we refer the reader to [4]. In particular, if $n_i > 0$, the benzenoid system is classified as *pericondensed*.

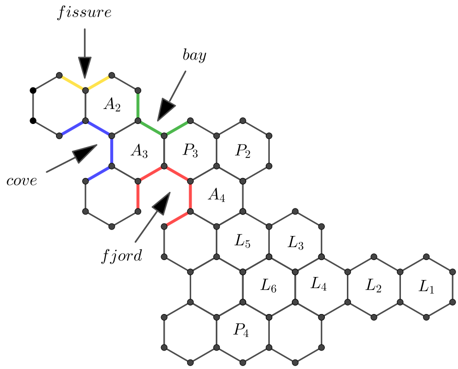


Fig. 1. The twelve possible types of hexagons in benzenoid system and some structural features on the perimeter.

The hexagons in a benzenoid system are classified as L_1, L_2, L_3, L_4, L_5, L_6, A_2, A_3, A_4, P_2, P_3 and P_4, depending on the number and position of the hexagons adjacent to it. Their definition is clear from Fig. 1, where an example is also provided.

Fig. 1 also illustrates the structural features on the perimeter of the benzenoid system: fissures, bays, coves, and fjords. The numbers of these features in H are denoted by $f(H)$, $B(H)$, $C(H)$, and $F(H)$, respectively. The number of inlets of H is

$$r(H) = f(H) + B(H) + C(H) + F(H).$$

In 2016, Cruz et al. [2] proved that $r(H) \geq \lceil \sqrt{3(h-1)} \rceil$ for each $H \in HS_h$. The *bay regions* of H, denoted by $b(H)$, and defined as

$$b(H) = B(H) + 2C(H) + 3F(H), \tag{3}$$

which counts the number of edges on the perimeter, connecting two vertices of degree 3. If $b(H) = 0$, then we say that H is a *convex benzenoid system*.

The results on the convex benzenoid system are referred to in [1].

In [17], Rada et al. presented lower and upper bounds for the Sombor index and the elliptic Sombor index of catacondensed benzenoid systems. In this paper, we focus on analyzing the Sombor index and the elliptic Sombor index for benzenoid systems, including both catacondensed and pericondensed structures. First, we characterize the extremal graphs that achieve the upper bounds of the topological index TI for benzenoid systems, where TI satisfies the condition $0 < q < \frac{f(2,2)}{2}$ or $-\frac{f(2,2)}{4} < q < 0$, respectively. This result contains the upper bound of the Sombor index identified by Cruz et al. [3]. In addition, Cruz et al. [3] also proposed the following problem:

Problem 1. *Among all hexagonal systems with h hexagons, which hexagonal systems have minimal value of SO?*

In the fourth section of this paper, we provide a lower bound for the Sombor index on benzenoid systems and analyze the benzenoid systems that attain the minimal value of the Sombor index.

2 Preliminary results

A hexagon of H, containing some external edge of H, is said to be on the boundary of H. In this section, we obtain two useful lemmas.

Lemma 1. *Let $H \in \mathcal{HS}_h$ and let h_0 be a hexagon on the boundary of H such that $H \setminus h_0$ is connected. If H' is the benzenoid system obtained from H by moving h_0 to an inlet of H such that $n_i(H') > n_i(H)$, then $r(H) - 4 \leq r(H') \leq r(H) + 2$.*

Proof. Since $H \setminus h_0$ is connected and h_0 is on the boundary of H, h_0 must be a hexagon of type L_1, L_3, L_5, P_2, or P_4. However, if h_0 is a hexagon of type L_5, then there does not exist an inlet r_0 in H such that, by moving h_0 to r_0, a new benzenoid system H' is obtained, satisfying $n_i(H') > n_i(H)$. Thus, we need to consider the cases when h_0 is a hexagon of type L_1, L_3, P_2, or P_4.

Case 1: h_0 is a hexagon of type L_1.

Obviously, moving h_0 to any inlet of H results in a benzenoid system H' such that $n_i(H') > n_i(H)$. We classify three types of hexagons in mode L_1 as L_1^0, L_1^{-1}, and L_1^{-2} (see Fig. 2), such that, when a hexagon of type L_1^0, L_1^{-1}, or L_1^{-2} is removed, the number of inlets remains unchanged, decreases by one, or decreases by two, respectively.

Fig. 2 also shows the three possible forms of each inlet in H: a_1, a_2, and a_3 for fissures; b_1, b_2, and b_3 for bays; and c_1, c_2, and c_3 for coves. These forms depend on whether the number of inlets increases by one, remains unchanged, or decreases by one when adding a hexagon to a fissure, bay, or cove, respectively. Specially, the three possible forms of fjords in H are f_1, f_2, and f_3, determined by whether the number of inlets remains unchanged, decreases by one, or decreases by two when adding a hexagon to a fjord, respectively. These notations will also be used in later proofs.

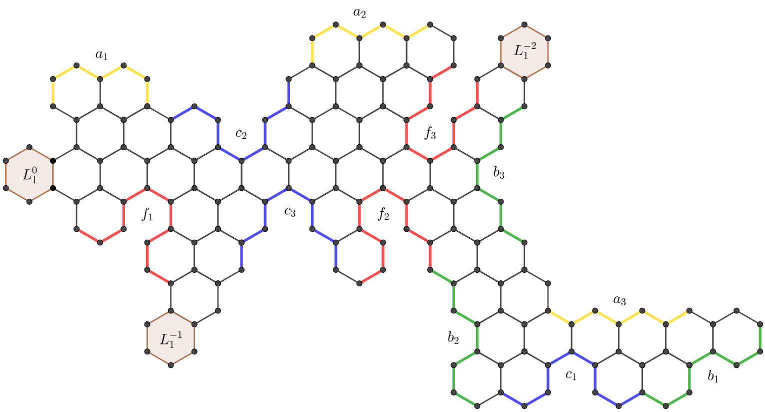


Fig. 2. The three types of hexagons in mode L_1, and the three possible forms of fissure, bay, cove and fjord on the perimeter of H.

Subcase 1.1: h_0 is the type of L_1^{-2}.

If H' is obtained from H by moving L_1^{-2} to a_1, b_1 or c_1, then $r(H') = r(H) - 1$. If H' is obtained from H by moving L_1^{-2} to a_2, b_2, c_2 or f_1, then $r(H') = r(H) - 2$. If H' is obtained from H by moving L_1^{-2} to a_3, b_3, c_3 or f_2, then $r(H') = r(H) - 3$. If H' is obtained from H by moving h_0 to f_3, then $r(H') = r(H) - 4$.

Subcase 1.2: h_0 is the type of L_1^{-1}.

If H' is obtained from H by moving L_1^{-1} to a_1, b_1 or c_1, then $r(H') = r(H)$. If H' is obtained from H by moving L_1^{-1} to a_2, b_2, c_2 or f_1, then $r(H') = r(H) - 1$. If H' is obtained from H by moving L_1^{-1} to a_3, b_3, c_3 or f_2, then $r(H') = r(H) - 2$. If H' is obtained from H by moving L_1^{-1} to f_3, then $r(H') = r(H) - 3$.

Subcase 1.3: h_0 is the type of L_1^0.

If H' is obtained from H by moving L_1^0 to a_1, b_1 or c_1, then $r(H') = r(H) + 1$. If H' is obtained from H by moving L_1^0 to a_2, b_2, c_2 or f_1, then $r(H') = r(H)$. If H' is obtained from H by moving L_1^0 to a_3, b_3, c_3 or f_2, then $r(H') = r(H) - 1$. If H' is obtained from H by moving L_1^0 to f_3, then $r(H') = r(H) - 2$.

Case 2: h_0 is a hexagon of type P_2.

Clearly, placing h_0 in a bay, cove or fjord of H will result in a benzenoid system H' with $n_i(H') > n_i(H)$. The hexagons in mode P_2 also have three types: P_2^{+1}, P_2^0, and P_2^{-1} (see Fig. 3). When a hexagon of type P_2^{+1}, P_2^0, or P_2^{-1} is removed, the number of inlets increases by one, remains unchanged, or decreases by one, respectively.

Subcase 2.1: h_0 is the type of P_2^{-1}.

If H' is obtained from H by moving P_2^{-1} to b_1 or c_1, then $r(H') = r(H)$. If H' is obtained from H by moving h_0 to b_2, c_2 or f_1, then $r(H') = r(H) - 1$. If H' is obtained from H by moving P_2^{-1} to b_3, c_3 or f_2, then $r(H') = r(H) - 2$. If H' is obtained from H by moving P_2^{-1} to f_3, then $r(H') = r(H) - 3$.

Subcase 2.2: h_0 is the type of P_2^0.

If H' is obtained from H by moving P_2^0 to b_1 or c_1, then $r(H') = r(H) + 1$. If H' is obtained from H by moving P_2^0 to b_2, c_2 or f_1, then $r(H') = r(H)$. If H' is obtained from H by moving P_2^0 to b_3, c_3 or f_2, then $r(H') = r(H) - 1$. If H' is obtained from H by moving P_2^0 to f_3, then $r(H') = r(H) - 2$.

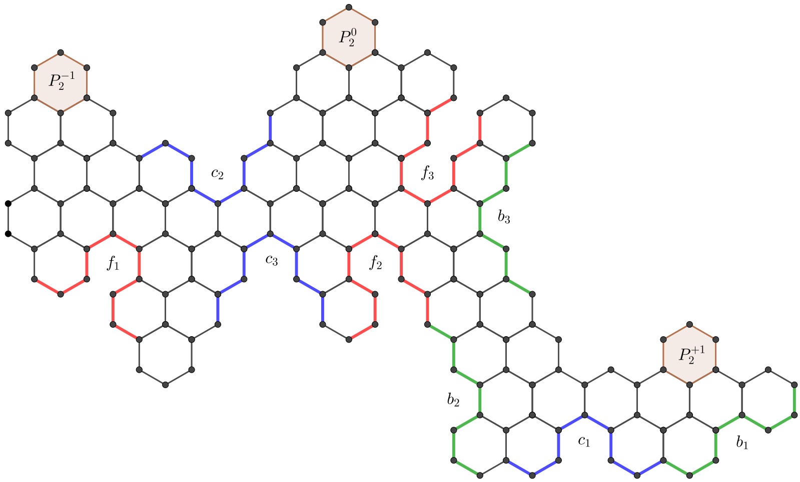


Fig. 3. The three types of hexagons in mode P_2, and the three possible forms of bay, cove and fjord on the perimeter of H.

Subcase 2.3: h_0 is the type of P_2^{+1}.

If H' is obtained from H by moving P_2^{+1} to b_1 or c_1, then $r(H') = r(H) + 2$. If H' is obtained from H by moving P_2^{+1} to b_2, c_2 or f_1, then $r(H') = r(H) + 1$. If H' is obtained from H by moving P_2^{+1} to b_3, c_3 or f_2, then $r(H') = r(H)$. If H' is obtained from H by moving P_2^{+1} to f_3, then $r(H') = r(H) - 1$.

Case 3: h_0 is a hexagon of type L_3.

Obviously, moving h_0 to a cove or fjord of H will result in a benzenoid system H' such that $n_i(H') > n_i(H)$. The three types of hexagons in mode L_3 are L_3^{+1}, L_3^0, and L_3^{-1} (see Fig. 4).

Subcase 3.1: h_0 is the type of L_3^{-1}.

If H' is obtained from H by moving L_3^{-1} to c_1, then $r(H') = r(H)$. If H' is obtained from H by moving L_3^{-1} to c_2 or f_1, then $r(H') = r(H) - 1$. If H' is obtained from H by moving L_3^{-1} to c_3 or f_2, then $r(H') = r(H) - 2$. If H' is obtained from H by moving L_3^{-1} to f_3, then $r(H') = r(H) - 3$.

Subcase 3.2: h_0 is the type of L_3^0.

If H' is obtained from H by moving L_3^0 to c_1, then $r(H') = r(H) + 1$. If H' is obtained from H by moving L_3^0 to c_2 or f_1, then $r(H') = r(H)$. If H' is obtained from H by moving L_3^0 to c_3 or f_2, then $r(H') = r(H) - 1$. If H' is obtained from H by moving L_3^0 to f_3, then $r(H') = r(H) - 2$.

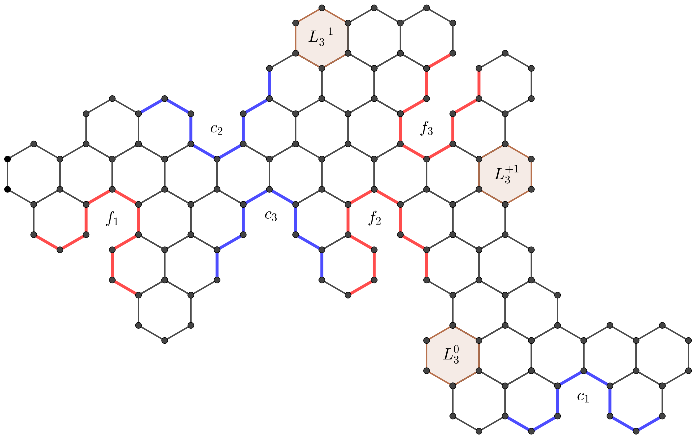


Fig. 4. The three types of hexagons in mode L_3, and the three possible forms of cove and fjord on the perimeter of H.

Subcase 3.3: h_0 is the type of L_3^{+1}.

If H' is obtained from H by moving L_3^{+1} to c_1, then $r(H') = r(H) + 2$. If H' is obtained from H by moving L_3^{+1} to c_2 or f_1, then $r(H') = r(H)+1$. If H' is obtained from H by moving L_3^{+1} to c_3 or f_2, then $r(H') = r(H)$. If H' is obtained from H by moving L_3^{+1} to f_3, then $r(H') = r(H) - 1$.

Case 4: h_0 is a hexagon of type P_4.

It is evident that placing P_4 into a fjord of H produces a benzenoid system H' with $n_i(H') > n_i(H)$. Fig. 5 shows the three possible forms P_4^{+1}, P_4^0, and P_4^{-1} of a hexagon of type P_4 in H, as well as the three distinct forms of fjord in H: f_1, f_2 and f_3.

Subcase 3.1: h_0 is the type of P_4^{-1}.

If H' is obtained from H by moving P_4^{-1} to f_1, then $r(H') = r(H) - 1$. If H' is obtained from H by moving P_4^{-1} to f_2, then $r(H') = r(H) - 2$. If H' is obtained from H by moving P_4^{-1} to f_3, then $r(H') = r(H) - 3$.

Subcase 3.2: h_0 is the type of P_4^0.

If H' is obtained from H by moving P_4^0 to f_1, then $r(H') = r(H)$. If H' is obtained from H by moving P_4^0 to f_2, then $r(H') = r(H) - 1$. If H' is obtained from H by moving P_4^0 to f_3, then $r(H') = r(H) - 2$.

Subcase 3.3: h_0 is the type of P_4^{+1}.

If H' is obtained from H by moving P_4^{+1} to f_1, then $r(H') = r(H) + 1$. If H' is obtained from H by moving P_4^{+1} to f_2, then $r(H') = r(H)$. If H' is obtained from H by moving P_4^{+1} to f_3, then $r(H') = r(H) - 1$.

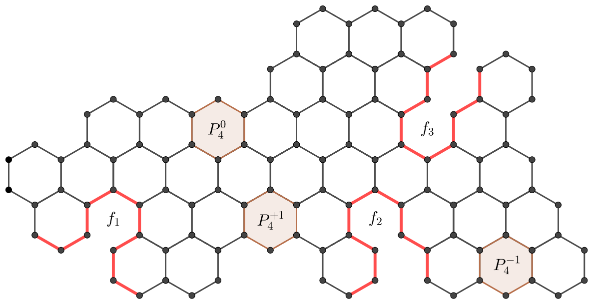


Fig. 5. The three types of hexagons in mode P_4, and the three possible forms of fjord on the perimeter of H.

■

It is well known that the number of $(2,2)$-edges in a benzenoid system is at least six. Similar to Lemma 1, we obtain the following lemma.

Lemma 2. *Let H be a pericondensed benzenoid system with h hexagons, and let h_0 be a hexagon on the boundary of H that contains internal vertices of H, such that $H \setminus h_0$ is connected. If H'' is the benzenoid system obtained from H by moving h_0 to a $(2,2)$-edge in H, then $r(H) - 2 \le r(H'') \le r(H) + 4$.*

Proof. Let h_0 be a hexagon on the boundary of H that contains internal vertices of H. Since $H \setminus h_0$ is connected, h_0 must be of type L_1, L_3, L_5, P_2 or P_4. From the proof of Lemma 1, it follows that the number of inlets in H decreases by at most 2 or increases by at most 2 after removing h_0. However, after attaching a hexagon to the $(2,2)$-edge of H, the inlets of

H may remain unchanged, increase by 1, or increase by 2. Let H'' be the benzenoid system obtained from H by moving h_0 to a $(2,2)$-edge in H. Then $r(H) - 2 \leq r(H'') \leq r(H) + 4$. ■

3 The upper bound of Sombor index and elliptic Sombor index of benzenoid systems

Let $H \in \mathcal{HS}_h$. The benzenoid system possess only vertices of degree 2 and 3. Consequently, all their edges are of type $(2,2)$, $(2,3)$ and $(3,3)$, and so for H,

$$TI(H) = f(2,2)m_{2,2} + f(2,3)m_{2,3} + f(3,3)m_{3,3}, \tag{4}$$

where TI is a topological index of the form (1). For convenience, let $\varphi_{2,2} = f(2,2)$, $\varphi_{2,3} = f(2,3)$ and $\varphi_{3,3} = f(3,3)$. We can obtain an expression for the topological index of H in terms $r(H)$ and $n_i(H)$ as shown below.

Theorem 2. *Let $H \in HS_h$. Then*

$$\begin{aligned} TI(H) &= (2\varphi_{2,2} + 3\varphi_{3,3})h + (2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3})r(H) - \varphi_{2,2}n_i(H) \\ &\quad +(4\varphi_{2,2} - 3\varphi_{3,3}). \end{aligned}$$

Proof. The result follows from (4) and the previously known relations given in [12]:

$$\begin{cases} m_{2,2}(H) = n(H) - 2h - r(H) + 2, \\ m_{2,3}(H) = 2r(H), \\ m_{3,3}(H) = 3h - r(H) - 3, \end{cases}$$

and [7]

$$n(H) = 4h + 2 - n_i(H). \tag{5}$$

■

Let $K = \frac{\varphi_{2,2}}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}$. The following theorem can be established.

Theorem 3. *Let H be a pericondensed benzenoid system with h hexagons, and let h_0 be a hexagon on the boundary of H that contains internal vertices of H, such that $H \backslash h_0$ is connected. If H'' is the benzenoid system obtained from H by moving h_0 to a $(2,2)$-edge in H, then*

$$TI(H'') > TI(H),$$

where TI is a topological index of the form (4) such that $K < -4$ or $K > 2$.

Proof. By Theorem 2, we have

$$\begin{aligned} TI(H'') - TI(H) &= (2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3})(r(H'') - r(H)) \\ &- \varphi_{2,2}(n_i(H'') - n_i(H)). \end{aligned}$$

To establish $TI(H'') > TI(H)$, it suffices to show that $TI(H'') - TI(H) > 0$, i.e.

$$(2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3})(r(H'') - r(H)) > \varphi_{2,2}(n_i(H'') - n_i(H)). \tag{6}$$

If $K = \frac{\varphi_{2,2}}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}} < -4$, then $2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3} < 0$. Therefore, (6) is equivalent to

$$r(H'') - r(H) < \frac{\varphi_{2,2}(n_i(H'') - n_i(H))}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}.$$

Suppose that $n_i(H'') = n_i(H) - a$, where $1 \leq a \leq 4$. We have

$$r(H'') < r(H) + \frac{-\varphi_{2,2}a}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}. \tag{7}$$

Since $\frac{\varphi_{2,2}}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}} < -4$, we obtain $\frac{-\varphi_{2,2}a}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}} > 4$. By Lemma 2, $r(H'') \leq r(H) + 4$. Thus the inequality (7) holds for any pericondensed benzenoid system H. Thus, (6) holds.

If $K = \frac{\varphi_{2,2}}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}} > 2$, then $2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3} > 0$. Hence, (6) reduces to the following inequality

$$r(H'') - r(H) > \frac{\varphi_{2,2}(n_i(H'') - n_i(H))}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}.$$

Since $n_i(H'') = n_i(H) - a$, we have

$$r(H'') > r(H) + \frac{-\varphi_{2,2}a}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}. \tag{8}$$

Since $\frac{\varphi_{2,2}}{2\varphi_{2,3}-\varphi_{2,2}-\varphi_{3,3}} > 2$ and $1 \leq a \leq 4$, we obtain $\frac{-\varphi_{2,2}a}{2\varphi_{2,3}-\varphi_{2,2}-\varphi_{3,3}} < -2$. By Lemma 2, $r(H'') \geq r(H) - 2$. So, the inequality (8) holds for any pericondensed benzenoid system H. Thus, (6) holds as well. The proof is complete. ■

Recall that a catacondensed benzenoid system H is a benzenoid system with $n_i(H) = 0$. We can immediately obtain the following corollary from the above Theorem.

Corollary 1. *Let TI be a topological index of the form (4), subject to the condition that $K < -4$ or $K > 2$. If $H_1 \in HS_h$ is a pericondensed benzenoid system, then there exists an $H_2 \in HS_h$ that is a catacondensed benzenoid system such that $TI(H_1) < TI(H_2)$.*

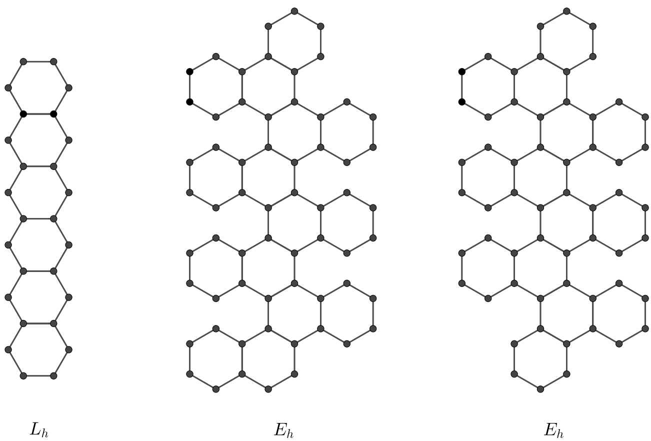


Fig. 6. The linear benzenoid chain L_h, and the catacondensed benzenoid system E_h correspond to the cases where h is odd and even, respectively.

Two special catacondensed benzenoid systems are L_h and E_h, shown in Fig. 6. It was shown in [13] that if H is a catacondensed benzenoid system with h hexagons then,

$$r(E_h) = \lceil \frac{h}{2} + 1 \rceil \leq r(H) \leq 2(h-1) = r(L_h). \tag{9}$$

Let $q = 2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}$. For a catacondensed benzenoid system, we immediately obtain the following theorem.

Theorem 4. *Let H be a catacondensed benzenoid system with h hexagons, and let TI be a topological index of the form (4). Then*

(1) if $q > 0$, then $TI(H) < TI(L_h)$;

(2) if $q < 0$, then $TI(H) < TI(E_h)$.

Proof. According to the definition of catacondensed benzenoid system and Theorem 2, the topological index $TI(H)$ can be expressed as:

$$\begin{aligned} TI(H) &= (2\varphi_{2,2} + 3\varphi_{3,3})h + (2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3})r(H) \\ &+ (4\varphi_{2,2} - 3\varphi_{3,3}). \end{aligned}$$

The result is obtained by applying inequality (9) to this expression. ■

By combining Corollary 1 with Theorem 4, we obtain one of our main results.

Corollary 2. *Let $H \in HS_h$, and let TI be a topological index of the form (4). Then*

(1) if $0 < q < \frac{\varphi_{2,2}}{2}$, then $TI(H) < TI(L_h)$;

(2) if $-\frac{\varphi_{2,2}}{4} < q < 0$, then $TI(H) < TI(E_h)$.

Example 1. Recall that the Sombor index of a benzenoid system H, is defined as

$$SO(H) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2}.$$

Note that in this case

$$q = 2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3} = 2\sqrt{13} - 2\sqrt{2} - 3\sqrt{2} \approx 0.14. \tag{10}$$

Since $0 < q < \frac{\varphi_{2,2}}{2} = \sqrt{2}$. We have $SO(H) \leq SO(L_h)$.

This result is consistent with the result in [3], which are shown below.

Theorem 5. *[3] Let H be a benzenoid system with h hexagons. Then $SO(H) \leq SO(L_h)$.*

Example 2. Consider now the elliptic Sombor index of a benzenoid system H, is defined as

$$ESO(H) = \sum_{uv \in E} (d_u + d_v)\sqrt{d_u^2 + d_v^2}.$$

Thus,

$$q = 2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3} = 10\sqrt{13} - 8\sqrt{2} - 18\sqrt{2} \approx -0.714.$$

Clearly, $-2\sqrt{2} = -\frac{\varphi_{2,2}}{4} < q < 0$. We have $SO(H) \leq SO(E_h)$.

4 The lower bound of Sombor index and elliptic Sombor index of benzenoid systems

4.1. Lower bound of elliptic Sombor index of benzenoid systems

In [14], Rada et al. proved the following theorem.

Theorem 6. *([14]) Let $H \in \mathcal{HS}_h$, and let TI be a topological index of the form (4). If $-f(2,2) \leq q \leq 0$, then*

$$TI(H) \geq TI(W),$$

where W is the convex benzenoid system with h hexagons and $2h + 1 - \lceil \sqrt{12h - 3} \rceil$ internal vertices.

In particularly, for elliptic Sombor index, $-f(2,2) \leq q \leq 0$. Thus, we have the following theorem.

Theorem 7. *If $H \in HS_h$, then*

$$ESO(H) \geq 54\sqrt{2}h + (10\sqrt{13} - 18\sqrt{2})\lceil\sqrt{12h-3}\rceil - 30\sqrt{13} + 48\sqrt{2},$$

with equality if and only if H is a convex benzenoid system with $2h+1-\lceil\sqrt{12h-3}\rceil$ internal vertices.

Proof. Let H_0 be a convex benzenoid system with h hexagons and $2h+1-\lceil\sqrt{12h-3}\rceil$ internal vertices. By Theorem 6, it follows that

$$ESO(H) \geq ESO(H_0).$$

From the relations in [15],

$$m_{2,2}(H_0) = 6 + b(H_0). \tag{11}$$

Since $b(H_0) = 0$, we have $r(H_0) = f(H_0)$. Therefore,

$$m_e(H_0) = m_{2,2}(H_0) + 2f(H_0) = 6 + 2r(H_0).$$

Furthermore,

$$n(H_0) = n_i(H_0) + n_e(H_0) = n_i(H_0) + m_e(H_0) = n_i(H_0) + 6 + 2r(H_0). \tag{12}$$

Using equations (5) and (12), we derive

$$r(H_0) = 2h - n_i(H_0) - 2. \tag{13}$$

By substituting $n_i(H_0) = 2h + 1 - \lceil\sqrt{12h-3}\rceil$ into (13) and applying Theorem 2, we obtain

$$ESO(H_0) = 54\sqrt{2}h + (10\sqrt{13} - 18\sqrt{2})\lceil\sqrt{12h-3}\rceil - 30\sqrt{13} + 48\sqrt{2}.$$

■

4.2. Lower bound of Sombor index of benzenoid systems

Unfortunately, for the Sombor index, we have $q > 0$. Therefore, we now focus on determining the lower bound of the Sombor index of benzenoid systems.

Lemma 3. *If $H \in \mathcal{HS}_h$, then*

$$2\lceil\sqrt{12h-3}\rceil \leq m_e(H) \leq 4h-2,$$

with left equality if and only if $n_i(H) = 2h + 1 - \lceil\sqrt{12h-3}\rceil$, and with right equality if and only if $n_i(H) = 0$.

Proof. Combing $n(H) = n_i(H) + n_e(H)$ with (5), we get

$$n_e(H) = 4h + 2 - 2n_i(H). \tag{14}$$

Since $m_e(H) = n_e(H)$, by inequality (2), it follows that

$$2\lceil\sqrt{12h-3}\rceil \leq m_e(H) \leq 4h-2.$$

■

Theorem 8. *Let $H \in \mathcal{HS}_h$ and let h_0 be a hexagon on the boundary of H such that $H \setminus h_0$ is connected. If H' is the benzenoid system obtained from H by moving h_0 to an inlet of H such that $n_i(H') > n_i(H)$, then*

$$TI(H') < TI(H),$$

where TI be a topological index of the form (4) such that $K > 2$.

Proof. By Theorem 2, we have

$$\begin{aligned} TI(H') - TI(H) &= (2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3})(r(H') - r(H)) \\ &- \varphi_{2,2}(n_i(H') - n_i(H)). \end{aligned}$$

To establish $TI(H') < TI(H)$, it suffices to show that $TI(H') - TI(H) < 0$, which is

$$(2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3})(r(H') - r(H)) < \varphi_{2,2}(n_i(H') - n_i(H)). \tag{15}$$

Since $K = \frac{\varphi_{2,2}}{2\varphi_{2,3}-\varphi_{2,2}-\varphi_{3,3}} > 2$, it follows that $2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3} > 0$, Therefore, the inequality (15) is equivalent to

$$r(H') - r(H) < \frac{\varphi_{2,2}(n_i(H') - n_i(H))}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}.$$

Suppose that $n_i(H') = n_i(H) + a$, where $1 \leq a \leq 4$. We have

$$r(H') < r(H) + \frac{\varphi_{2,2}a}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}}. \tag{16}$$

Since $\frac{\varphi_{2,2}}{2\varphi_{2,3}-\varphi_{2,2}-\varphi_{3,3}} > 2$, we have $\frac{\varphi_{2,2}a}{2\varphi_{2,3}-\varphi_{2,2}-\varphi_{3,3}} > 2$. By Lemma 1, $r(H') < r(H) + 2$. Thus, the inequality (16) holds for any benzenoid system H. Thus, inequality (15) is satisfied, completing the proof. ■

Based on the proof of Lemma 1, we derive the following conclusions: (1) moving a hexagon of type L_1 into any inlet of H results in a benzenoid system H' such that $n_i(H') > n_i(H)$; (2) for any cove or fjord of H, there exists a hexagon h_0 such that moving h_0 to a cove or fjord of H produces a benzenoid system H' with $n_i(H') > n_i(H)$. Therefore, we have the following corollary.

Corollary 3. *Let TI be a topological index of the form (4) with $K > 2$. If $H_1 \in \mathcal{HS}_h$ contains a cove, a fjord, or a hexagon of type L_1, then there exists an $H_2 \in \mathcal{HS}_h$ that lacks these features and satisfies $TI(H_1) > TI(H_2)$.*

Example 3. For the Sombor index of a benzenoid system,

$$K = \frac{\varphi_{2,2}}{2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}} = \frac{2\sqrt{2}}{2\sqrt{13} - 2\sqrt{2} - 3\sqrt{2}} \approx 20.198 > 2.$$

Thus, the benzenoid system that minimizes the Sombor index does not contain coves and fjords. Below, we provide an expression for the Sombor index on a benzenoid system without cove and fjord.

Theorem 9. *If $H \in \mathcal{HS}_h$ with $C(H) = F(H) = 0$, then*

$$SO(H) = 9\sqrt{2}h + (2\sqrt{13} - 3\sqrt{2})f(H) + (2\sqrt{13} - \sqrt{2})B(H) + 3\sqrt{2}.$$

Proof. By equations (3) and (11), we have $m_{2,2}(H) = 6 + B(H)$. Furthermore,

$$n_e(H) = m_e(H) = m_{2,2}(H) + 2f(H) + 3B(H) = 2f(H) + 4B(H) + 6. \quad (17)$$

Combing $n(H) = n_i(H) + n_e(H)$ with (5) and (17), we get

$$n_i(H) = 2h - f(H) - 2B(H) - 2. \quad (18)$$

Since $r(H) = f(H) + B(H)$, By Theorem 2, it follows that

$$SO(H) = 9\sqrt{2}h + (2\sqrt{13} - 3\sqrt{2})f(H) + (2\sqrt{13} - \sqrt{2})B(H) + 3\sqrt{2}.$$

■

Next, we give a lower bound for the Sombor index on benzenoid systems without cove and fjord.

Theorem 10. *If $H \in \mathcal{HS}_h$ with $C(H) = F(H) = 0$, then*

$$SO(H) > 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})\lceil\sqrt{12h-3}\rceil - 3\sqrt{13} + \frac{9\sqrt{2}}{2}.$$

Proof. By equation (17), we have $f(H) + 2B(H) = \frac{m_e - 6}{2}$. By Theorem 9, we have

$$\begin{aligned} SO(H) &= 9\sqrt{2}h + (2\sqrt{13} - 3\sqrt{2})f(H) + (2\sqrt{13} - \sqrt{2})B(H) + 3\sqrt{2} \\ &> 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})f(H) + (2\sqrt{13} - \sqrt{2})B(H) + 3\sqrt{2} \\ &= 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})(f(H) + 2B(H)) + 3\sqrt{2} \\ &= 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})\frac{m_e - 6}{2} + 3\sqrt{2} \end{aligned}$$

By Lemma 3, $m_e(H) \geq 2\lceil\sqrt{12h-3}\rceil$, we have $SO(H) > 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})(\lceil\sqrt{12h-3}\rceil - 3) + 3\sqrt{2}$. Thus, the result holds. ■

By combining Corollary 3 with Theorem 10, we obtain a lower bound for the Sombor index on benzenoid systems as follows.

Corollary 4. *If $H \in \mathcal{HS}_h$, then*

$$SO(H) > 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})\lceil\sqrt{12h-3}\rceil - 3\sqrt{13} + \frac{9\sqrt{2}}{2}.$$

4.3. The benzenoid systems have minimal value of Sombor index

As is known, for an $H_1 \in \mathcal{HS}_h$ with $n_i(H_1) < 2h + 1 - \lceil\sqrt{12h-3}\rceil$, then there exists an $H_2 \in HS_h$ with $n_i(H_2) > n_i(H_1)$. Suppose that $n_i(H_2) - n_i(H_1) > a$ where $a > 0$. As shown in Example 3, and the proof of Theorem 8, it is sufficient to show that $r(H_2) < r(H_1) + 20a$ in order to establish $SO(H_2) < SO(H_1)$. This statement is generally true, but we have not yet found an appropriate way to prove it. Thus, we propose the following conjecture.

Conjecture 1. *If $H_1 \in \mathcal{HS}_h$ with $n_i(H_1) < 2h + 1 - \lceil\sqrt{12h-3}\rceil$, then there exists an $H_2 \in \mathcal{HS}_h$ with $n_i(H_2) > n_i(H_1)$ such that $SO(H_2) < SO(H_1)$.*

The correctness of the above conjecture means that the benzenoid system attains the minimum of Sombor index is the anacondensed benzenoid system.

Here, we address and rectify an error found in Theorem 5.3 in [3]. According to [3], the expression for $TI(H)$ is given by:

$$\begin{aligned} TI(H) &= (4\varphi_{2,3} + \varphi_{3,3})h + (\varphi_{2,2} - 2\varphi_{2,3} + \varphi_{3,3})b(H) \\ &\quad +(\varphi_{3,3} - 2\varphi_{2,3})n_i(H) + (6\varphi_{2,2} - 4\varphi_{2,3} - \varphi_{3,3}). \end{aligned}$$

Since H is a catacondensed benzenoid system, we analyze the term $q = 2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}$ and find that:

- if $q > 0$, then $\varphi_{2,2} - 2\varphi_{2,3} + \varphi_{3,3} < 0$, and TI is minimized when $b(H)$ is maximized.

- Similarly, if $q < 0$, then $\varphi_{2,2} - 2\varphi_{2,3} + \varphi_{3,3} > 0$, and TI attains its minimum when $b(H)$ is minimized.

Therefore, the corrected statement of Theorem 5.3 in [3] is as follows.

Theorem 11. *Let TI be a topological index of the form (4). Let $q = 2\varphi_{2,3} - \varphi_{2,2} - \varphi_{3,3}$. Then*

(1) if $q = 0$, then TI is constant over anacondensed benzenoid system;

(2) if $q > 0$, then V_h(resp.U_h) attains the maximal (resp. minimal) value of TI over anacondensed benzenoid system;

(3) if $q < 0$, then U_h(resp.V_h) attains the maximal (resp. minimal) value of TI over anacondensed benzenoid system.

By combining (10) with Theorem 11, we guess that U_h, as defined in [3], attains the minimum Sombor index.

In particular, in [3], Cruz et al. proved that there is a unique anacondensed benzenoid system with $h = 3k(k-1)+1$, as depicted in the figure below.

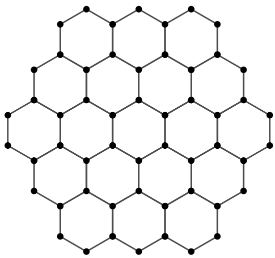
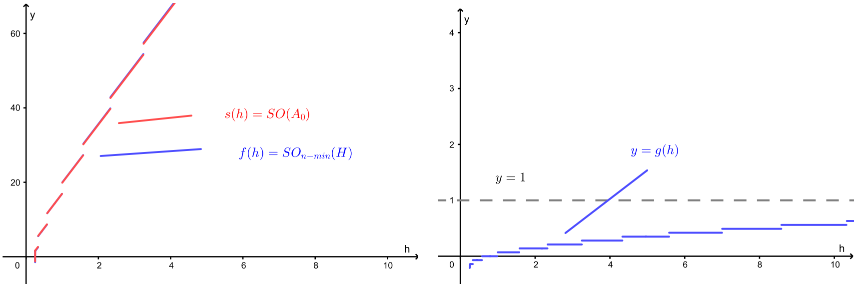


Fig. 7. The anacondensed benzenoid system with $h = 3k(k-1)+1$ when $k = 3$.

We use A_0 to denote the anacondensed benzenoid system with $h = 3k(k-1)+1$. Since $n_i(A_0) = 2h + 1 - \lceil\sqrt{2h-3}\rceil$, by (13) and Theorem 2, we get

$$SO(A_0) = 9\sqrt{2}h + (2\sqrt{13} - 3\sqrt{2})\lceil\sqrt{12h-3}\rceil - 6\sqrt{13} + 12\sqrt{2}.$$

Let $SO_{n-min}(H) = 9\sqrt{2}h + (\sqrt{13} - \frac{\sqrt{2}}{2})\lceil\sqrt{12h-3}\rceil - 3\sqrt{13} + \frac{9\sqrt{2}}{2}$, which represents the lower bound of the Sombor index of benzenoid systems, as derived in Corollary 4. Let $f(h) = SO_{n-min}(H)$ and $s(h) = SO(A_0)$. We can see $f(h)$ and $s(h)$ nearly overlap from the Fig. 8 (a). Let $g(h) = SO(A_0) - SO_{n-min}(H)$. From the Fig. 8 (b), we can see that $g(h)$ is growing slowly.



(a) (b)

Fig. 8. (a) show the function of $f(h)$ and $s(H)$, and (b) show the function of $g(h)$.

To further demonstrate that $SO_{n-min}(H)$ is very close to the tight lower bound of the Sombor index on the benzenoid system, let

$$\begin{aligned} t(h) &= \frac{SO(A_0) - SO_{n-min}(H)}{SO(A_0)} \\ &= \frac{(\sqrt{13} - \frac{5\sqrt{2}}{2})\lceil\sqrt{12h-3}\rceil - 3\sqrt{13} + \frac{15\sqrt{2}}{2}}{9\sqrt{2}h + (2\sqrt{13} - 3\sqrt{2})\lceil\sqrt{12h-3}\rceil - 6\sqrt{13} + 12\sqrt{2}}. \end{aligned}$$

Since

$$\lim_{h\to\infty} \frac{(\sqrt{13} - \frac{5\sqrt{2}}{2})\lceil\sqrt{12h-3}\rceil - 3\sqrt{13} + \frac{15\sqrt{2}}{2}}{9\sqrt{2}h + (2\sqrt{13} - 3\sqrt{2})\lceil\sqrt{12h-3}\rceil - 6\sqrt{13} + 12\sqrt{2}} = 0,$$

the difference between $SO(A_0)$ and $SO_{n-min}(H)$, when compared to $SO(A_0)$, is almost negligible.

To sum up, we find that although the lower bound of the Sombor index for the benzenoid systems obtained in Corollary 4 is not sharp, it appears to differ very little from the true lower bound.

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