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On Extremal Sombor Indices of Chemical Graphs, and Beyond

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Abstract

For a (chemical) graph G with vertex set V_G and edge set E_G, the Sombor index is defined as $SO(G) = \sum\limits_{uv \in E_G} \sqrt{d^2(u) + d^2(v)}$, where $d(u)$ denotes the degree of vertex u in G. In this paper, we determine the second and third minimum (resp. maximum) Sombor index of catacondensed hexagonal systems and phenylenes, the second minimum Sombor index of cata-catacondensed fluoranthene-type benzenoid systems. We also determine the minimum (resp. maximum) Sombor index of caterpillar trees with given degree sequence. At last, the first three maximum and the minimum Sombor index of star-like trees are determined.

1 Introduction

Let G be a simple connected graph with vertex set V_G and edge set E_G. The degree of a vertex u is defined as $d(u)$. If $d(u) \leq 4$ for all $u \in V_G$, then

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we call G is a chemical graph (or molecular graph). We write $uv \in E_G$ if $u \sim v$ in G. Let m_{ij} be the number of edges if the degrees of two end vertices are i and j. Denote by S_n and P_n, the star graph and path with order n, respectively. In this paper, all notations and terminologies used but not defined can refer to Bondy and Murty [2].

The distance $d_G(u, v)$ between vertex u and v is the length of shortest path from u to v. The diameter $diam(G)$ is defined as $diam(G) = \max\{d_G(u, v)|u, v \in V_G\}$. A tree T is a star-like tree if $diam(T) \leq 4$. Note that the star-like tree we considered here are different from the star-like tree of [4] which is a tree with exactly one vertex of degree greater than 2. If $d_1, d_2, \cdots, d_n$ is the degrees of n vertices in G and $d_1 \geq d_2 \geq \cdots \geq d_n$, then we call $\pi = (d_1, d_2, \cdots, d_n)$ the degree sequence of G.

Inspired by Euclidean metric, in 2020, Gutman proposed the Sombor index [9], which is defined as

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

Since then, the Sombor index has attracted much attention of researchers. Redžepović et al. [20] researched the chemical applicability of the Sombor indices. Deng et al. [7] determined the maximum Sombor index in chemical trees. Li et al. [15] considered the extremal Sombor index of trees with given diameter. Very recently, Gutman [10] showed that geometry-based reasonings reveal the geometric background of several classical topological indices, and led to a series of new SO-like degree-based graph invariants. One can refer to [16–18, 21, 22] for more details about the Sombor index.

The remainder of this paper is organized as follow. In Section 2.1, we determine the second and third minimum (resp. maximum) Sombor index of catacondensed hexagonal systems and phenylenes. In Section 2.2, we determine the second minimum Sombor index of cata-catacondensed fluoranthene-type benzenoid systems. In Section 3, we determine the minimum (resp. maximum) Sombor index of caterpillar trees with given degree sequence. In Section 4, the first three maximum and minimum Sombor index of star-like trees are determined.

2 Hexagonal systems and phenylenes

In this section, we determine the extremal Sombor index of catacondensed hexagonal systems, phenylenes and cata-catacondensed fluoranthen e-type benzenoid systems.

2.1 Catacondensed hexagonal systems and phenylenes

A hexagonal system is a special chemical graph. A hexagonal system [11,12] (or called a benzenoid system) is a finite connected plane graph with out cut vertices, in which all interior regions are mutually congruent regular hexagons. Let $\mathcal{HS}_h$ be the set of hexagonal systems with h hexagons.

We use $ID(H)$ to denote the inner dual graph [11] of a hexagonal system H, which is the graph whose vertices are the hexagons of H and two vertices are adjacent in $ID(H)$ if the corresponding hexagons in H are adjacent. If the inner dual $ID(H)$ is a tree with h vertices, then we call H is a catacondensed hexagonal system with h hexagons, and denote by $\mathcal{CHS}_h$ the set of catacondensed hexagonal systems with h hexagons. Further, if the inner dual $ID(H)$ is a path with h vertices, then we call H is a hexagonal chain with h hexagons, and denoted by L_h.

The types of hexagons in a catacondensed hexagonal system can be divided into linear (L_1 and L_2) and angular (A_2 and A_3) (see Figure 1, and which is defined in [13]). We use $l_1(H)$, $l_2(H)$, $a_2(H)$, $a_3(H)$ to denote the number of L_1-, L_2-, A_2-, A_3-hexagons in H, respectively. A fissure is a path with degree sequence $(2,3,2)$ if it goes along the perimeter of a catacondensed hexagonal system, and bay with degree sequence $(2,3,3,2)$, cove with degree sequence $(2,3,3,3,2)$, fjord with degree sequence $(2,3,3,3,3,2)$, respectively (see Figure 1). The numbers of fissures, bays, coves, fjords in a catacondensed hexagonal system H are denoted by $f(H)$, $B(H)$, $C(H)$, $F(H)$, respectively. Then the number of inlets of H is $r(H) = f(H) + B(H) + C(H) + F(H)$.

Let H be a catacondensed hexagonal system. Then by the definition of the Sombor index, we have $SO(H) = 2\sqrt{2}m_{22} + \sqrt{13}m_{23} + 3\sqrt{2}m_{33}$.

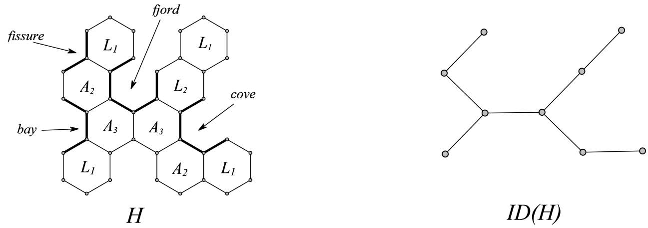

Figure 1. A catacondensed hexagonal system H and its $ID(H)$.

Lemma 2.1. [19] *Let $H \in \mathcal{HS}_h$ with n vertices and r inlets. Then*

$$\begin{cases} m_{22} = n - 2h - r + 2, \\ m_{23} = 2r, \\ m_{33} = 3h - r - 3. \end{cases}$$

Note that $n = 4h + 2$ for a catacondensed hexagonal system with h hexagons, then by Lemma 2.1, we immediately have

Lemma 2.2. *If $H \in \mathcal{HS}_h$ with n vertices and r inlets, then*

$$SO(H) = 2\sqrt{2}n + 5\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})r - 5\sqrt{2}.$$

Especially, if $H \in \mathcal{CHS}_h$, then we have

$$SO(H) = 13\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})r - \sqrt{2}. \tag{1}$$

Lemma 2.3. [25] *Let $H \in \mathcal{CHS}_h$ with $a_2(H) = a_2$, $a_3(H) = a_3$ and r inlets. Then $r + 3a_3 + a_2 = 2(h - 1)$.*

Lemma 2.4. [24] *Let $H \in \mathcal{CHS}_h$ with $a_2(H) = a_2$, $a_3(H) = a_3$, $l_2(H) = l_2$ and r inlets. Then $a_2 + 2a_3 + l_2 = h - 2$ and*

$$r = \frac{1}{2}(h + 2 + a_2 + 3l_2) \geq \begin{cases} \frac{h+2}{2}, & if\ h\ is\ even, \\ \frac{h+3}{2}, & if\ h\ is\ odd, \end{cases} \tag{2}$$

with equality if and only if $\begin{cases} a_2 = l_2 = 0, & if\ h\ is\ even, \\ a_2 = 1, l_2 = 0, & if\ h\ is\ odd. \end{cases}$

By Lemmas 2.3 and 2.4 and Equation (1), we have

Theorem 2.5. [5] *Let $h \geq 3$ and $H \in \mathcal{CHS}_h$. Then*
(i) $SO(H) \leq (4\sqrt{13}+3\sqrt{2})h + 9\sqrt{2} - 4\sqrt{13}$, *with equality if and only if* $H \cong L_h$.
(ii) $$SO(H) \geq \begin{cases} 13\sqrt{2}h + (2\sqrt{13}-5\sqrt{2})\frac{h+2}{2} - \sqrt{2}, & if\ h\ is\ even, \\ 13\sqrt{2}h + (2\sqrt{13}-5\sqrt{2})\frac{h+3}{2} - \sqrt{2}, & if\ h\ is\ odd, \end{cases}$$
with equality if and only if $\begin{cases} a_2 = 0, a_3 = \frac{h-2}{2}, & if\ h\ is\ even, \\ a_2 = 1, a_3 = \frac{h-3}{2}, & if\ h\ is\ odd. \end{cases}$

Remark 2.6. *Note that the graphs in $\mathcal{CHS}_h$ with the minimum Sombor index satisfied:* $\begin{cases} a_2 = 0, a_3 = \frac{h-2}{2}, & if\ h\ is\ even, \\ a_2 = 1, a_3 = \frac{h-3}{2}, & if\ h\ is\ odd. \end{cases}$ *It is obvious that the Figure 6 of [5] are not correct. We redrawn it* (see Figure 2).

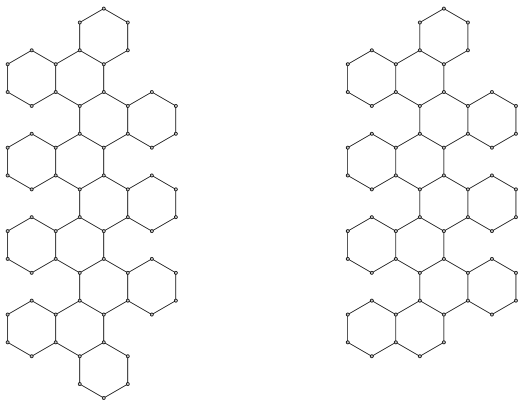

Figure 2. Minimum graphs in $\mathcal{CHS}_h$ with $h = 16$ and $h = 15$.

In the following, we consider the second and third maximum graphs in $\mathcal{CHS}_h$ with respect to the Sombor index. Let $\mathcal{L}_h^2$ be the set of the second maximum catacondensed hexagonal systems in $\mathcal{CHS}_h$.

Theorem 2.7. *Let $H \in \mathcal{CHS}_h \setminus \{L_h\}$ with $a_2(H) = a_2$, $a_3(H) = a_3$ and r inlets.*
(i) $SO(H) \leq 13\sqrt{2}h + (2\sqrt{13}-5\sqrt{2})(2h-3) - \sqrt{2}$, *with equality if and only if $a_2 = 1, a_3 = 0$ in H.*
(ii) *If $H \in \mathcal{CHS}_h \setminus (\{L_h\} \cup \mathcal{L}_h^2)$, then $SO(H) \leq 13\sqrt{2}h + (2\sqrt{13}-5\sqrt{2})(2h-4) - \sqrt{2}$, with equality if and only if $a_2 = 2, a_3 = 0$ in H.*

Proof. By Theorem 2.5, $SO(H) \leq SO(L_h)$, with equality if and only if $r = 2(h-1)$.

If $r \neq 2(h-1)$, then $r \leq 2(h-1)-1 = 2h-3$, with equality if and only if $a_2 = 1, a_3 = 0$ in H. Thus $SO(H) \leq 13\sqrt{2}h + (2\sqrt{13}-5\sqrt{2})(2h-3) - \sqrt{2}$, with equality if and only if $a_2 = 1, a_3 = 0$ in H.

If $r \neq 2(h-1)$, $r \neq 2h-3$, then $r \leq 2h-4$ with equality if and only if $a_2 = 2, a_3 = 0$ in H. Thus $SO(H) \leq 13\sqrt{2}h + (2\sqrt{13}-5\sqrt{2})(2h-4) - \sqrt{2}$ with equality if and only if $a_2 = 2, a_3 = 0$ in H.

Note that it is easy to confirm that the graphs with the second and the third maximum Sombor index exist (see (1) and (2) of Figure 3). ■

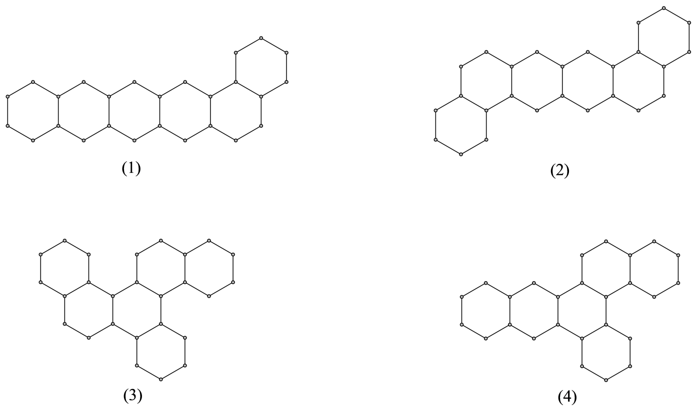

Figure 3. Examples for the second maximum, the third maximum, the second minimum and the third minimum graphs in $\mathcal{CHS}_6$.

Next, we consider the second and the third minimum graphs in $\mathcal{CHS}_h$ with respect to the Sombor index.

Theorem 2.8. *Let $H \in \mathcal{CHS}_h$ $(h \geq 5)$ with $a_2(H) = a_2$, $a_3(H) = a_3$ and r inlets.*
(i) If h is even, then H has the second minimum Sombor index if and only if $a_2 = 2, a_3 = \frac{1}{2}(h-4)$ in H.
(ii) If h is odd, then H has the second minimum Sombor index if and only if $a_2 = 0, a_3 = \frac{1}{2}(h-3)$ or $a_2 = 3, a_3 = \frac{1}{2}(h-5)$ in H.

Proof. (i) If h is even, by Lemma 2.4, H has the minimum Sombor index if and only if $r = \frac{1}{2}(h+2)$. If $r \neq \frac{1}{2}(h+2)$, then $r \geq \frac{1}{2}(h+4)$ with equality if and only if $a_2 = 2, a_3 = \frac{1}{2}(h-4)$ in H. Thus $SO(H) \geq 13\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})\frac{h+4}{2} - \sqrt{2}$, with equality if and only if $a_2 = 2, a_3 = \frac{1}{2}(h-4)$ in H.

(ii) If h is odd, by Lemma 2.4, H has the minimum Sombor index if and only if $r = \frac{1}{2}(h+3)$. If $r \neq \frac{1}{2}(h+3)$, then $r \geq \frac{1}{2}(h+5)$ with equality if and only if $a_2 = 0, a_3 = \frac{1}{2}(h-3)$ or $a_2 = 3, a_3 = \frac{1}{2}(h-5)$ in H. Thus $SO(H) \geq 13\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})\frac{h+5}{2} - \sqrt{2}$, with equality if and only if $a_2 = 0, a_3 = \frac{1}{2}(h-3)$ or $a_2 = 3, a_3 = \frac{1}{2}(h-5)$ in H.

Note that it is easy to confirm that the graphs with second minimum Sombor index exist (see (3) of Figure 3). ■

Further, similar to the proof of Theorem 2.8, we have

Theorem 2.9. *Let $H \in \mathcal{CHS}_h$ $(h \geq 5)$ with $a_2(H) = a_2$, $a_3(H) = a_3$ and r inlets.*
(i) *If h is even, then H has the third minimum Sombor index if and only if $a_2 = 1, a_3 = \frac{1}{2}(h-4)$ in H.*
(ii) *If h is odd, then H has the third minimum Sombor index if and only if $a_2 = 2, a_3 = \frac{1}{2}(h-5)$ in H.*

Note that it is easy to confirm that the graphs with the third minimum Sombor index of Theorem 2.9 exist (see (4) of Figure 3).

Phenylenes (denoted by PH) are polycyclic conjugated molecules possessing both quadrilaterals and hexagons. Each quadrilateral is adjacent to two disjoint hexagons, and no two hexagons are adjacent. By squeezing out the squares from a phenylene, we can obtain a catacondensed hexagonal system which is also called the hexagonal squeeze (denoted by HS) of the corresponding phenylene. A hexagonal squeeze is also a catacondensed hexagonal system. An example of the PH and its corresponding HS see Figure 4.

Let $\mathcal{PH}$ be the set of phenylenes. Firstly, we consider the relationship between the Sombor index of phenylenes and its hexagonal squeeze. Let $H \in \mathcal{PH}$, then by the definition of the Sombor index, we have

$$SO(H) = 2\sqrt{2}m_{22} + \sqrt{13}m_{23} + 3\sqrt{2}m_{33}.$$

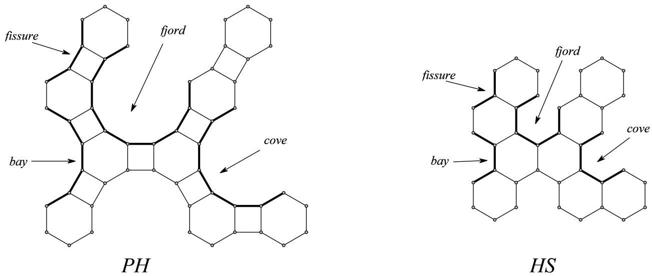

Figure 4. A phenylene (PH) and its hexagonal squeeze (HS).

Lemma 2.10. [19] *Let $H \in \mathcal{PH}$ with h hexagons and r inlets. Then*

$$\begin{cases} m_{22} = 2h - r + 4, \\ m_{23} = 2r, \\ m_{33} = 6h - r - 6. \end{cases}$$

Note that $n = 6h$ for phenylene with h hexagons, then by Lemma 2.10, we immediately have

Theorem 2.11. *Let $H \in \mathcal{PH}$ with h hexagons and r inlets. Then*

$$SO(H) = 22\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})r - 10\sqrt{2}.$$

Combining the conclusions of Theorem 2.11 and Lemma 2.2, we have

Corollary 2.12. *Let $H \in \mathcal{PH}$ with h hexagons, $H^* \in \mathcal{HS}$ be the corresponding hexagonal squeeze of H. Then $SO(H) = SO(H^*) + 9\sqrt{2}(h-1)$.*

By Corollary 2.12, similarly, we can determine the extremal Sombor index of phenylenes with h hexagons. We omit the proof of Theorems 2.13-2.15.

Theorem 2.13. *Let $h \geq 3$ and $H \in \mathcal{PH}$, $H^* \in \mathcal{HS}$ be the corresponding hexagonal squeeze of H. Then*
(i) $SO(H) \leq (4\sqrt{13}+12\sqrt{2})h - 4\sqrt{13}$, *with equality if and only if $H^* \cong L_h$.*
(ii) $SO(H) \geq \begin{cases} 22\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})\frac{h+2}{2} - 10\sqrt{2}, & if\ h\ is\ even, \\ 22\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})\frac{h+3}{2} - 10\sqrt{2}, & if\ h\ is\ odd, \end{cases}$

with equality if and only if $\begin{cases} a_2(H^*) = 0, a_3(H^*) = \frac{h-2}{2}, & if\ h\ is\ even, \\ a_2(H^*) = 1, a_3(H^*) = \frac{h-3}{2}, & if\ h\ is\ odd. \end{cases}$

Theorem 2.14. *Let $h \geq 3$ and $H \in \mathcal{PH}$, $H^* \in \mathcal{HS}$ be the corresponding hexagonal squeeze of H. Then*
(i) H has the second maximum Sombor index if and only if $a_2(H^*) = 1, a_3(H^*) = 0$ in H^*.
(ii) H has the third maximum Sombor index if and only if $a_2(H^*) = 2, a_3(H^*) = 0$ in H^*.

Theorem 2.15. *Let $h \geq 5$ and $H \in \mathcal{PH}$, $H^* \in \mathcal{HS}$ be the corresponding hexagonal squeeze of H. Then*
(i) *If h is even, then H has second minimum Sombor index if and only if $a_2(H^*) = 2, a_3(H^*) = \frac{1}{2}(h-4)$ in H^*.*
(ii) *If h is odd, then H has second minimum Sombor index if and only if $a_2(H^*) = 0, a_3(H^*) = \frac{1}{2}(h-3)$ or $a_2(H^*) = 3, a_3(H^*) = \frac{1}{2}(h-5)$ in H^*.*
(iii) *If h is even, then H has third minimum Sombor index if and only if $a_2(H^*) = 1, a_3(H^*) = \frac{1}{2}(h-4)$ in H^*.*
(iv) *If h is odd, then H has third minimum Sombor index if and only if $a_2(H^*) = 2, a_3(H^*) = \frac{1}{2}(h-5)$ in H^*.*

2.2 Cata-catacondensed fluoranthene-type benzenoid systems

Let X be a benzenoid system, $d(u) = d(v) = 2$, $d(w) = 3$ for $uw, vw \in E(X)$ (see Figure 5). Let Y be another benzenoid system, $d(x) = d(y) = 2$ for $xy \in E(Y)$ (see Figure 5). The the fluoranthene-type benzenoid system (simply for f-benzenoid system) $F(X, Y)$ is the graph obtained from X and Y by connecting vertices u and x, v and y, respectively. If X and Y are both catacondensed benzenoid system, then we call $F(X, Y)$ cata-catacondensed fluoranthene-type benzenoid system (simply for cata-catacondensed f-benzenoid system). Let $\mathcal{FC}_h$ be the set of cata-cataconden sed f-benzenoid systems with h hexagons.

Lemma 2.16. [13] *Let F be a f-benzenoid system with n vertices and $h \geq 3$ hexagons and r inlets. Then $SO(F) = 2\sqrt{2}n + (2\sqrt{13} - 5\sqrt{2})r + 5\sqrt{2}h$.*

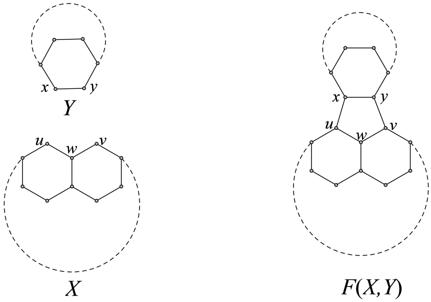

Figure 5. benzenoid systems X, Y and f-benzenoid system $F(X, Y)$.

For $F \in \mathcal{FC}_h$ with n vertices and h hexagons, then $n = 4h + 4$, thus

Corollary 2.17. [13] *Let $F \in \mathcal{FC}_h$ with r inlets. Then* $SO(F) = (2\sqrt{13} - 5\sqrt{2})r + 13\sqrt{2}h + 8\sqrt{2}$.

Lemma 2.18. [8] *Let $h \geq 3$ and $F \in \mathcal{FC}_h$, FL_h and E_h be defined in [13] (see Figures 4,8,9 of [13]). Then*
(i) $r(F) \leq r(FL_h) = 2h - 3$;
(ii) $r(F) \geq r(E_h) = \begin{cases} \frac{1}{2}(h+4), & if\ h\ is\ even, \\ \frac{1}{2}(h+3), & if\ h\ is\ odd. \end{cases}$

Theorem 2.19. [13] *Let $h \geq 3$ and $F \in \mathcal{FC}_h$. Then*
(i) $SO(F) \leq SO(FL_h) = 14\sqrt{2} + \sqrt{13}(4h - 6) + 3\sqrt{2}(h + 3)$;
(ii) $SO(F) \geq SO(E_h) = \begin{cases} (\frac{21}{2}\sqrt{2} + \sqrt{13})h + 4\sqrt{13} - 2\sqrt{2}, & if\ h\ is\ even, \\ (\frac{21}{2}\sqrt{2} + \sqrt{13})h + 4\sqrt{13} - \frac{1}{2}\sqrt{2}, & if\ h\ is\ odd. \end{cases}$

Let $F(X, Y)$ be the cata-catacondensed fluoranthene-type benzenoid systems with h hexagons, a_2 A_2-hexagons, a_3 A_3-hexagons and l_2 L_2-hexagons. Let a_2^1, a_2^2 be the numbers of A_2-hexagons in X and Y, l_2^1, l_2^2 the numbers of L_2-hexagons in X and Y, respectively. Let $d(u), d(v), d(x), d(y)$ be the degree of vertices u, v, x, y in cata-catacondensed f-benzenoid system $F(X, Y)$, see Figure 5.

Lemma 2.20. [8] *Let $F \in \mathcal{FC}_h$ with $h \geq 3$. Then*
(i) *if h is even and $r \neq \frac{1}{2}(h + 4)$, then $r \geq \frac{1}{2}(h + 6)$, with equality if and only if one of the following holds:*
(1) $d(u) = d(v) = d(x) = d(y) = 2, l_2 = l_2^1 = l_2^2 = 0, a_2 = a_2^1 = a_2^2 = 0$;

(2) $d(u) = d(x) = d(y) = 2, d(v) = 3, a_2 = a_2^1 + a_2^2 = 1, l_2 = l_2^1 = l_2^2 = 0$;
(3) $d(v) = d(x) = d(y) = 2, d(u) = 3, a_2 = a_2^1 + a_2^2 = 1, l_2 = l_2^1 = l_2^2 = 0$;
(4) $d(u) = d(x) = 3, d(v) = d(y) = 2, l_2 = l_2^1 = 1, a_2 = a_2^1 + a_2^2 = 1$;
(5) $d(x) = d(y) = 2, d(u) = d(v) = 3, a_2 = a_2^1 + a_2^2 = 3, l_2 = l_2^1 = l_2^2 = 0$;
(6) $d(u) = d(y) = 3, d(v) = d(x) = 2, a_2 = a_2^1 + a_2^2 = 0, l_2 = l_2^1 = 1$;
(7) $d(v) = d(y) = 3, d(u) = d(x) = 2, l_2 = l_2^1 = 1, a_2 = a_2^1 = a_2^2 = 0$;
(8) $d(v) = d(y) = d(x) = 3, d(u) = 2, l_2 = l_2^1 = 2, a_2 = a_2^1 = a_2^2 = 0$;
(9) $d(v) = d(y) = d(u) = 3, d(x) = 2, a_2^2 \geq 1, a_2 = a_2^1 + a_2^2 = 2, l_2 = l_2^1 = 1$;
(10)$d(v) = d(x) = d(u) = 3, d(y) = 2, a_2^2 \geq 1, a_2 = a_2^1 + a_2^2 = 2, l_2 = l_2^1 = 1$;
(11) $d(y) = d(u) = d(x) = 3, d(v) = 2, l_2 = l_2^1 = 2, a_2 = a_2^1 = a_2^2 = 0$;
(12) $d(u) = d(v) = d(x) = d(y) = 3, l_2 = l_2^1 = 2, a_2^1 \geq 1, a_2 = a_2^1 + a_2^2 = 2$.

(ii) *if h is odd and $r \neq \frac{1}{2}(h+3)$, then $r \geq \frac{1}{2}(h+5)$, with equality if and only if one of the following holds:*
(1) $d(u) = d(y) = 3, d(v) = d(x) = 2, l_2 = 0, a_2 = a_2^1 + a_2^2 = 2, a_2^1 \geq 1$;
(2) $d(u) = d(x) = d(y) = 2, d(v) = 3, a_2 = a_2^1 + a_2^2 = 1, l_2 = l_2^1 = l_2^2 = 0$;
(3) $d(v) = d(x) = d(y) = 2, d(u) = 3, a_2 = a_2^1 + a_2^2 = 1, l_2 = l_2^1 = l_2^2 = 0$;
(4) $d(u) = d(x) = 3, d(v) = d(y) = 2, l_2 = l_2^1 = 1, a_2 = a_2^1 + a_2^2 = 0$;
(5) $d(u) = d(y) = 2, d(x) = d(v) = 3, l_2 = l_2^1 = 1, a_2 = a_2^1 + a_2^2 = 0$;
(6) $d(u) = d(y) = d(v) = 3, d(x) = 2, l_2 = l_2^1 = 1, a_2 = a_2^1 + a_2^2 = 2$;
(7) $d(u) = d(y) = 3, d(v) = d(x) = 2, l_2 = l_2^1 = 1, a_2 = a_2^1 + a_2^2 = 0$;
(8) $d(u) = d(v) = d(y) = d(x) = 3, l_2 = l_2^1 = 2, a_2^1 \geq 0, a_2 = a_2^1 = 1$.

By Corollary 2.17 and Lemma 2.20, we can determine the second minimum Sombor index in $\mathcal{FC}_h$.

Theorem 2.21. *Let $F \in \mathcal{FC}_h \setminus \{E_h\}$. Then*
(i) *if h is even, then $SO(F) \geq (2\sqrt{13} - 5\sqrt{2})\frac{h+6}{2} + 13\sqrt{2}h + 8\sqrt{2}$, with equality if and only if the same with case* (i) *of Lemma 2.20.*
(ii) *if h is odd, then $SO(F) \geq (2\sqrt{13} - 5\sqrt{2})\frac{h+5}{2} + 13\sqrt{2}h + 8\sqrt{2}$, with equality if and only if the same with case* (ii) *of Lemma 2.20.*

Our purpose for introducing Lemma 2.20 is to show that the extremal graphs exist.

3 Caterpillar trees of given degree sequence

In this section, we determine the minimum and maximum Sombor index of caterpillar trees with given degree sequence.

Definition 3.1. *Let $\pi = (d_1, d_2, \cdots, d_n)$ be a non-negative nonincreasing sequence. If there exists a graph whose degree sequence is π, the we call π is a graphical sequence.*

The caterpillar tree (also called Gutman tree) is the tree obtained from a path $P = v_1 v_2 \cdots v_l$ by connecting pendent vertices to vertices, say $v_1, v_2, \cdots, v_l$, of the path P. Let $d(v_i) = x_i + 1 \geq 2$ for $i = 1, 2, \cdots, l$. We denote the caterpillar trees of Figure 6 by $CT(x_1, x_2, \cdots, x_l)$.

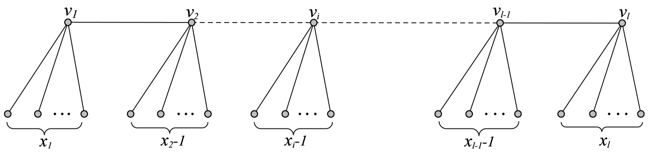

Figure 6. $CT(x_1, x_2, \cdots, x_l)$.

The following result is obvious, we omit the proof.

Lemma 3.2. *Let $x > a \geq 1, y > 0$, $f(x, y) = \sqrt{x^2 + y^2} - \sqrt{(x - a)^2 + y^2}$. Then $f(x, y)$ is strictly increasing with x, strictly decreasing with y.*

Let $\pi = (d_1, d_2, \cdots, d_n)$. Then we use $\mathcal{CT}_\pi$ to denote the set of caterpillar trees with given degree sequence π.

Lemma 3.3. *Let $d_1 > d_2 > \cdots > d_l \geq 2 > d_{l+1} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, and $(x_1, x_2, \cdots, x_l)$ be a permutation of $(d_1, d_2, \cdots, d_l)$. If the caterpillar tree $CT(x_1 - 1, x_2 - 1, \cdots, x_l - 1)$ in $\mathcal{CT}_\pi$ has the maximum Sombor index, then $\min\{x_1, x_l\} > x_i$ for $i = 2, 3, \cdots, l - 1$.*

Proof. For any $2 \leq i \leq l - 1$, we compare the sequence $(x_1, \cdots, x_{i-1}, x_i, x_{i+1}, \cdots, x_l)$ with sequence $(x_i, x_{i-1}, \cdots, x_1, x_{i+1}, \cdots, x_l)$. Since $CT(x_1 -$

$1, x_2 - 1, \cdots, x_l - 1)$ has the maximum Sombor index, then

$$\begin{aligned}
&SO(CT(x_i - 1, x_{i-1} - 1, x_{i-2} - 1, \cdots, x_1 - 1, x_{i+1} - 1, \cdots, x_l - 1)) \\
&- SO(CT(x_1 - 1, \cdots, x_{i-2} - 1, x_{i-1} - 1, x_i - 1, x_{i+1} - 1, \cdots, x_l - 1)) \\
&= (x_i - 1)\sqrt{x_i^2 + 1} + (x_1 - 2)\sqrt{x_1^2 + 1} + \sqrt{x_1^2 + x_{i+1}^2} \\
&\quad - \{(x_1 - 1)\sqrt{x_1^2 + 1} + (x_i - 2)\sqrt{x_i^2 + 1} + \sqrt{x_i^2 + x_{i+1}^2}\} \\
&= (\sqrt{x_1^2 + x_{i+1}^2} - \sqrt{x_i^2 + x_{i+1}^2}) - (\sqrt{x_1^2 + 1} - \sqrt{x_i^2 + 1}) \leq 0.
\end{aligned}$$

Since $x_{i+1} \geq 2$, then by Lemma 3.2, we have $x_1 > x_i$. Similarly, we have $x_l > x_i$. Thus $\min\{x_1, x_l\} > x_i$ for $i = 2, 3, \cdots, l - 1$. ■

Lemma 3.4. *Let $d_1 > d_2 > \cdots > d_l \geq 2 > d_{l+1} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, and $(x_1, x_2, \cdots, x_l)$ be a permutation of $(d_1, d_2, \cdots, d_l)$. If the caterpillar tree $CT(x_1-1, x_2-1, \cdots, x_l-1)$ in $\mathcal{CT}_\pi$ has the maximum Sombor index, then $x_i < x_j \Leftrightarrow x_{i-1} > x_{j+1}$ for $2 \leq i < j \leq l - 1$.*

Proof. For any $2 \leq i < j \leq l - 1$, we compare the sequence $(x_1, \cdots, x_{i-1}, x_i, \cdots, x_{j-1}, x_j, x_{j+1}, \cdots, x_l)$ with the sequence $(x_1, \ldots, x_{i-1}, x_j, x_{j-1}, \ldots, x_i, x_{j+1}, \ldots, x_l)$. Since $CT(x_1 - 1, x_2 - 1, \ldots, x_l - 1)$ has the maximum Sombor index, then
$SO(CT(x_1 - 1, \cdots, x_{i-1} - 1, x_j - 1, x_{j-1} - 1, \cdots, x_i - 1, x_{j+1} - 1, \cdots, x_l - 1)) - SO(CT(x_1 - 1, \cdots, x_{i-1} - 1, x_i - 1, \cdots, x_{j-1} - 1, x_j - 1, x_{j+1} - 1, \cdots, x_l - 1)) = (\sqrt{x_{i-1}^2 + x_j^2} - \sqrt{x_{j+1}^2 + x_j^2}) - (\sqrt{x_{i-1}^2 + x_i^2} - \sqrt{x_{j+1}^2 + x_i^2}) \leq 0$.

Then by Lemma 3.2, we have $x_i < x_j \Leftrightarrow x_{i-1} > x_{j+1}$ for $2 \leq i < j \leq l - 1$. ■

Example 3.5. *Let $d_1 > d_2 > \cdots > d_9 \geq 2 > d_{10} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, and $(x_1, x_2, \cdots, x_9)$ be a permutation of $(d_1, d_2, \cdots, d_9)$. If the caterpillar tree $CT(x_1-1, x_2-1, \cdots, x_9-1)$ in $\mathcal{CT}_\pi$ has the maximum Sombor index, then $(x_1, x_2, \cdots, x_9) = (d_1, d_9, d_3, d_7, d_5, d_6, d_4, d_8, d_2)$ or $(d_2, d_8, d_4, d_6, d_5, d_7, d_3, d_9, d_1)$.*

Proof. By Lemma 3.3, we have $\min\{x_1, x_9\} > x_i$ for $i = 2, 3, \cdots, 8$. Without loss of generality, we suppose $x_1 > x_9$, thus $x_1 = d_1, x_9 = d_2$.

Since $x_1 > x_9$, then by Lemma 3.4, we have $x_2 < x_8$. Since $x_i < x_9$ for $i = 2, 3, \cdots, 6$, then by Lemma 3.4, we have $x_8 < x_j$ for $j = 3, 4, \cdots, 7$. Thus $x_2 = d_9, x_8 = d_8$.

Since $x_2 < x_8$, then by Lemma 3.4, we have $x_3 > x_7$. Since $x_8 < x_i$ for $i = 3, 4, 5$, then by Lemma 3.4, we have $x_7 > x_j$ for $j = 4, 5, 6$. Thus $x_3 = d_3, x_7 = d_4$.

Since $x_3 > x_7$, then by Lemma 3.4, we have $x_4 < x_6$. Since $x_4 < x_7$, then by Lemma 3.4, we have $x_5 > x_6$. Thus $x_4 = d_7, x_6 = d_6, x_5 = d_5$.

In summary, we have $(x_1, x_2, \cdots, x_9) = (d_1, d_9, d_3, d_7, d_5, d_6, d_4, d_8, d_2)$.

If $x_1 < x_9$, similarly, we have $(x_1, x_2, \cdots, x_9) = (d_2, d_8, d_4, d_6, d_5, d_7, d_3, d_9, d_1)$. ■

Due to symmetry in caterpillar trees, we always suppose $x_1 > x_l$ in the rest of this paper. Using the conclusions of Lemmas 3.3 and 3.4 repeatedly, we have

Theorem 3.6. *Let $d_1 > d_2 > \cdots > d_l \geq 2 > d_{l+1} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, $(x_1, x_2, \cdots, x_l)$ be a permutation of $(d_1, d_2, \cdots, d_l)$, and the caterpillar tree $CT(x_1 - 1, x_2 - 1, \cdots, x_l - 1)$ in $\mathcal{CT}_\pi$ have the maximum Sombor index. If $l = 4m + r$ with $r = 0, 1, 2, 3$, then one of the following holds:*

(i) $(x_1, x_2, \cdots, x_{4m}) = (d_1, d_{4m}, d_3, d_{4m-2}, \cdots, d_{2m-1}, d_{2m+2}, d_{2m+1}, d_{2m}, \cdots, d_{4m-3}, d_4, d_{4m-1}, d_2)$;

(ii) $(x_1, x_2, \cdots, x_{4m+1}) = (d_1, d_{4m+1}, d_3, d_{4m-1}, \cdots, d_{2m-1}, d_{2m+3}, d_{2m+1}, d_{2m+2}, d_{2m}, \cdots, d_{4m-2}, d_4, d_{4m}, d_2)$;

(iii) $(x_1, x_2, \cdots, x_{4m+2}) = (d_1, d_{4m+2}, d_3, d_{4m}, \cdots, d_{2m-1}, d_{2m+4}, d_{2m+1}, d_{2m+2}, d_{2m+3}, d_{2m}, \cdots, d_{4m-1}, d_4, d_{4m+1}, d_2)$;

(iv) $(x_1, x_2, \cdots, x_{4m+3}) = (d_1, d_{4m+3}, d_3, d_{4m+1}, \cdots, d_{2m-1}, d_{2m+5}, d_{2m+1}, d_{2m+3}, d_{2m+2}, d_{2m+4}, d_{2m}, \cdots, d_{4m}, d_4, d_{4m+2}, d_2)$.

Proof. We only consider the case of $l = 4m$. The proof of other cases are similar to the case of $l = 4m$, so we omit it.

By Lemma 3.3, we have $\min\{x_1, x_{4m}\} > x_i$ for $i = 2, 3, \cdots, 4m - 1$. Without loss of generality, we suppose $x_1 > x_{4m}$, thus $x_1 = d_1, x_{4m} = d_2$.

Since $x_1 > x_{4m}$, then by Lemma 3.4, we have $x_2 < x_{4m-1}$. Since $x_i < x_{4m}$ for $i = 2, 3, \cdots, 4m-3$, then by Lemma 3.4, we have $x_{4m-1} < x_j$

for $j = 3, 4, \cdots, 4m-2$. Thus $x_2 = d_{4m}, x_{4m-1} = d_{4m-1}$.

Since $x_2 < x_{4m-1}$, then by Lemma 3.4, we have $x_3 > x_{4m-2}$. Since $x_{4m-1} < x_i$ for $i = 3, 4, \cdots, 4m-4$, then by Lemma 3.4, we have $x_{4m-2} > x_j$ for $j = 4, 5, \cdots, 4m-3$. Thus $x_3 = d_3, x_{4m-2} = d_4$.

Since $x_3 > x_{4m-2}$, then by Lemma 3.4, we have $x_4 < x_{4m-3}$. Since $x_i < x_{4m-2}$ for $i = 4, 5, \cdots, 4m-5$, then by Lemma 3.4, we have $x_{4m-3} < x_j$ for $j = 5, 6, \cdots, 4m-4$. Thus $x_4 = d_{4m-2}, x_{4m-3} = d_{4m-3}$.

Using Lemma 3.4 repeatedly, we obtain $(x_1, x_2, \cdots, x_{4m}) = (d_1, d_{4m}, d_3, d_{4m-2}, \cdots, d_{2m-1}, d_{2m+2}, d_{2m+1}, d_{2m}, \cdots, d_{4m-3}, d_4, d_{4m-1}, d_2)$. ■

Similar to the proof of Lemmas 3.3 and 3.4, we have

Lemma 3.7. *Let $d_1 > d_2 > \cdots > d_l \geq 2 > d_{l+1} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, and $(x_1, x_2, \cdots, x_l)$ be a permutation of $(d_1, d_2, \cdots, d_l)$. If the caterpillar tree $CT(x_1-1, x_2-1, \cdots, x_l-1)$ in $\mathcal{CT}_\pi$ has the mimimum Sombor index, then $\max\{x_1, x_l\} < x_i$ for $i = 2, 3, \cdots, l-1$.*

Lemma 3.8. *Let $d_1 > d_2 > \cdots > d_l \geq 2 > d_{l+1} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, and $(x_1, x_2, \cdots, x_l)$ be a permutation of $(d_1, d_2, \cdots, d_l)$. If the caterpillar tree $CT(x_1-1, x_2-1, \cdots, x_l-1)$ in CT_π has the minimum Sombor index, then $x_i < x_j \Leftrightarrow x_{i-1} < x_{j+1}$ for $2 \leq i < j \leq l-1$.*

Example 3.9. *Let $d_1 > d_2 > \cdots > d_9 \geq 2 > d_{10} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, and $(x_1, x_2, \cdots, x_9)$ be a permutation of $(d_1, d_2, \cdots, d_9)$. If the caterpillar tree $CT(x_1-1, x_2-1, \cdots, x_9-1)$ in $\mathcal{CT}_\pi$ has the minimum Sombor index, then $(x_1, x_2, \cdots, x_9) = (d_8, d_6, d_4, d_2, d_1, d_3, d_5, d_7, d_9)$.*

Proof. By Lemma 3.7, we have $\max\{x_1, x_9\} < x_i$ for $i = 2, 3, \cdots, 8$. Without loss of generality, we suppose $x_1 > x_9$, thus $x_1 = d_8, x_9 = d_9$.

Since $x_1 > x_9$, then by Lemma 3.8, we have $x_2 > x_8$. Since $x_1 < x_i$ for $i = 4, 5, \cdots, 8$, then by Lemma 3.8, we have $x_2 < x_j$ for $j = 3, 4, \cdots, 7$. Thus $x_2 = d_6, x_8 = d_7$.

Since $x_2 > x_8$, then by Lemma 3.8, we have $x_3 > x_7$. Since $x_2 < x_i$ for $i = 5, 6, 7$, then by Lemma 3.8, we have $x_3 < x_j$ for $j = 4, 5, 6$. Thus $x_3 = d_4, x_7 = d_5$.

Since $x_3 > x_7$, then by Lemma 3.8, we have $x_4 > x_6$. Since $x_3 < x_6$, then by Lemma 3.8, we have $x_4 < x_5$. Thus $x_4 = d_2, x_6 = d_3, x_5 = d_1$.

Combining the above arguments, we have $(x_1, x_2, \cdots, x_9) = (d_8, d_6, d_4, d_2, d_1, d_3, d_5, d_7, d_9)$. ■

Using the conclusions of Lemmas 3.7, 3.8 repeatedly, we have

Theorem 3.10. *Let $d_1 > d_2 > \cdots > d_l \geq 2 > d_{l+1} = \cdots = d_n = 1$, $\pi = (d_1, d_2, \cdots, d_n)$, $(x_1, x_2, \cdots, x_l)$ be a permutation of $(d_1, d_2, \cdots, d_l)$, and the caterpillar tree $CT(x_1 - 1, x_2 - 1, \cdots, x_l - 1)$ in $\mathcal{CT}_\pi$ have the minimum Sombor index. If $l = 2k + r$ with $r = 0, 1$, then one of the following holds:*
(i) $(x_1, x_2, \cdots, x_{2k}) = (d_{2k-1}, d_{2k-3}, d_{2k-5}, \cdots, d_5, d_3, d_1, d_2, d_4, d_6, \cdots, d_{2k-4}, d_{2k-2}, d_{2k})$.
(ii) $(x_1, x_2, \cdots, x_{2k+1}) = (d_{2k}, d_{2k-2}, d_{2k-4}, \cdots, d_6, d_4, d_2, d_1, d_3, d_5, \cdots, d_{2k-3}, d_{2k-1}, d_{2k+1})$.

Proof. We only consider the case of $l = 2k$. The proof of the other case is similar to the case of $l = 2k$, so we omit it.

By Lemma 3.7, we have $\max\{x_1, x_{2k}\} < x_i$ for $i = 2, 3, \cdots, 2k - 1$. Without loss of generality, we suppose $x_1 > x_{2k}$, thus $x_1 = d_{2k-1}, x_{2k} = d_{2k}$.

Since $x_1 > x_{2k}$, then by Lemma 3.8, we have $x_2 > x_{2k-1}$. Since $x_1 < x_i$ for $i = 4, 5, \cdots, 2k - 1$, then by Lemma 3.8, we have $x_2 < x_j$ for $j = 3, 4, \cdots, 2k - 2$. Thus $x_2 = d_{2k-3}, x_{2k-1} = d_{2k-2}$.

Since $x_2 > x_{2k-1}$, then by Lemma 3.8, we have $x_3 > x_{2k-2}$. Since $x_2 < x_i$ for $i = 5, 6, \cdots 2k - 2$, then by Lemma 3.8, we have $x_3 < x_j$ for $j = 4, 5, \cdots 2k - 3$. Thus $x_3 = d_{2k-5}, x_7 = d_{2k-4}$.

Using Lemma 3.8 repeatedly, we can finally obtain that $(x_1, x_2, \cdots, x_{2k}) = (d_{2k-1}, d_{2k-3}, d_{2k-5}, \cdots, d_5, d_3, d_1, d_2, d_4, d_6, \cdots, d_{2k-4}, d_{2k-2}, d_{2k})$. ■

4 Star-like trees

In [6], Cruz et al. determined the extremal Sombor index of trees with at most three branch vertices. In this section, we determine the first three maximum and minimum Sombor index in star-like trees.

Definition 4.1. [14] *A tree T is called a star-like tree if $diam(T) \leq 4$.*

Definition 4.2. [14] *Let $(c_1, c_2, \cdots, c_d)$ be a partition of n with $c_1 + c_2 + \cdots + c_d = n$. A star-like tree is constructed as follows:*
(i) *Let $S_1, S_2, \cdots, S_d$ be stars with $c_1 - 1, c_2 - 1, \cdots, c_d - 1$ edges, respectively, and v_i be the center of S_i for $1 \leq i \leq d$.*
(ii) *Add a vertex v_0 to the union $S_1 \cup S_2 \cup \cdots \cup S_d$ and connect v_0 to $v_1, v_2, \cdots, v_d$.*

Then we can obtain a star-like tree T with order $n+1$ and $diam(T) \leq 4$. For convenience, we denote the star-like tree T by $S(c_1, c_2, \cdots, c_d)$ (see Figure 7). Let $\mathcal{S}_{n,d} = \{S(c_1, c_2, \cdots, c_d) | c_1 + c_2 + \cdots + c_d = n\}$. Without loss of generality, we suppose that $c_1 \geq c_2 \geq \cdots \geq c_d$.

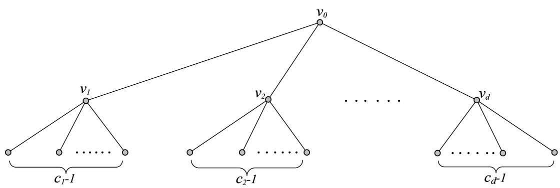

Figure 7. $S(c_1, c_2, \cdots, c_d)$.

Note that the double star tree is a special star-like tree whose diameter is 3. In [3, 15], the authors considered the extremal double star trees with respect to Sombor index. In the following, we generalize their results, determine the first three maximum and the minimum star-like trees with respect to Sombor index.

Lemma 4.3. *Let $x \geq 2$ and $g(x) = (x-1)\sqrt{(x+1)^2+1} - (x-2)\sqrt{x^2+1}$. Then $g(x)$ is a strictly increasing function with x.*

Proof. Since $((x^2-1)\sqrt{x^2+1})^2 - (x(x-2)\sqrt{(x+1)^2+1})^2 = 2x^5 + x^4 - 9x^2 + 1 > 0$ for $x \geq 2$, then $g'(x) = (\sqrt{(x+1)^2+1} - \sqrt{x^2+1}) + \frac{(x^2-1)\sqrt{x^2+1} - x(x-2)\sqrt{(x+1)^2+1}}{\sqrt{(x+1)^2+1}\sqrt{x^2+1}} > 0$ for $x \geq 2$, thus $g(x)$ is a strictly increasing function with x. ■

Since $\mathcal{S}_{n,n-2} = \{S(3,1,1,\cdots,1), S(2,2,1,1,\cdots,1)\}$, $\mathcal{S}_{n,n-3} = \{S(4,1,1,\cdots,1), S(3,2,1,1,\cdots,1), S(2,2,2,1,1\cdots,1)\}$, it is trivial when $d = n-2$ or $d = n-3$. Thus we only consider the extremal Sombor index in $\mathcal{S}_{n,d}$ with $2 \leq d \leq n-4$.

Let $S_{n,d}^0 = S(l+1, l+1, \cdots, l+1, l, l, \cdots, l)$ $(l = \lfloor \frac{n}{d} \rfloor)$, $S_{n,d}^1 = S(n-d+1, 1, 1, \cdots, 1)$, $S_{n,d}^2 = S(n-d, 2, 1, 1, \cdots, 1)$, $S_{n,d}^3 = S(n-d-1, 3, 1, 1, \cdots, 1)$. Then we have

Theorem 4.4. *Let $2 \le d \le n-4$, $T \in \mathcal{S}_{n,d} \setminus \{S_{n,d}^0, S_{n,d}^1, S_{n,d}^2, S_{n,d}^3\}$. Then $SO(S_{n,d}^0) < SO(T) < SO(S_{n,d}^3) < SO(S_{n,d}^2) < SO(S_{n,d}^1)$.*

Proof. (i) If $T_1 = S(c_1, c_2, \cdots, c_d) \in \mathcal{S}_{n,d} \setminus \{S_{n,d}^1\}$, then there exists some $2 \le t \le d$ satisfying $c_t \ge 2$. Let $i = \max\{t | c_t \ge 2\}$, and $T_2 = S(c_1 + 1, c_2, \cdots, c_{i-1}, c_i - 1, c_{i+1}, \cdots, c_d) \in \mathcal{S}_{n,d}$. By Lemmas 3.2, 4.3, we have

$$\begin{aligned}
& SO(T_2) - SO(T_1) \\
= \; & c_1\sqrt{(c_1+1)^2+1^2} - (c_1-1)\sqrt{c_1^2+1^2} + (c_i-2)\sqrt{(c_i-1)^2+1^2} \\
& -(c_i-1)\sqrt{c_i^2+1^2} + \sqrt{d^2+(c_1+1)^2} - \sqrt{d^2+c_1^2} \\
& +\sqrt{d^2+(c_i-1)^2} - \sqrt{d^2+c_i^2} \\
= \; & \{(\sqrt{(c_1+1)^2+1^2} - \sqrt{c_1^2+1^2}) - (\sqrt{c_i^2+1^2} - \sqrt{(c_i-1)^2+1^2})\} \\
& +\{(\sqrt{d^2+(c_1+1)^2} - \sqrt{d^2+c_1^2}) - (\sqrt{d^2+c_i^2} - \sqrt{d^2+(c_i-1)^2})\} \\
& +\{((c_1-1)\sqrt{(c_1+1)^2+1^2} - (c_1-2)\sqrt{c_1^2+1^2}) \\
& -((c_i-2)\sqrt{c_i^2+1^2} - (c_i-3)\sqrt{(c_i-1)^2+1^2})\} > 0.
\end{aligned}$$

Using the transformation from $S(c_1, c_2, \cdots, c_d)$ to $S(c_1+1, c_2, \cdots, c_{i-1}, c_i - 1, c_{i+1}, \cdots, c_d)$ repeatedly, we can finally obtain $S_{n,d}^1$. Thus $S_{n,d}^1$ has the maximum Sombor index.

(ii) If $T_3 = S(c_1, c_2, \cdots, c_d) \in \mathcal{S}_{n,d} \setminus \{S_{n,d}^0\}$, then there exists $c_i \ge c_j + 2$. Let $\alpha = (c_1, c_2, \cdots, c_{i-1}, c_i, c_{i+1}, \cdots, c_{j-1}, c_j, c_{j+1}, \cdots, c_d)$ and $\beta = (c_1, c_2, \cdots, c_{i-1}, c_i - 1, c_{i+1}, \cdots, c_{j-1}, c_j + 1, c_{j+1}, \cdots, c_d)$. Let the sequence after reordering the numbers in sequence β be $(c_1', c_2', \cdots, c_d')$ satisfying $c_1' \ge c_2' \ge \cdots \ge c_d'$. Let $T_4 = S(c_1', c_2', \cdots, c_d')$, then similarly we have $SO(T_4) < SO(T_3)$.

Using the transformation from $S(c_1, c_2, \cdots, c_d)$ to $S(c_1, c_2, \cdots, c_{i-1}, c_i - 1, c_{i+1}, \cdots, c_{j-1}, c_j + 1, c_{j+1}, \cdots, c_d)$ repeatedly, we can finally obtain $S_{n,d}^0$. Thus $S_{n,d}^0$ has the minimum Sombor index.

(iii) If $T_5 = S(c_1, c_2, \cdots, c_d) \in \mathcal{S}_{n,d} \backslash \{S^1_{n,d}, S^2_{n,d}\}$, then $c_2 \geq 3$ or $c_3 \geq 2$. Let $T_6 = S(c_1+1, c_2-1, c_3, \cdots, c_d) \in \mathcal{S}_{n,d}$ or $S(c_1+1, c_2, c_3-1, \cdots, c_d) \in \mathcal{S}_{n,d} \in \mathcal{S}_{n,d}$. We denote the graph obtained from reordering the sequence of graph T_6 as $T'_6 = S(c''_1, c''_2, \cdots, c''_d)$ satisfying $c''_1 \geq c''_2 \geq \cdots \geq c''_d$, then similarly we have $SO(T'_6) > SO(T_5)$.

Using the above transformation repeatedly, we can finally obtain $S^2_{n,d}$. Thus $S^2_{n,d}$ has the second maximum Sombor index.

(iv) If $T_7 = S(c_1, c_2, \cdots, c_d) \in \mathcal{S}_{n,d} \backslash \{S^1_{n,d}, S^2_{n,d}, S^3_{n,d}\}$, then $c_2 = 2, c_3 \geq 2$ or $c_2 = 3, c_3 \geq 2$ or $c_2 \geq 4$. Similarly, using the transformation of case (i), we can find T_8 with $SO(T_8) > SO(T_7)$.

Using the transformation of case (i) repeatedly, we can finally obtain $S^3_{n,d}$. Thus $S^3_{n,d}$ has the third maximum Sombor index. ■

Note that the star-like trees we considered here are different from the of star-like trees of [4]. In [4], Betancur et al. determined the extremal vertex-degree-based topological indices over starlike trees. It is easy to verify that the conclusions of [4] are suitable for Sombor index.

5 Conclusions

A bivariable function $f(x, y)$ defined on $\mathbb{N} \times \mathbb{N}$ is called de-escalating if $f(a, b) + f(c, d) \leq f(c, b) + f(a, d)$ for any $a \geq c$ and $b \geq d$.

Definition 5.1. [23] **(Greedy Tree)** *With given vertex degrees, the greedy tree is achieved through the following* ***greedy algorithm****:*

(i) Label the vertex with the largest degree as v (the root);

(ii) Label the neighbors of v as $v_1, v_2, \cdots$, assign the largest degrees available to them such that degree $d(v_1) \geq d(v_2) \geq \cdots$;

(iii) Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \cdots$, such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \cdots$, then do the same for $v_2, v_3, \cdots$;

(iv) Repeat (iii) for all the newly labled vertices. Always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

By Lemma 3.2, it is easy to know that $\sqrt{x^2+y^2}$ is de-escalating. Thus by the conclusions of [27], we have

Theorem 5.2. *The Sombor index is minimized by the greedy tree among trees with given degree sequence.*

A nonincreasing sequence of nonnegative integer π is called a unicyclic degree sequence (denoted by $\mathcal{U}_\pi$) if there exists a unicyclic graph having π as its vertex sequence [26]. Since $\sqrt{x^2+y^2}$ is de-escalating, then by the conclusions of [26], we have

Theorem 5.3. *Given a unicyclic degree sequence π, the Sombor index is minimized by $\mathcal{U}_\pi^*$ (see [26] for the definition) in $\mathcal{U}_\pi$.*

In [16], authors calculate the (reduced) Sombor index of a set of benzenoid hydrocarbons (see Table 1 of [16]). The Sombor index (resp. reduced Sombor index) of the 4-th and 12-th benzenoid hydrocarbons should be 72.6850 (resp. 43.3444) and 98.2809 (resp. 60.5444). The correlation coefficient R between boiling points and Sombor indices (resp. reduced Sombor indices) is about 0.9929 (resp. 0.9892).

In [1], authors calculate the Sombor index of a set of octane isomers (see Table 12 of [1]). The Sombor index of the 13-th octane isomer of [1] should be 24.2477. The absolute value of correlation coefficient $|R|$ between acentric factor (resp. entropy, enthalpy of vaporization, standard enthalpy of vaporization) and Sombor indices is about 0.9594 (resp. 0.9465, 0.9031, 0.9469).

In this paper, we characterize some extremal chemical graphs and trees with respect to Sombor index. In the future, we will consider more chemical and mathematical properties of the Sombor index.

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