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QUASI-TREE GRAPHS WITH THE MINIMAL SOMBOR INDICES

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Abstract. The Sombor index $SO(G)$ of a graph G is the sum of the edge weights $\sqrt{d_G^2(u)+d_G^2(v)}$ of all edges uv of G, where $d_G(u)$ denotes the degree of the vertex u in G. A connected graph $G=(V,E)$ is called a quasi-tree if there exists $u\in V(G)$ such that $G-u$ is a tree. Denote $\mathscr{Q}(n,k)=\{G\colon G$ is a quasi-tree graph of order n with $G-u$ being a tree and $d_G(u)=k\}$. We determined the minimum and the second minimum Sombor indices of all quasi-trees in $\mathscr{Q}(n,k)$. Furthermore, we characterized the corresponding extremal graphs, respectively.

Keywords: Sombor index; quasi-tree; tree

MSC 2020: 05C07, 05C09, 05C35

1. Introduction

We first introduce some terminology. Let $G=(V(G),E(G))$ be a simple undirected graph of order n. Denote $V(G)=\{v_1,v_2,\ldots,v_n\}$. For $v_i\in V(G)$, we use $N_G(v_i)$ to denote the *set of neighbors* of v_i in G, and the *degree* of v_i, written by $d_G(v_i)$ or d_i, is the number of edges incident with v_i. An *i-vertex* is a vertex of degree i. Let $V_i(G)$ be the set of all i-vertices in G. For a subgraph H of G, let $N_H(v_i)=N_G(v_i)\cap V(H)$ and $d_H(v_i)=|N_H(v_i)|$ for $v_i\in V(G)$. To *subdivide* an edge e in G is to delete e, add a new vertex x, and join x to the ends of e. We will use $G-v_i$ or $G-v_iv_j$ to denote the graph that arises from G by deleting the vertex $v_i\in V(G)$ or the edge $v_iv_j\in E(G)$. Similarly, $G+v_iv_j$ is a graph that arises from G by adding an edge $v_iv_j\notin E(G)$.

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A *tree* is a connected acyclic graph. If there exists a vertex $v_i \in V(G)$ such that $G - v_i$ is a tree, then G is called a *quasi-tree*. Let $\mathscr{Q}(n,k) = \{G\colon G$ is a quasi-tree graph of order n with $G - v_i$ being a tree and $d_i = k\}$. If $k = 1$, then $\mathscr{Q}(n,1)$ is the set of all trees of order n.

By P_n/C_n, we denote a *path/cycle* of order n. Let T be a tree, and let $P_{l+1} = v_1v_2\dots v_{l+1}$ $(l \geqslant 1)$ be a path of T with $d_T(v_1) = 1$, $d_T(v_2) = \dots = d_T(v_l) = 2$ and $d_T(v_{l+1}) \geqslant 3$. Then we call P_{l+1} a *pendant chain* of T and we also call that l the length of the pendant chain P_{l+1}. For a tree T, if v is a vertex of T with exactly $d_T(v) - 1 \geqslant 2$ pendant chains, then the subgraph induced by the union of vertex sets of its $d_T(v) - 1$ pendant chains is said to be a *pendant spider of T at v*. If T is not a path, then T has some pendant spiders.

Proposition 1.1 ([1]). *For a tree T we have $d_T(v) \leqslant |V_1(T)|$ for any $v \in V(T)$. Moreover, $|V_1(T)| = 2$ if and only if $T \cong P_n$.*

A vertex-degree-based-topological index was recently introduced by Gutman (see [8]), called the *Sombor index*, and defined for a graph G as

$$SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}.$$

Since then, the problem concerning graphs with the maximal or minimal Sombor index of a given class of graphs has been studied extensively, and numerous results have been obtained, see [2]–[14]. For a comprehensive survey and more details on Sombor index, we refer the reader to [10] and references therein.

In [6], [8], Gutman presented some properties of the Sombor index and characterized the maximal and minimal graphs with respect to the Sombor indices. Zhou et al. in [14] obtained the maximum and minimum Sombor indices of trees and unicyclic graphs, respectively. Recently, Das and Gutman in [6] gave the maximum and minimum Sombor indices of all quasi-tree graphs, and also obtained the second maximum and minimum extremal trees, respectively. In this paper, we determined the minimum and the second minimun Sombor indices of all quasi-tree graphs in the set $\mathscr{Q}(n,k)$.

2. Preliminaries

In this section, we first define some quasi-tree graphs (see Figure 1) in order to formulate our results.

A *fan* F_t is a graph obtained from a path P_t and an isolated vertex v by adding edges joining v to every vertex of P_t.

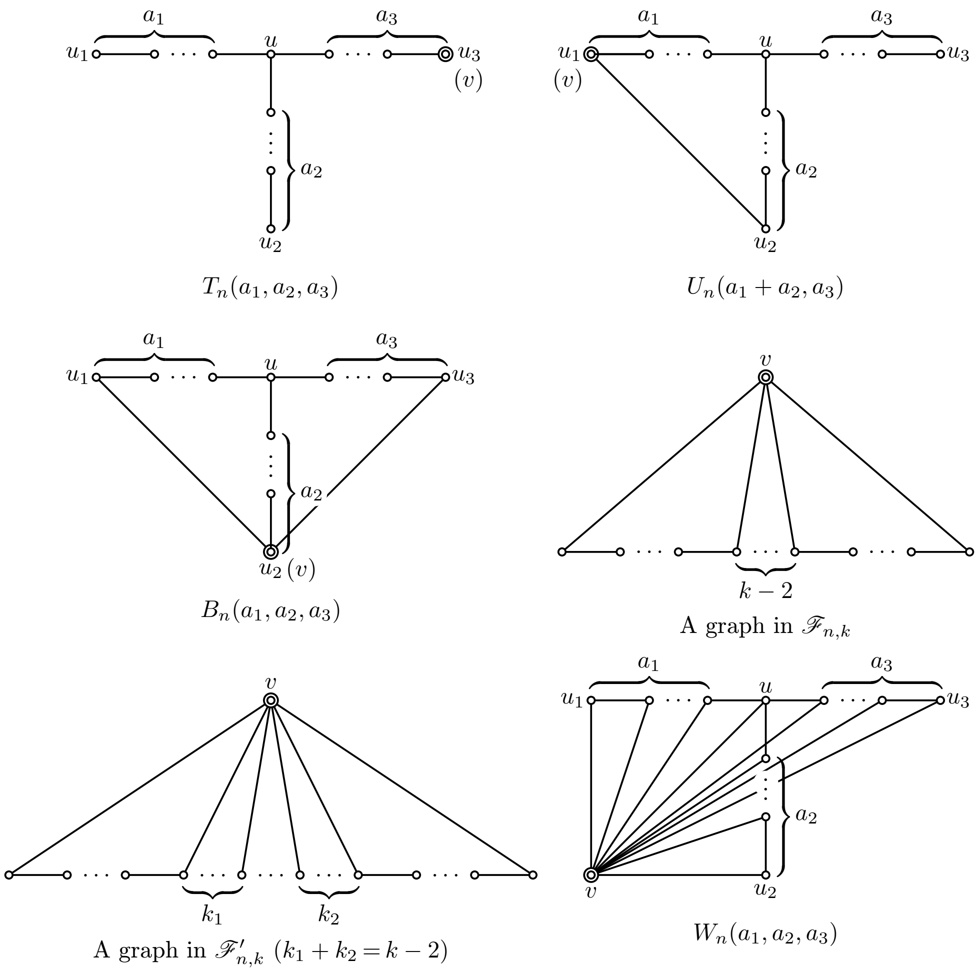

Figure 1. Some quasi-tree graphs in $\mathscr{Q}(n, k)$.

Let $\mathscr{F}_{n,1} = \{P_n\}$, $\mathscr{F}_{n,n-1} = \{F_{n-1}\}$, and $\mathscr{F}_{n,k}$ $(2 \leqslant k \leqslant n-2)$ be a family of graphs of order n obtained from F_k by a sequence of edge subdivisions, where the subdivided edges are incident with some 2-vertices.

A *T-shaped tree* is a tree with exactly one of its vertices being 3-vertex. Let $T_n(a_1, a_2, a_3)$ be a T-shape tree of order n such that $T_n(a_1, a_2, a_3) - u = P_{a_1} \cup P_{a_2} \cup P_{a_3}$, where u is the 3-vertex. Let $u_i \in V_1(T_n(a_1, a_2, a_3)) \cap V(P_{a_i})$ for $i = 1, 2, 3$. Denote

$$\begin{aligned} W_n(a_1, a_2, a_3) &:= K_1 \vee T_{n-1}(a_1, a_2, a_3), \\ U_n(a_1, a_2, a_3) &:= T_n(a_1, a_2, a_3) + u_1u_2, \\ B_n(a_1, a_2, a_3) &:= T_n(a_1, a_2, a_3) + \{u_1u_2, u_2u_3\}. \end{aligned}$$

Let $F_{n,k}^s$ be a graph of order n obtained from $F_{n-s,k} \in \mathscr{F}_{n-s,k}$ by subdividng an edge of $E(F_{n-s,k})$, whose ends are 3-vertices, s times. Denote

$$\begin{aligned}
\mathscr{F}'_{n,1} &:= \{T_n(a_1,a_2,a_3)\colon \min\{a_1,a_2,a_3\} \geqslant 2\},\\
\mathscr{F}'_{n,2} &:= \{U_n(a_1,a_2,a_3)\colon a_3 \geqslant 2\},\\
\mathscr{F}'_{n,3} &:= \{B_n(a_1,a_2,a_3)\colon a_2 \geqslant 2\},\\
\mathscr{F}'_{n,k} &:= \{F_{n,k}^s\colon 1 \leqslant s \leqslant n-1-k\} \quad \text{for } 4 \leqslant k \leqslant n-2,\\
\mathscr{F}'_{n,n-1} &:= \{W_n(a_1,a_2,a_3)\colon \min\{a_1,a_2,a_3\} \geqslant 2\}.
\end{aligned}$$

By a straightforward calculation, we give the following proposition.

Proposition 2.1.

(i) *If* $\min\{a_1,a_2,a_3\} \geqslant 2$, *then* $SO(T_n(a_1,a_2,a_3)) < SO(T_n(a'_1,a'_2,1))$, *and* $SO(W_n(a_1,a_2,a_3)) < SO(W_n(a'_1,a'_2,1))$, *where* $a'_1,a'_2 \geqslant 1$ *and* $a'_1+a'_2 = a_1+a_2+a_3-1$.

(ii) *If* $a_3 \geqslant 2$, *then* $SO(U_n(a_1,a_2,a_3)) < SO(U_n(a'_1,a'_2,1))$, *where* $a'_1+a'_2 = a_1+a_2+a_3-1$.

Next, we develop some useful tools in the following lemmas that will be used in the proof of main results.

Lemma 2.1. *Let* $g^{(r)}(x,y) = \sqrt{x^2+y^2} - \sqrt{x^2+(y-r)^2}$ *with* $2y > r > 0$. *Then* $g^{(r)}(x,y)$ *is monotonic decreasing in* $x \geqslant 1$ *and monotonic increasing in* $y \geqslant 1$. *Moreover,* $g^{(r)}(x,y)$ *is monotonic increasing in* $r < y$.

P r o o f. Since $2y > r > 0$, $y^2 > (y-r)^2$, we have

$$\begin{aligned}
\frac{\partial g^{(r)}(x,y)}{\partial x} &= \frac{x}{\sqrt{x^2+y^2}} - \frac{x}{\sqrt{x^2+(y-r)^2}} < 0,\\
\frac{\partial g^{(r)}(x,y)}{\partial y} &= \frac{y}{\sqrt{x^2+y^2}} - \frac{y-r}{\sqrt{x^2+(y-r)^2}} = \frac{1}{\sqrt{1+x^2/y^2}} - \frac{1}{\sqrt{1+x^2/(y-r)^2}} > 0,\\
\frac{\partial g^{(r)}(x,y)}{\partial r} &= \frac{y-r}{\sqrt{x^2+(y-r)^2}} > 0.
\end{aligned}$$

Thus, the function $g^{(r)}(x,y)$ is monotonic decreasing in $x \geqslant 1$, monotonic increasing in $y \geqslant 1$ and monotonic increasing in $r < y$. $\square$

Lemma 2.2. *Let* G *be a graph and let* $uv, xy \in E(G)$ *with* $d_G(u) \geqslant d_G(x)$ *and* $d_G(v) \leqslant d_G(y)$. *Set* $G' = G - \{uv,xy\} + \{uy,xv\}$. *Then*

$$SO(G') \leqslant SO(G).$$

Moreover, the equality holds if and only if $d_G(u) = d_G(x)$ *or* $d_G(v) = d_G(y)$.

Proof. Note that $V(G) = V(G')$ and $d_G(w) = d_{G'}(w)$ for all $w \in V(G)$. Then

$$\begin{aligned} SO(G') - SO(G) = {} & \sqrt{d_G^2(x) + d_G^2(v)} + \sqrt{d_G^2(u) + d_G^2(y)} \\ & - \sqrt{d_G^2(x) + d_G^2(y)} - \sqrt{d_G^2(u) + d_G^2(v)}. \end{aligned}$$

Clearly, $SO(G') = SO(G)$ if and only if $d_G(u) = d_G(x)$ or $d_G(v) = d_G(y)$. So we can assume that $d_G(v) < d_G(y)$ and $d_G(u) > d_G(x)$. Let $r := d_G(y) - d_G(v) > 0$, then by Lemma 2.1,

$$SO(G') - SO(G) = g^{(r)}(d_G(u), d_G(y)) - g^{(r)}(d_G(x), d_G(y)) < 0$$

as $d_G(u) > d_G(x)$. Therefore, the proof of Lemma 2.2 is complete. □

3. Main results

In this section, we will determine the minimum and the second minimum Sombor indices of all quasi-tree graphs in $\mathscr{Q}(n,k)$, and characterize corresponding extremal graphs.

Denote $\varphi(n,1) := 2\sqrt{5} + (n-3)\sqrt{8}$, $\varphi(n,k) := (k-2)\sqrt{k^2+9} + 2\sqrt{k^2+4} + (k-3)\sqrt{18} + (n-k-1)\sqrt{8} + 2\sqrt{13}$ for $2 \leqslant k \leqslant n-1$.

Theorem 3.1. *Let $G \in \mathscr{Q}(n,k)$ with $1 \leqslant k \leqslant n-1$. Then*

$$SO(G) \geqslant \varphi(n,k) \tag{1}$$

with equality in (1) *if and only if $G \in \mathscr{F}_{n,k}$.*

Proof. First we note that if $G \in \mathscr{F}_{n,k}$, then $SO(G) = \varphi(n,k)$. Now we will show that if $G \in \mathscr{Q}(n,k)$, then $SO(G) \geqslant \varphi(n,k)$ and the equality holds only if $G \in \mathscr{F}_{n,k}$.

Choose $G \in \mathscr{Q}(n,k)$ such that $SO(G)$ is as small as possible. Assume that $G - v_n$ is a tree. Denote $T := G - v_n$. Let $V'(T) = \{v_i \in V(T) \colon d_i \geqslant 3\}$.

Claim 3.1. *If $\delta(G) = 1$, then $\Delta(G) \leqslant 2$.*

Proof of Claim 3.1. Let $v_1 \in V(G)$ with $d_1 = 1$. If $\Delta(G) \geqslant 3$, then $V'(T) \neq \emptyset$. Moreover, we can assume that $v_1 \in V_1(T)$ and $v_1 v_n \notin E(G)$. Choose $v_i \in V'(T)$ such that $d_T(v_i, v_1)$ is as small as possible. Then $d_i \geqslant 3$, furthermore, $(d_i-1)^2+4 < d_i^2+1$. Let $P := v_1 v_2 \ldots v_i$ be the only (v_1, v_i)-path in T. We consider two cases.

Case 1: $v_nv_i \in E(G)$. In this case, we set $G' = G - v_nv_i + v_1v_n$. Then $G' \in \mathscr{Q}(n,k)$. If $v_1v_i \in E(G)$, then

$$\begin{aligned} SO(G') - SO(G) = & \sum_{v_j \in N_G(v_i) \setminus \{v_n, v_1\}} \left(\sqrt{(d_i-1)^2 + d_j^2} - \sqrt{d_i^2 + d_j^2} \right) \\ & + \sqrt{(d_i-1)^2 + 4} - \sqrt{d_i^2 + 1} + \sqrt{k^2 + 4} - \sqrt{k^2 + d_i^2} \\ < & \; 0, \end{aligned}$$

a contradiction.

If $v_1v_i \notin E(G)$, then $d_2 = \ldots = d_{i-1} = 2$ by the choice of v_i. By Lemma 2.1,

$$\begin{aligned} SO(G') - SO(G) = & \sum_{v_j \in N_G(v_i) \setminus \{v_{i-1}, v_n\}} \left(\sqrt{(d_i-1)^2 + d_j^2} - \sqrt{d_i^2 + d_j^2} \right) \\ & + \sqrt{k^2 + 4} + \sqrt{2^2 + 2^2} - \sqrt{1^2 + 2^2} \\ & + \sqrt{(d_i-1)^2 + 2^2} - \sqrt{k^2 + d_i^2} - \sqrt{d_i^2 + 2^2} \\ < & \sqrt{2^2 + 2^2} - \sqrt{1^2 + 2^2} + \sqrt{(d_i-1)^2 + 2^2} - \sqrt{d_i^2 + 2^2} \\ = & \; g^{(1)}(2,2) - g^{(1)}(2,d_i) < 0, \end{aligned}$$

a contradiction.

Case 2: $v_nv_i \notin E(G)$. In this case, let $v_{i'} \in N_G(v_i) \setminus V(P)$, and let $G'' = G - v_iv_{i'} + v_1v_{i'}$. Then $G'' \in \mathscr{Q}(n,k)$. If $v_1v_i \in E(G)$, then

$$\begin{aligned} SO(G'') - SO(G) = & \sum_{v_j \in N_G(v_i) \setminus \{v_i'\}} \left(\sqrt{(d_i-1)^2 + d_j^2} - \sqrt{d_i^2 + d_j^2} \right) + \sqrt{d_{i'}^2 + 2^2} \\ & - \sqrt{d_{i'}^2 + d_i^2} + \sqrt{(d_i-1)^2 + 4} - \sqrt{d_i^2 + 1} \\ < & \; 0, \end{aligned}$$

a contradiction. If $v_1v_i \notin E(G)$, then $d_2 = \ldots = d_{i-1} = 2$ by the choice of v_i. By Lemma 2.1,

$$\begin{aligned} SO(G'') - SO(G) = & \sum_{v_j \in N_G(v_i) \setminus \{v_{i-1}, v_i'\}} \left(\sqrt{(d_i-1)^2 + d_j^2} - \sqrt{d_i^2 + d_j^2} \right) \\ & + \sqrt{d_{i'}^2 + 2^2} - \sqrt{d_{i'}^2 + d_i^2} + \sqrt{2^2 + 2^2} \\ & - \sqrt{1^2 + 2^2} + \sqrt{(d_i-1)^2 + 2^2} - \sqrt{d_i^2 + 2^2} \\ < & \sqrt{2^2 + 2^2} - \sqrt{1^2 + 2^2} + \sqrt{(d_i-1)^2 + 2^2} - \sqrt{d_i^2 + 2^2} \\ = & \; g^{(1)}(2,2) - g^{(1)}(2,d_i) < 0, \end{aligned}$$

a contradiction. □

If $k = 1$, then $\delta(G) = 1$ clearly, and thus $G \cong P_n$ by Claim 3.1, the assertion holds for $k = 1$. So, in the following, we assume that $k \geqslant 2$.

Claim 3.2. *If $k \geqslant 2$, then $\delta(G) = 2$.*

P r o o f of Claim 3.2. If $\delta(G) = 1$, then by Claim 3.1, $\Delta(G) \leqslant 2$, which implies $\Delta(T) = 2$, that is, T is a path. Since $k \geqslant 2$, we have $v_n v_i \in E(G)$ for some $v_i \in V(T) \setminus V_1(T)$. Thus, $d_i = 3$, a contradiction with $\Delta(G) \leqslant 2$. □

If $k = 2$, then $G \cong C_n$ by Claim 3.2. Thus, the assertion holds for $k = 2$.

Claim 3.3. *If $k \geqslant 3$, then $T \cong P_{n-1}$.*

P r o o f of Claim 3.3. If $T \ncong P_{n-1}$, then there exists v_i such that $d_T(v_i) \geqslant 3$ and $|V_1(T)| \geqslant 3$. Choose $v_i \in V'(T)$ such that T has a pendant spider at v_i. Let $P^1 = v_{a_1} v_{a_2} \ldots v_{a_s} v_i$ and $P^2 = v_{b_1} v_{b_2} \ldots v_{b_t} v_i$ be two pendant chains with $d_T(v_{a_1}) = d_T(v_{b_1}) = 1$, where $s, t \geqslant 1$, and let $v_{i+1} \in N_G(v_i) \setminus \{v_{a_s}, v_{b_t}\}$. Then $d_T(v_{a_l}) = d_T(v_{b_j}) = 2$ for $2 \leqslant l \leqslant s$ and $2 \leqslant j \leqslant t$. Furthermore, $d_{a_1} = d_{b_1} = 2$ and $d_{a_l}, d_{b_j} \leqslant 3$ for all $2 \leqslant l \leqslant s$ and $2 \leqslant j \leqslant t$.

By Proposition 1.1, $k \geqslant |V_1(T)| \geqslant d_T(v_l)$ for any $v_l \in V(T)$. Moreover, we will show that if $d_i = 3$, then $k > d_{i+1}$. If $d_{i+1} \leqslant 2$, then $k \geqslant 3 > 2 \geqslant d_{i+1}$. So we can assume $d_{i+1} \geqslant 3$. If $v_n v_{i+1} \in E(G)$, then $k \geqslant 1 + |V_1(T)| \geqslant 1 + d_{i+1}$, and if $v_n v_{i+1} \notin E(G)$, then $k \geqslant |V_1(T)| \geqslant d_i + d_{i+1} - 2 > d_{i+1}$ as $|V_1(T^j)| \geqslant d_{T^j}(v_j) = d_T(v_j) - 1$ by Proposition 1.1, where T^j ($j \in \{i, i+1\}$) is the component containing v_j of $T - v_i v_{i+1}$.

We set $G^* = G - v_i v_{b_t} + v_{a_1} v_{b_t}$, then $G^* \in \mathscr{Q}(n,k)$. Then we consider two cases.

Case 1: $s = 1$, i.e., $v_{a_1} v_i \in E(G)$. If $d_i = 3$, then $k > d_{i+1}$, and by Lemma 2.1,

$$\begin{aligned} SO(G^*) - SO(G) &= \sqrt{d_{i+1}^2 + 4} - \sqrt{d_{i+1}^2 + 9} + \sqrt{k^2 + 9} - \sqrt{k^2 + 4} \\ &= g^{(1)}(k, 3) - g^{(1)}(d_{i+1}, 3) < 0, \end{aligned}$$

a contradiction.

If $d_i \geqslant 4$, we have $(d_i - 1)^2 + 9 < d_i^2 + 4$, then by Lemma 2.1,

$$\begin{aligned} SO(G^*) - SO(G) = &\sum_{v_j \in N_G(v_i) \setminus \{v_{b_t}\}} \Big(\sqrt{(d_i - 1)^2 + d_j^2} - \sqrt{d_i^2 + d_j^2}\Big) \\ &+ \sqrt{k^2 + 3^2} - \sqrt{k^2 + 2^2} + \sqrt{d_{b_t}^2 + 3^2} - \sqrt{d_{b_t}^2 + d_i^2} \\ &+ \sqrt{(d_i - 1)^2 + 3^2} - \sqrt{d_i^2 + 2^2} \\ < &\sqrt{k^2 + 3^2} - \sqrt{k^2 + 2^2} + \sqrt{d_{b_t}^2 + 3^2} - \sqrt{d_{b_t}^2 + d_i^2} \\ = &\, g^{(1)}(k, 3) - g^{(d_i - 3)}(d_{b_t}, d_i) \leqslant g^{(1)}(k, 3) - g^{(1)}(d_{b_t}, d_i) \leqslant 0 \end{aligned}$$

as $d_i \geqslant 3$ and $k \geqslant d_{b_t}$, a contradiction.

Case 2: $v_1v_i \notin E(G)$ $(s \geqslant 2)$. In this case, $d_{a_2} \leqslant 3$ and $k \geqslant |V_1(T)| \geqslant d_T(v_i)$. If $d_i = 3$, then $v_nv_i \notin E(G)$ as $d_T(v_i) \geqslant 3$. Set $G^{**} = G - \{v_nv_{a_1}, v_iv_{b_t}\} + \{v_nv_i, v_{a_1}v_{b_t}\}$, then $G^{**} \in \mathscr{Q}(n,k)$. By Lemma 2.2, $SO(G^{**}) < SO(G)$, a contradiction.

So we may assume that $d_i \geqslant 4$, then $k \geqslant |V_1(T)| \geqslant d_T(v_i) \geqslant 3 \geqslant d_{a_2}$, and by Lemma 2.1, we have

$$\begin{aligned} SO(G^*) - SO(G) = & \sum_{v_j \in N_G(v_i)\setminus\{v_{b_t}\}} \left(\sqrt{(d_i-1)^2+d_j^2} - \sqrt{d_i^2+d_j^2}\right) \\ & + \sqrt{k^2+3^2} - \sqrt{k^2+2^2} + \sqrt{d_{a_2}^2+3^2} - \sqrt{d_{a_2}^2+2^2} \\ & + \sqrt{d_{b_t}^2+3^2} - \sqrt{d_{b_t}^2+d_i^2} + \sqrt{(d_i^2-1)^2+d_{a_s}^2} - \sqrt{d_i^2+d_{s_s}^2} \\ < & \sqrt{k^2+3^2} - \sqrt{k^2+2^2} + \sqrt{d_{a_2}^2+3^2} - \sqrt{d_{a_2}^2+2^2} \\ = & \, g^{(1)}(k,3) - g^{(1)}(d_{a_2},3) \leqslant 0, \end{aligned}$$

a contradiction. □

By Claim 3.3, we let $T = v_1v_2\dots v_{n-1}$. Denote $X = \{v_l \in V(T) \colon d_l \geqslant 3\}$.

Claim 3.4. *If $k \geqslant 3$, then $G[X]$ is connected.*

Proof of Claim 3.4. Suppose $G[X]$ is disconnected. Then $G[X]$ contains at least two components. Let $P' = v_iv_{i+1}\dots v_j$ and $P'' = v_av_{a+1}\dots v_b$ be the two components of $G[X]$ with $j < a-1$. Then $d_{i-1} = d_{a-1} = 2$. Set $G^* = G - \{v_{i-1}v_i, v_{a-1}v_a\} + \{v_iv_a, v_{i-1}v_{a-1}\}$. Then $G^* \in \mathscr{Q}(n,k)$. Note that $d_i = d_a = 3$, and thus, by Lemma 2.2, $SO(G^*) < SO(G)$, a contradiction. □

By Claims 3.3 and 3.4, $G \in \mathscr{F}_{n,k}$. Therefore, the proof of Theorem 3.1 is complete. □

Denote $\varphi'(n,1) = (n-7)\sqrt{8} + 3\sqrt{13} + 3\sqrt{5}$, $\varphi'(n,2) = (n-4)\sqrt{8} + 3\sqrt{13} + \sqrt{5}$ and $\varphi'(n,3) = (n-5)\sqrt{8} + 6\sqrt{13}$. For $4 \leqslant k \leqslant n-2$, let $\varphi'(n,k) = (k-2)\sqrt{k^2+9} + 2\sqrt{k^2+4} + (k-4)\sqrt{18} + (n-k-2)\sqrt{8} + 4\sqrt{13}$. Let $\varphi'(n,n-1) = (n-5)\sqrt{(n-1)^2+9} + 3\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+16} + (n-8)\sqrt{18} + 3\sqrt{13} + 15$.

Theorem 3.2. *Let $G \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$ with $1 \leqslant k \leqslant n-1$. Then*

$$SO(G) \geqslant \varphi'(n,k).$$

Moreover, the equality holds if and only if $G \in \mathscr{F}'_{n,k}$.

Proof. First we note that if $G \in \mathscr{F}'_{n,k}$, then $SO(G) = \varphi'(n,k)$. Now we will show that if $G \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$, then $SO(G) \geqslant \varphi'(n,k)$ and the equality holds only if $G \in \mathscr{F}'_{n,k}$.

Choose $G \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$ such that $SO(G)$ is as small as possible. Without loss of generality, assume that $G - v_n$ is a tree. Denote $T = G - v_n$. We consider the following two cases.

Case 1: T is a path. In this case, $k \leqslant n-2$ as $G \notin \mathscr{F}_{n,k}$. Let $T := v_1v_2\ldots v_{n-1}$ and $N_G(v_n) = \{v_{i_1}, v_{i_2}, \ldots, v_{i_k}\}$ with $i_1 < i_2 < \ldots < i_k$ and $i_1 \geqslant n - i_k$.

Claim 3.5. *If $i_1 \geqslant 2$ and $k \geqslant 2$, then $i_k = n-1$.*

Proof of Claim 3.5. Suppose that $i_k \leqslant n-2$. Set $G^* = G - v_{i_k}v_n + v_nv_{n-1}$. Then $G^* \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$ as $v_1v_n \notin E(G)$. If $i_k = n-2$, then

$$\begin{aligned}SO(G^*) - SO(G) &= \sqrt{k^2+2^2} - \sqrt{k^2+3^2} + \sqrt{8} - \sqrt{10}\\ &\quad + \sqrt{d_{n-3}^2+2^2} - \sqrt{d_{n-3}^2+3^2}\\ &< 0,\end{aligned}$$

and if $i_k < n-2$, then

$$\begin{aligned}SO(G^*) - SO(G) &= \sqrt{k^2+2^2} - \sqrt{k^2+3^2} + \sqrt{d_{i_k-1}^2+2^2} - \sqrt{d_{i_k-1}^2+3^2}\\ &\quad + 2\sqrt{8} - \sqrt{13} - \sqrt{5}\\ &< 2\sqrt{8} - \sqrt{13} - \sqrt{5} \approx 0.1848 < 0.\end{aligned}$$

Hence, in either case, we have a contradiction. $\square$

Claim 3.6. *If $i_1 \geqslant 2$, then $i_1 \geqslant 3$ for $k \leqslant n-3$.*

Proof of Claim 3.6. Suppose that $i_1 = 2$. If $k = 1$, then $SO(G) = 2\sqrt{10} + \sqrt{5} + \sqrt{13} + (n-5)\sqrt{8} = \varphi'(n,1) + 2(\sqrt{10} + \sqrt{8} - \sqrt{13} - \sqrt{5}) > \varphi'(n,1)$. If $k = 2$, then by Claim 3.5, $v_nv_{n-1} \in E(G)$, and thus $SO(G) = 2\sqrt{13} + \sqrt{10} + (n-3)\sqrt{8} = \varphi'(n,2) + \sqrt{10} + \sqrt{8} - \sqrt{13} - \sqrt{5} > \varphi'(n,2)$. So we can assume that $k \geqslant 3$. Then by Claim 3.5, $v_nv_{n-1} \in E(G)$.

Since $k \leqslant n-3$, there exists some i ($3 \leqslant i \leqslant n-2$) such that v_i is a 2-vertex. Choose $v_i \in V_2(G)$ with the minimum i. Then v_{i-1} is a 3-vertex and $d_{i+1} \geqslant 2$. Set $G^* = G - v_2v_n + v_nv_i$. Then $G^* \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$ and

$$\begin{aligned}SO(G^*) - SO(G) &= \sqrt{d_{i+1}^2+3^2} - \sqrt{d_{i+1}^2+2^2} + \sqrt{1^2+2^2} - \sqrt{1^2+3^2}\\ &= g^{(1)}(d_{i+1},3) - g^{(1)}(1,3) < 0,\end{aligned}$$

a contradiction. $\square$

If $k = 1$, then by Claim 3.6 and the symmetry, $3 \leqslant i_1 \leqslant n-3$, thus $G \cong T_n(a_1, a_2, 1)$, where $a_1, a_2 \geqslant 2$, we have $SO(G) = 2\sqrt{5} + \sqrt{10} + 2\sqrt{13} + (n-6)\sqrt{8} = \varphi'(n,1) + \sqrt{10} + \sqrt{8} - \sqrt{13} - \sqrt{5} > \varphi'(n,1)$, and if $k = 2$, then by Claims 3.5 and 3.6, $i_1 \geqslant 3$ and $i_k = n-1$, that is, $G \in \mathscr{F}'(n,2)$. So in the following, we can assume $k \geqslant 3$. Let $X := N_G(v_n) \setminus \{v_1, v_{n-1}\}$. If $i_1 \geqslant 2$, then by an argument similar to the proof of Claim 3.4, $G[X]$ is a path, and hence,

$$\begin{aligned} SO(G) &= (k-1)\sqrt{k^2+9} + \sqrt{k^2+4} + (k-2)\sqrt{18} + (n-k-3)\sqrt{8} + 2\sqrt{13} + \sqrt{5} \\ &= \varphi'(n,k) + \sqrt{k^2+9} - \sqrt{k^2+4} + 2\sqrt{18} - 2\sqrt{13} - \sqrt{8} + \sqrt{5} \\ &< \varphi'(n,k) + 2\sqrt{18} - 2\sqrt{13} - \sqrt{8} + \sqrt{5} \approx \varphi'(n,k) + 0.6818 > \varphi'(n,k). \end{aligned}$$

So we can assume that $i_1 = 1$ and $i_k = n-1$. Then $k \geqslant 4$ and $G[X]$ is disconnected as $G \notin \mathscr{F}_{n,k}$. Furthermore, $G[X]$ contains exactly two components. Otherwise, let $v_i v_{i+1} \ldots v_j$ and $v_a v_{a+1} \ldots v_b$ be two components with $j < a-1$. Then $d_{i-1} = d_{a-1} = 2$. Set $G^* = G - \{v_{i-1}v_i, v_{a-1}v_a\} + \{v_i v_a, v_{i-1}v_{a-1}\}$. Then $G^* \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$. By Lemma 2.2, $SO(G^*) < SO(G)$, a contradiction. So $G \in \mathscr{F}'_{n,k}$.

Case 2: T is not a path. In this case, there exists a vertex $v_i \in V(T)$ such that $d_T(v_i) \geqslant 3$. Choose v_i with $d_T(v_i) \geqslant 3$ such that T has a pendant spider at v_i. Then by an argument similar to the proof of Claims 3.1–3.3, we have the following:

Claim 3.7.

(i) $T \cong T_{n-1}(a_1, a_2, a_3)$.

(ii) *If* $k \geqslant |V_1(T)|$, *then* $V_1(T) \subseteq N_G(v_n)$.

(iii) *If* $k \leqslant |V_1(T)|$, *then* $N_G(v_n) \subseteq V_1(T)$.

By Claim 3.7 and Proposition 2.1, if $k = 1$, then $G \cong T_n(a_1, a_2, a_3)$ with $\min\{a_1, a_2, a_3\} \geqslant 2$; if $k = 2$, then $G \cong U_n(a_1, a_2, a_3)$ with $a_3 \geqslant 2$; if $k = 3$, then $G \cong B_n(a_1, a_2, a_3)$ with $a_2 \geqslant 2$; and if $k = n-1$, then $G \cong W_n(a_1, a_2, a_3)$ with $\min\{a_1, a_2, a_3\} \geqslant 2$. Thus, $G \in \mathscr{F}'(n,k)$ for $k \in \{1, 2, 3, n-1\}$.

So, in the following, we assume $4 \leqslant k \leqslant n-2$. Then by Claim 3.7 (ii), $d_l = 2$ for any $v_l \in V_1(T)$. Let $X' = \{v_j \in V(T) \colon d_j \geqslant 3\}$. Note that each vertex of $N_G(v_n) \setminus (V_1(T) \cup \{v_i\})$ is a 3-vertex, and hence $k-3 \leqslant |X'| \leqslant k-2$ and $G[V_2(G)]$ contains at least three components G_1^2, G_2^2 and G_3^2 as $|V_1(T)| = 3$.

If $G[X']$ is disconnected, let G_1^3 and G_2^3 be two components of $G[X']$, then there exists a $v_j \in V(G_j^3)$ such that $v_j v_{j'} \in E(G)$, where $v_{j'} \in V(G_j^2)$ for $j = 1, 2$. Set $G^* = G - \{v_1 v_{1'}, v_2 v_{2'}\} + \{v_1 v_2, v_{1'} v_{2'}\}$. Then $G^* \in \mathscr{Q}(n,k) \setminus \mathscr{F}_{n,k}$. Note that $d_1 = d_2 = 3$ and $d_{1'} = d_{2'} = 2$, and thus, by Lemma 2.2, $SO(G^*) < SO(G)$, a contradiction. Therefore, $G[X']$ is connected. Clearly, $G[X']$ is acyclic. Thus,

$G[X']$ is a tree and $k-4 \leqslant |E(G[X'])| \leqslant k-3$. If $|E(G[X'])| = k-3$, i.e., $v_n v_i \notin E(G)$, then

$$\begin{aligned} SO(G) &= (k-3)\big(\sqrt{3^2+3^2} + \sqrt{k^2+9}\big) + 3\big(\sqrt{k^2+4} + \sqrt{3^2+2^2}\big) + (n-k-2)\sqrt{8} \\ &= \varphi'(n,k) + \sqrt{k^2+2^2} - \sqrt{3^2+2^2} - \sqrt{k^2+3^2} + \sqrt{3^2+3^2} \\ &= \varphi'(n,k) + g^{(k-3)}(2,k) - g^{(k-3)}(3,k) > \varphi'(n,k), \end{aligned}$$

where the last inequality follows from Lemma 2.1. So we can assume that

$$|E(G[X'])| = k-4,$$

then $v_n v_i \in E(G)$, that is, $d_i = 4$. If $k = 4$, then

$$\begin{aligned} SO(G) &= \sqrt{32} + 6\sqrt{20} + (n-5)\sqrt{8} \\ &= \varphi'(n,4) + 4\sqrt{4^2+2^2} + \sqrt{4^2+4^2} + \sqrt{2^2+2^2} - 2\sqrt{4^2+3^2} - 4\sqrt{3^2+2^2} \\ &\approx \varphi'(n,4) + 1.9516 > \varphi'(n,4). \end{aligned}$$

If $k \geqslant 5$, let $t = |N_G(v_i) \cap V_3(G)|$, then

$$\begin{aligned} SO(G) &= (k-4)\sqrt{k^2+3^2} + \sqrt{k^2+4^2} + 3\sqrt{k^2+2^2} + t\big(\sqrt{3^2+4^2} + \sqrt{3^2+2^2}\big) \\ &\quad + (k-4-t)\sqrt{3^2+3^2} + (3-t)\sqrt{4^2+2^2} + (n-k-1)\sqrt{8} \\ &\geqslant (k-4)\sqrt{k^2+3^2} + \sqrt{k^2+4^2} + 3\sqrt{k^2+2^2} + 3\big(\sqrt{3^2+4^2} + \sqrt{3^2+2^2}\big) \\ &\quad + (k-7)\sqrt{3^2+3^2} + (n-k-1)\sqrt{8} \\ &= \varphi'(n,k) - 2\sqrt{k^2+3^2} + \sqrt{k^2+4^2} + \sqrt{k^2+2^2} + 15 - \sqrt{13} - 3\sqrt{18} + \sqrt{8} \\ &\approx \varphi'(n,k) + g^{(1)}(k,4) - g^{(1)}(k,3) + 1.4950 > \varphi'(n,k). \end{aligned}$$

Therefore, the proof of Theorem 3.2 is complete. $\square$

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References

[1] *J. A. Bondy, U. S. R. Murty*: Graph Theory. Graduate Texts in Mathematics 244. Springer, Berlin, 2008. zbl MR doi

[2] *H. Chen, W. Li, J. Wang*: Extremal values on the Sombor index of trees. MATCH Commun. Math. Comput. Chem. *87* (2022), 23–49. zbl doi

[3] *R. Cruz, I. Gutman, J. Rada*: Sombor index of chemical graphs. Appl. Math. Comput. *399* (2021), Article ID 126018, 10 pages. zbl MR doi

[4] *R. Cruz, J. Rada*: Extremal values of the Sombor index in unicyclic and bicyclic graphs. J. Math. Chem. *59* (2021), 1098–1116. zbl MR doi
[5] *R. Cruz, J. Rada, J. M. Sigarreta*: Sombor index of trees with at most three branch vertices. Appl. Math. Comput. *409* (2021), Article ID 126414, 9 pages. zbl MR doi
[6] *K. C. Das, I. Gutman*: On Sombor index of trees. Appl. Math. Comput. *412* (2022), Article ID 126575, 8 pages. zbl MR doi
[7] *H. Deng, Z. Tang, R. Wu*: Molecular trees with extremal values of Sombor indices. Int. J. Quantum Chem. *121* (2021), Article ID e26622, 9 pages. doi
[8] *I. Gutman*: Geometric approach to degree-based topological indices: Sombor indices. MATCH Commun. Math. Comput. Chem. *86* (2021), 11–16. zbl
[9] *H. Liu, H. Chen, Q. Xiao, X. Fang, Z. Tang*: More on Sombor indices of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons. Int. J. Quantum Chem. *121* (2021), Article ID e26689, 9 pages. doi
[10] *H. Liu, I. Gutman, L. You, Y. Huang*: Sombor index: Review of extremal results and bounds. J. Math. Chem. *60* (2022), 771–798. zbl MR doi
[11] *J. Rada, J. M. Rodríguez, J. M. Sigarreta*: General properties on Sombor indices. Discrete Appl. Math. *299* (2021), 87–97. zbl MR doi
[12] *T. Réti, T. Došlić, A. Ali*: On the Sombor index of graphs. Contrib. Math. *3* (2021), 11–18. doi
[13] *Z. Wang, Y. Mao, Y. Li, B. Furtula*: On relations between Sombor and other degree-based indices. J. Appl. Math. Comput. *68* (2022), 1–17. zbl MR doi
[14] *T. Zhou, Z. Lin, L. Miao*: The Sombor index of trees and unicyclic graphs with given maximum degree. DML, Discrete Math. Lett. *7* (2021), 24–29. MR doi

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