MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **89** (2023) 741–758
ISSN: 0340–6253
doi: 10.46793/match.89-3.741Z

Extremal Values of the Sombor Index in Tricyclic Graphs

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(Received December 3, 2022)

Abstract

A vertex-degree-based molecular structure descriptor was introduced by Ivan Gutman, named the Sombor index. The Sombor index of a graph G is defined as $SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$, where $d_G(u)$ denotes the degree of the vertex u in G. In this paper we determine the extremal values of Sombor index of tricyclic graphs.

1 Introduction

In this paper, we only consider connected, simple and undirected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. For $v \in V(G)$, $N_G(v)$ denotes the set of all neighbors of v, and $d_G(v) = |N_G(v)|$ denotes the degree of vertex v in G. If $d_G(v) = 1$, then v is called a pendent vertex (or a leaf) of G and the unique edge incident with a pendent vertex v is called a pendent edge of G. If there is an edge from vertex u to vertex v, we indicate this by writing uv (or vu). For $uv \in E(G)$, denote by $G - uv$ the subgraph of G obtained from G by deleting the edge uv. For two nonadjacent vertices u and v of G, denote

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by $G + uv$ the graph obtained from G by adding the edge uv. We refer the reader to [1] for terminology and notation not given here.

The topological indices and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, predicting biological activity of chemical compounds, establishing relationships between structure and properties of molecules, and making their chemical applications. The Sombor index of a graph G is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

in [2], which is a vertex-degree-based molecular structure descriptor was proposed by Ivan Gutman. This topological index was motivated by the geometric interpretation of the degree radius of an edge uv of G, which is the distance from the origin to the ordered pair $(d_G(u), d_G(v))$. The Sombor index gave rise to numerous publications on its mathematical properties and chemical applications [3–12].

In recent years, the extreme value problem has been a hot topic in Sombor index research. In the review [13] authors collected an enormous number of bounds and extremal results related to the Sombor index and its variants. Until now the graphs extremal Sombor index were determined in the acyclic [2], unicyclic and bicyclic [14], and tetracyclic [15] cases. The tricyclic case has not been considered so far. Inspired by the works about unicyclic and bicyclic graphs extremal Sombor index done by Cruz and Rada [14], we are concerned with the Sombor index of tricyclic graphs. The main goal of this paper is to characterize the connected tricyclic graphs with minimum and maximum Sombor index. For convenience, let $\mathcal{G}_{n,3}$ be the set of all the tricyclic graphs with n vertices.

2 Tricyclic graphs with the minimum Sombor index

In this section, we study the tricyclic graphs with the minimum Sombor index. In order to find the minimum Sombor index over the set of $\mathcal{G}_{n,3}$, we will introduce two transformations that decrease the Sombor index.

Lemma 2.1. *Let G be a connected graph and $w \in V(G)$ such that $d_G(w) \geq 3$. The two paths of G are $wu_1u_2\cdots u_{r-1}u_r$ and $wv_1v_2\cdots v_{q-1}v_q$ such that $d_G(u_r) = d_G(v_q) = 1$, and $d_G(u_i) = d_G(v_j) = 2$ whenever $0 < i < r$, $0 < j < q$. Let $G' = G - wv_1 + u_rv_1$. Then, $SO(G) > SO(G')$.*

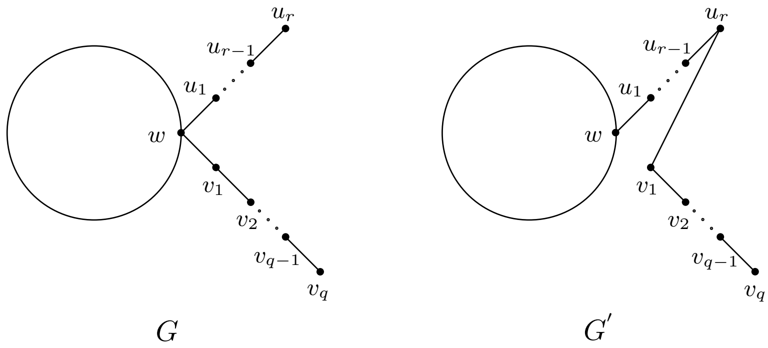


Figure 1. Graphs used in Lemma 2.1.

Proof. Let $G_0 = G - \{u_1, \cdots, u_r, v_1, \cdots, v_q\}$ and $x = d_G(w) \geq 3$. We distinguish the following three cases.

Case 1. If $r > 1$, $q > 1$, it follows that

$$\begin{aligned}
&SO(G) - SO(G') \\
&= \sum_{v \in N_{G_0}(w)} \left[\sqrt{d_G(v)^2 + x^2} - \sqrt{d_G(v)^2 + (x-1)^2}\right] \\
&+ \left[\sqrt{x^2 + 2^2} - \sqrt{(x-1)^2 + 2^2}\right] + \left[\sqrt{2^2 + 1^2} - \sqrt{2^2 + 2^2}\right] \\
&+ \left[\sqrt{x^2 + 2^2} - \sqrt{2^2 + 2^2}\right] \\
&> \sqrt{x^2 + 2^2} + \sqrt{2^2 + 1^2} - 2\sqrt{2^2 + 2^2} \\
&\geq \sqrt{13} + \sqrt{5} - 4\sqrt{2} \approx 0.1848 > 0
\end{aligned}$$

Case 2. If $r = 1$, $q = 1$. Since $\left[x^2 + 1\right] - \left[(x-1)^2 + 4\right] = 2x - 4 \geq 2$ for $x \geq 3$, which means $\sqrt{x^2 + 1} - \sqrt{(x-1)^2 + 4} > 0$ for $x \geq 3$. Then we have that

$$\begin{aligned}
&SO(G) - SO(G^{'}) \\
&= \sum_{v \in N_{G_0}(w)} \left[\sqrt{d_G(v)^2 + x^2} - \sqrt{d_G(v)^2 + (x-1)^2}\right] \\
&+ \left[\sqrt{x^2+1} - \sqrt{(x-1)^2 + 2^2}\right] + \left[\sqrt{x^2+1^2} - \sqrt{2^2+1^2}\right] \\
&> \sqrt{x^2+1} - \sqrt{(x-1)^2+4} > 0
\end{aligned}$$

Case 3. If $r = 1$, $q > 1$, it follows that

$$\begin{aligned}
&SO(G) - SO(G^{'}) \\
&= \sum_{v \in N_{G_0}(w)} \left[\sqrt{d_G(v)^2 + x^2} - \sqrt{d_G(v)^2 + (x-1)^2}\right] \\
&+ \left[\sqrt{x^2+1} - \sqrt{(x-1)^2 + 2^2}\right] + \left[\sqrt{x^2+2^2} - \sqrt{2^2+2^2}\right] \\
&> \sqrt{x^2+1} - 2\sqrt{2} \geq \sqrt{10} - 2\sqrt{2} \approx 0.3339 > 0
\end{aligned}$$

Thus, we complete the proof of Lemma 2.1. ∎

Lemma 2.2. *Let G be a connected graph with $wv \in E(G)$ such that $d_G(w) \geq 3$, $d_G(v) \geq 2$. The path of G is $wu_1u_2 \cdots u_{r-1}u_r$ such that $d_G(u_r) = 1$ and $d_G(u_i) = 2$ whenever $0 < i < r$. Let $G^{'} = G - wv + vu_r$. Then, $SO(G) > SO(G^{'})$.*

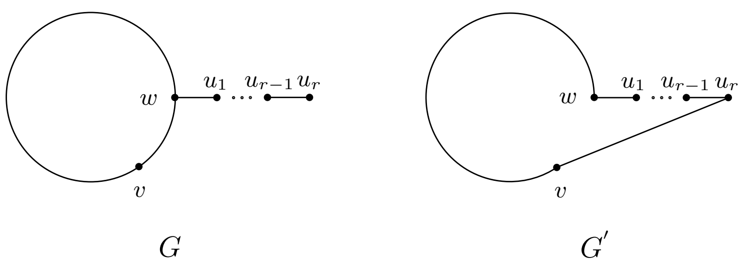


Figure 2. Graphs used in Lemma 2.2.

Proof. Let $G_1 = G - \{v, u_1, \cdots, u_r\}$ and $x = d_G(w) \geq 3$, $y = d_G(v) \geq 2$. We distinguish the following two cases.

Case 1. If $r > 1$, it follows that

$$\begin{aligned}
&SO(G) - SO(G^{'}) \\
&= \sum_{v_0 \in N_{G_1}(w)} \left[\sqrt{d_G(v_0)^2 + x^2} - \sqrt{d_G(v_0)^2 + (x-1)^2}\right] \\
&+ \left[\sqrt{x^2 + 2^2} - \sqrt{(x-1)^2 + 2^2}\right] + \left[\sqrt{x^2 + y^2} - \sqrt{2^2 + y^2}\right] \\
&+ \left[\sqrt{2^2 + 1^2} - \sqrt{2^2 + 2^2}\right] \\
&> \sqrt{x^2 + 4} - \sqrt{(x-1)^2 + 4} + \sqrt{5} - 2\sqrt{2} \\
&\geq \sqrt{13} + \sqrt{5} - 4\sqrt{2} \approx 0.1848 > 0
\end{aligned}$$

Case 2. If $r = 1$. Since $\left[x^2 + 1\right] - \left[(x-1)^2 + 4\right] = 2x - 4 \geq 2$ for $x \geq 3$, which means $\sqrt{x^2+1} - \sqrt{(x-1)^2 + 4} > 0$ for $x \geq 3$. Then we have

$$\begin{aligned}
&SO(G) - SO(G^{'}) \\
&= \sum_{v_0 \in N_{G_1}(w)} \left[\sqrt{d_G(v_0)^2 + x^2} - \sqrt{d_G(v_0)^2 + (x-1)^2}\right] \\
&+ \left[\sqrt{x^2 + 1} - \sqrt{(x-1)^2 + 2^2}\right] + \left[\sqrt{x^2 + y^2} - \sqrt{2^2 + y^2}\right] \\
&> \sqrt{x^2 + 1} - \sqrt{(x-1)^2 + 4} > 0
\end{aligned}$$

Thus, we complete the proof of Lemma 2.2. ■

Remark 1. By Lemma 2.1 and Lemma 2.2, a graph in $\mathcal{G}_{n,3}$ with minimum Sombor index must be a tricyclic graph without pendent vertices.

Thus, we only need to find the minimum Sombor index in the base tricyclic graphs of n vertices.

Recall that if $G \in \mathcal{G}_{n,3}$, the base $B(G)$ is the minimal tricyclic subgraph of G, which is the unique tricyclic subgraph of G containing no pendent vertex. A tricyclic graph G can be constructed from $B(G)$ by adding trees to some or all vertices of $B(G)$. According to [16], we know that there are precisely fifteen types of base tricyclic graphs in the set of $\mathcal{G}_{n,3}$, which are denoted by $\mathcal{T}_i(i = 1, 2, ..., 15)$, respectively. (see $Figure.3$)

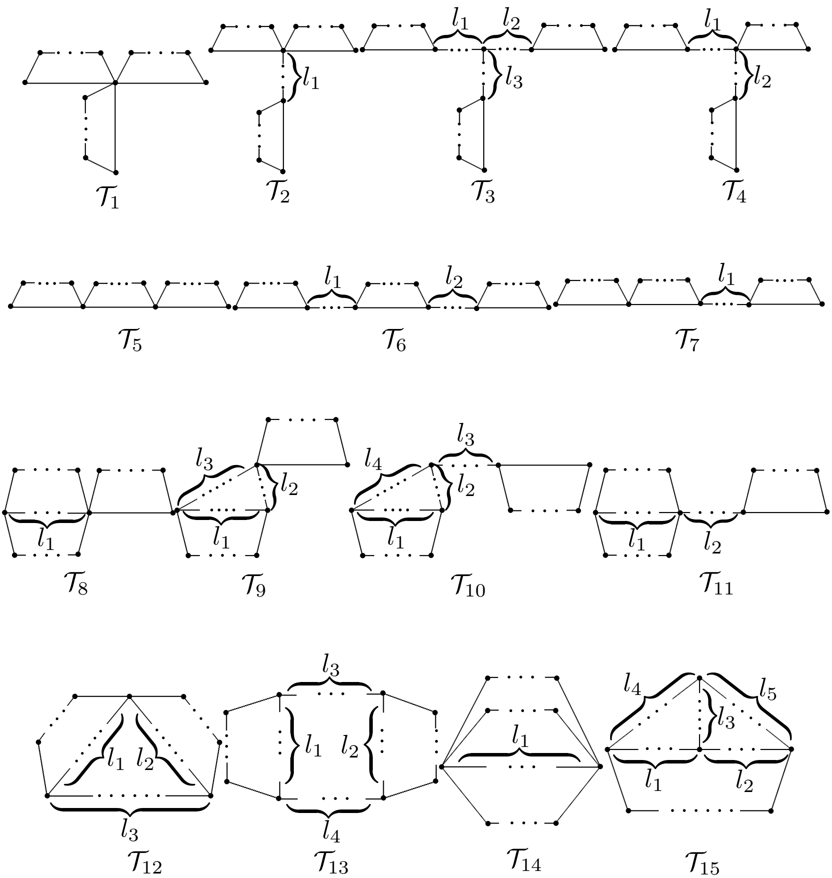


Figure 3. Bases in $\mathcal{G}_{n,3}$.

In order to calculate the values of the Sombor index for all classes of base tricyclic graphs with n vertices, we introduce the following definition.

Definition 1. $\mathcal{T}_i^n$ denotes the set of graphs in $\mathcal{T}_i(i = 1, 5)$ with n vertices. $\mathcal{T}_i^n(l_1)$ denotes the set of graphs in $\mathcal{T}_i(i = 2, 7, 8, 14)$ with n vertices. $\mathcal{T}_i^n(l_1, l_2)$ denotes the set of graphs in $\mathcal{T}_i(i = 4, 6, 11)$ with n vertices. $\mathcal{T}_i^n(l_1, l_2, l_3)$ denotes the set of graphs in $\mathcal{T}_i(i = 3, 9, 12)$ with n vertices.

$\mathcal{T}_i^n(l_1, l_2, l_3, l_4)$ denotes the set of graphs in $\mathcal{T}_i (i = 10, 13)$ with n vertices. $\mathcal{T}_{15}^n(l_1, l_2, l_3, l_4, l_5)$ denotes the set of graphs in $\mathcal{T}_{15}$ with n vertices. Note that $l_k \geq 1 (k = 1, \cdots, 5)$ is the length of the path connecting cycles or the common path formed by cycles.

We give the values list of the Sombor index of the graphs in these subclasses, shown in Table 1.

Table 1. The values of the Sombor index over the set of base tricyclic graphs with n vertices

The tricyclic graph G belong to	The value of the Sombor index of G
$\mathcal{T}_1^n$	$2\sqrt{2}n + 12\sqrt{10} - 8\sqrt{2}$
$\mathcal{T}_5^n$	$2\sqrt{2}n + 16\sqrt{5} - 12\sqrt{2}$
$\mathcal{T}_2^n(1) \cup \mathcal{T}_8^n(1)$	$2\sqrt{2}n + 4\sqrt{29} + \sqrt{34} + 2\sqrt{13} - 10\sqrt{2}$
$\mathcal{T}_2^n(\geq 2) \cup \mathcal{T}_8^n(\geq 2)$	$2\sqrt{2}n + 5\sqrt{29} + 3\sqrt{13} - 12\sqrt{2}$
$\mathcal{T}_3^n(\geq 2, 1, 1) \cup \mathcal{T}_6^n(1, 1) \cup \mathcal{T}_{10}^n(1, 1, \geq 2, \geq 2) \cup \mathcal{T}_{13}^n(1, 1, \geq 2, \geq 2) \cup \mathcal{T}_{15}^n(1, 1, \geq 2, \geq 2, \geq 2)$	$2\sqrt{2}n + 8\sqrt{13} - 10\sqrt{2}$
$\mathcal{T}_3^n(\geq 2, 1, \geq 2) \cup \mathcal{T}_6^n(1, \geq 2) \cup \mathcal{T}_{10}^n(\geq 2, 1, \geq 2, \geq 2) \cup \mathcal{T}_{13}^n(\geq 2, 1, \geq 2, \geq 2) \cup \mathcal{T}_{15}^n(\geq 2, 1, \geq 2, \geq 2, \geq 2)$	$2\sqrt{2}n + 10\sqrt{13} - 15\sqrt{2}$
$\mathcal{T}_3^n(\geq 2, \geq 2, \geq 2) \cup \mathcal{T}_6^n(\geq 2, \geq 2) \cup \mathcal{T}_{10}^n(\geq 2, \geq 2, \geq 2, \geq 2) \cup \mathcal{T}_{13}^n(\geq 2, \geq 2, \geq 2, \geq 2) \cup \mathcal{T}_{15}^n(\geq 2, \geq 2, \geq 2, \geq 2, \geq 2)$	$2\sqrt{2}n + 12\sqrt{13} - 20\sqrt{2}$
$\mathcal{T}_4^n(\geq 2, \geq 2) \cup \mathcal{T}_7^n(\geq 2) \cup \mathcal{T}_9^n(\geq 2, \geq 2, \geq 2) \cup \mathcal{T}_{11}^n(\geq 2, \geq 2) \cup \mathcal{T}_{12}^n(\geq 2, \geq 2, \geq 2)$	$2\sqrt{2}n + 8\sqrt{5} + 6\sqrt{13} - 16\sqrt{2}$
$\mathcal{T}_4^n(1, 1) \cup \mathcal{T}_9^n(\geq 2, 1, 1) \cup \mathcal{T}_{11}^n(1, 1) \cup \mathcal{T}_{12}^n(1, 1, \geq 2)$	$2\sqrt{2}n + 10 + 4\sqrt{5} + 4\sqrt{13} - 12\sqrt{2}$
$\mathcal{T}_4^n(\geq 2, 1) \cup \mathcal{T}_9^n(\geq 2, \geq 2, 1) \cup \mathcal{T}_{11}^n(\geq 2, 1) \cup \mathcal{T}_{12}^n(\geq 2, 1, \geq 2)$	$2\sqrt{2}n + 5 + 6\sqrt{5} + 5\sqrt{13} - 14\sqrt{2}$
$\mathcal{T}_7^n(1) \cup \mathcal{T}_9^n(1, \geq 2, \geq 2) \cup \mathcal{T}_{12}^n(\geq 2, \geq 2, 1)$	$2\sqrt{2}n + 8\sqrt{5} + 4\sqrt{13} - 11\sqrt{2}$
$\mathcal{T}_3^n(1, 1, 1) \cup \mathcal{T}_{10}^n(1, 1, \geq 2, 1) \cup \mathcal{T}_{13}^n(1, 1, \geq 2, 1) \cup \mathcal{T}_{15}^n(1, 1, \geq 2, 1, \geq 2)$	$2\sqrt{2}n + 6\sqrt{13} - 5\sqrt{2}$
$\mathcal{T}_9^n(1, 1, 1) \cup \mathcal{T}_{12}^n(1, 1, 1)$	$2\sqrt{2}n + 10 + 4\sqrt{5} + 2\sqrt{13} - 7\sqrt{2}$
$\mathcal{T}_9^n(1, \geq 2, 1) \cup \mathcal{T}_{12}^n(\geq 2, 1, 1)$	$2\sqrt{2}n + 5 + 6\sqrt{5} + 3\sqrt{13} - 9\sqrt{2}$
$\mathcal{T}_{10}^n(1, 1, 1, 1) \cup \mathcal{T}_{13}^n(1, 1, 1, 1) \cup \mathcal{T}_{15}^n(1, 1, 1, 1, \geq 2)$	$2\sqrt{2}n + 4\sqrt{13}$
$\mathcal{T}_{14}^n(1)$	$2\sqrt{2}n + 12\sqrt{5} - 6\sqrt{2}$
$\mathcal{T}_{14}^n(\geq 2)$	$2\sqrt{2}n + 16\sqrt{5} - 12\sqrt{2}$
$\mathcal{T}_{15}^n(1, 1, 1, 1, 1)$	$2\sqrt{2}n + 2\sqrt{13} + 5\sqrt{2}$

By comparing the values in Table 1, we get that the minimum Sombor index over the set of base tricyclic graphs with n vertices is attained in $\mathcal{T}_{15}^n(1, 1, 1, 1, 1)$. (see $Figure.4$)

From Lemma 2.1, 2.2 and Table 1, we can get the following theorem.

Theorem 2.3. *Let $G \in \mathcal{G}_{n,3}$, Then*

$$SO(G) \geq 2\sqrt{2}n + 2\sqrt{13} + 5\sqrt{2} = SO(\widetilde{G})$$

where $\widetilde{G}$ is the graph in $\mathcal{T}_{15}^n(1, 1, 1, 1, 1)$.

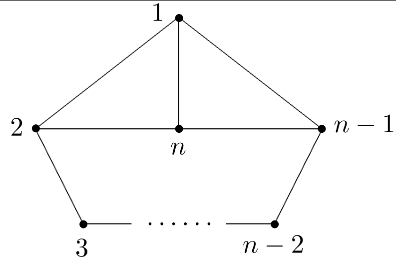


Figure 4. The tricyclic graph with minimum value of the Sombor index.

3 Tricyclic graphs with the maximum Sombor index

In this section, we study the tricyclic graphs with the maximum Sombor index and give some valuable lemmas used frequently in the sequel section.

Lemma 3.1. *Let* $\varphi(x,y) = \sqrt{x^2+y^2} - \sqrt{(x+1)^2+y^2}$, *where* $x \geq 1$ *and* $y \geq 1$. *Then, for any value of* $y \geq 1$, φ *is decreasing as a function of* x*; and for any value of* $x \geq 1$, φ *is increasing as a function of* y.

Proof. Since, $x^2\left[(x+1)^2+y^2\right] - (x+1)^2(x^2+y^2) = -y^2(2x+1) < 0$ for $x \geq 1$ and $y \geq 1$, which means $x\sqrt{(x+1)^2+y^2} - (x+1)\sqrt{x^2+y^2} < 0$ for $x \geq 1$ and $y \geq 1$.

Then we obtain the partial derivative of the function φ about x is

$$\frac{\partial\varphi(x,y)}{\partial x} = \frac{x\sqrt{(x+1)^2+y^2} - (x+1)\sqrt{x^2+y^2}}{\sqrt{x_2+y_2}\sqrt{(x+1)^2+y^2}} < 0$$

The partial derivative of the function φ about y is

$$\frac{\partial\varphi(x,y)}{\partial y} = \frac{y\sqrt{(x+1)^2+y^2} - y\sqrt{x^2+y^2}}{\sqrt{x_2+y_2}\sqrt{(x+1)^2+y^2}} > 0$$

for $x \geq 1$, and $y \geq 1$.

Thus we complete the proof of Lemma 3.1. ■

Lemma 3.2 ([17]). *Let* $x_1 \geq x_2 > s > 0$ *and* $c > 0$. *Then,*

$$\sqrt{(x_1+s)^2+c^2} + \sqrt{(x_2-s)^2+c^2} > \sqrt{x_1^2+c^2} + \sqrt{x_2^2+c^2}$$

Corollary 3.3. *Let $x \geq 2$, $y \geq 2$ and $z > 0$. Then*

$$\sqrt{(x+y-1)^2+z^2}+\sqrt{1+z^2} > \sqrt{x^2+z^2}+\sqrt{y^2+z^2}$$

Proof. Reference Lemma 3.2, let $x \geq y > y-1 \geq 1$, $z > 0$ and $x = x_1$, $y = x_2$, $s = y-1$, $c = z$, then we obtain $\sqrt{(x+y-1)^2+z^2}+\sqrt{1+z^2} > \sqrt{x^2+z^2}+\sqrt{y^2+z^2}$. ■

In order to find the maximum Sombor index over the set of $\mathcal{G}_{n,3}$, we introduce two transformations that increase the Sombor index in our following result.

To *identify* nonadjacent vertices u and v of a graph G is to replace these vertices by a single vertex w incident to all the edges which were incident in G to either u or v. The resulting graph $G/\{x,y\}$ has one less vertex than G; To *contract* an edge $e = uv$ of a graph G is to delete the edge and then identify its ends. The resulting graph G/uv has one less edge than G.

Lemma 3.4. *Let G be a connected graph and $u, v \in E(G)$ such that $d_G(u) \geq 2$ and $d_G(v) \geq 2$. Note that $N_G(u) \setminus \{v\} \cap N_G(v) \setminus \{u\} = \emptyset$. Let G' be a graph obtained by contracting the edge uv to a vertex w, further adding a pendent vertex adjacent to the vertex w. Then*

$$SO(G') > SO(G)$$

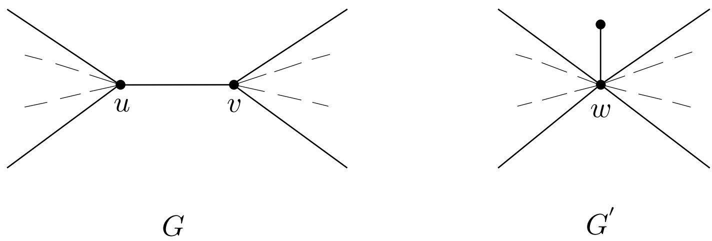


Figure 5. Graphs used in Lemma 3.4.

Proof. Let $x = d_G(u) \geq 2$, $y = d_G(v) \geq 2$

$$SO(G) - SO(G')$$

$$
\begin{aligned}
&= \sum_{v_0 \in N_G(u)\backslash\{v\}} \left[\sqrt{d_G(v_0)^2 + x^2} - \sqrt{d_G(v_0)^2 + (x+y-1)^2}\right] \\
&+ \sum_{v_1 \in N_G(v)\backslash\{u\}} \left[\sqrt{d_G(v_1)^2 + y^2} - \sqrt{d_G(v_1)^2 + (x+y-1)^2}\right] \\
&+ \left[\sqrt{x^2+y^2} - \sqrt{(x+y-1)^2 + 1^2}\right] \\
&< \sqrt{x^2+y^2} - \sqrt{(x+y-1)^2+1} \\
&= \sqrt{x^2+y^2} - \sqrt{x^2+y^2+2(x-1)(y-1)}
\end{aligned}
$$

Since x, $y \geq 2$, we obtain that $SO(G) - SO(G^{'}) < 0$. ■

Remark 2. Repeating the transformation in Lemma 3.4, any tree T of size t attached to a graph can be changed into a star S_{t+1}, and the Sombor index increases by Lemma 3.4. In addition, if G is a graph from $\mathcal{G}_{n,3}$ with maximum Sombor index, then the length of the base cycle in G is 3.

Lemma 3.5. *Let G be a connected graph and $u, v, m \in V(G)$, $uv \notin E(G)$ such that $d_G(u) \geq 2$, $d_G(v) \geq 2$. Note that $N_G(u) \cap N_G(v) = \{m\}$. Let $G^{'}$ be a graph obtained by identifying the vertices u, v and deleting one edge of mu and mv, further adding a pendent vertex adjacent to the vertex m. Then*

$$SO(G^{'}) > SO(G)$$

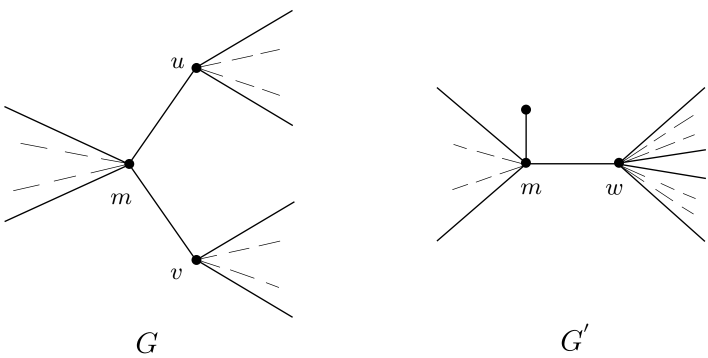


Figure 6. Graphs used in Lemma 3.5.

Proof. Let $x = d_G(u) \geq 2$, $y = d_G(v) \geq 2$, $z = d_G(m)$

$$\begin{aligned}
& SO(G) - SO(G^{'}) \\
&= \sum_{v_0 \in N_G(u)\setminus\{m\}} \left[\sqrt{d_G(v_0)^2 + x^2} - \sqrt{d_G(v_0)^2 + (x+y-1)^2}\right] \\
&+ \sum_{v_1 \in N_G(v)\setminus\{m\}} \left[\sqrt{d_G(v_1)^2 + y^2} - \sqrt{d_G(v_1)^2 + (x+y-1)^2}\right] \\
&+ \left[\sqrt{x^2+z^2} + \sqrt{y^2+z^2}\right] - \left[\sqrt{(x+y-1)^2+z^2} + \sqrt{1^2+z^2}\right] \\
&< \left[\sqrt{x^2+z^2} + \sqrt{y^2+z^2}\right] - \left[\sqrt{(x+y-1)^2+z^2} + \sqrt{1+z^2}\right]
\end{aligned}$$

Using Corollary 3.3, we obtain that $SO(G) - SO(G^{'}) < 0$. ■

Let $T_{14}(n, p_1, p_2, q_1, q_2, q_3) \in \mathcal{G}_{n,3}$, where $p_1, p_2, q_1, q_2, q_3 \geq 0$ are the number of pendent vertices and $p_1 + p_2 + q_1 + q_2 + q_3 = n - 5$, be a tricyclic graph shown in $Figure$.7.

Let $T_{15}(n, q_1, q_2, q_3, q_4) \in \mathcal{G}_{n,3}$, where $q_1, q_2, q_3, q_4 \geq 0$ are the number of pendent vertices and $q_1 + q_2 + q_3 + q_4 = n - 4$, be a tricyclic graph shown in $Figure$.7.

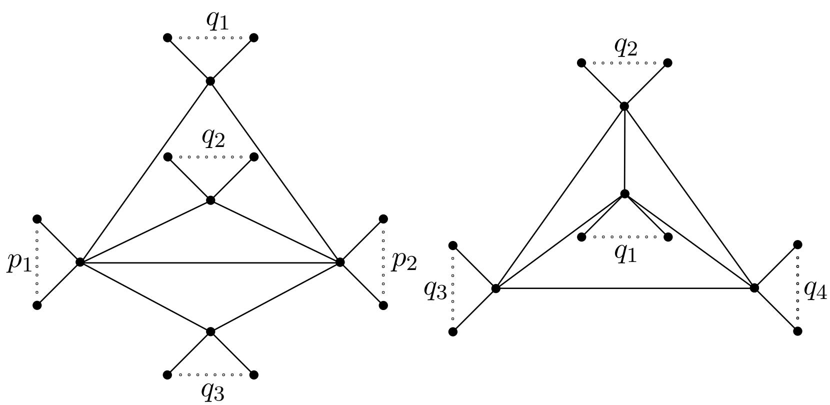


Figure 7. $T_{14}(n, p_1, p_2, q_1, q_2, q_3)$(left) and $T_{15}(n, q_1, q_2, q_3, q_4)$(right).

Remark 3. By Lemma 3.4 and Lemma 3.5, a graph in $\mathcal{G}_{n,3}$ with maximum Sombor index is of the form of $T_{14}(n, p_1, p_2, q_1, q_2, q_3)$ or $T_{15}(n, q_1, q_2, q_3, q_4)$.

To better understand the Remark 3, we give the *Example* 1.

Example 1. Let $G \in \mathcal{G}_{n,3}$ and G has a base graph in $\mathcal{T}_6$. Note that $a, b, c, d, e, f, g, h, i, j, k \geq 0$ are the number of pendent vertices and $j \geq c + d + 1$, $k \geq f + g + 1$.

Using Lemma 3.4, we can obtain $SO(G) < SO(G_1)$ and $SO(G_1) < SO(G_2)$ (See $Figure$.8).

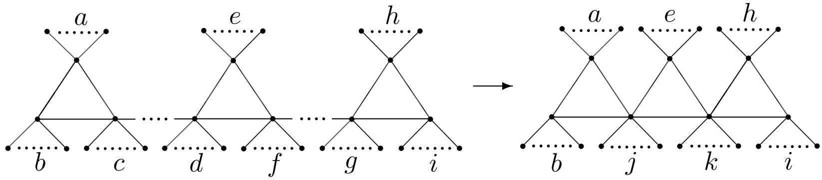


Figure 8. Graphs of the forms $G_1 \to G_2$.

Using Lemma 3.5, we can obtain $SO(G_2) < SO(G_3)$ and $SO(G_3) < SO(G_4)$ (See $Figure$.9).

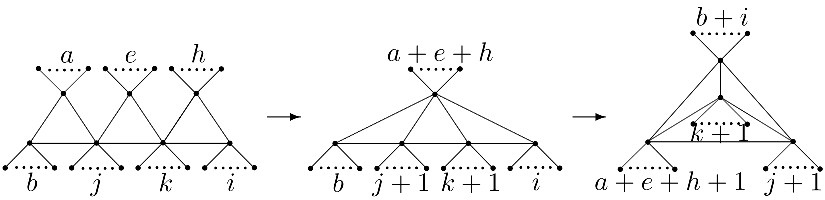


Figure 9. Graphs of the forms $G_2 \to G_3 \to G_4$.

Let $k + 1 = q_1$, $b + i = q_2$, $a + e + h + 1 = q_3$, and $j + 1 = q_4$, then we obtain $SO(G) < SO(T_{15}(n, q_1, q_2, q_3, q_4))$.

By the same way, we get that $SO(G) < SO(T_{15}(n, q_1, q_2, q_3, q_4))$ for those tricyclic graphs having a base graph in $\mathcal{T}_i (i = 1, 2, \cdots, 13)$. Moreover, when tricyclic graph G has a base graph in $\mathcal{T}_i (i = 1, 2, \cdots, 8, 11, 13)$, we also have that $SO(G) < SO(T_{14}(n, p_1, p_2, q_1, q_2, q_3))$.

Thus, we only need to find the maximum Sombor index in the forms of $T_{14}(n, p_1, p_2, q_1, q_2, q_3)$ and $T_{15}(n, q_1, q_2, q_3, q_4)$.

Denote by $f(x, y) = \sqrt{x^2 + y^2}$, where $x, y \geq 1$. Then we have $\varphi(x, y) = f(x, y) - f(x + 1, y)$.

Lemma 3.6. *Let $n \geq 5$. For any values of p_1, p_2, q_1, q_2, $q_3 \geq 0$ and $p_1+p_2+q_1+q_2+q_3 = n-5$. We have that*

$$SO(T_{14}(n,p_1,p_2,q_1,q_2,q_3)) < SO(T_{14}(n,n-5,0,0,0,0))$$

Proof. We first prove the following four inequalities:

(1) For any values of $p_1 \geq p_2 \geq 1$,

$$SO(T_{14}(n,p_1,p_2,q_1,q_2,q_3)) < SO(T_{14}(n,p_1+1,p_2-1,q_1,q_2,q_3))$$

$$\begin{aligned}
\Delta_1 = \quad & SO(T_{14}(n,p_1,p_2,q_1,q_2,q_3)) - SO(T_{14}(n,p_1+1,p_2-1,q_1,q_2,q_3)) \\
= \quad & p_1\left[f(p_1+4,1) - f(p_1+5,1)\right] - p_2\left[f(p_2+3,1) - f(p_2+4,1)\right] \\
& + \left[f(p_2+3,1) - f(p_1+5,1)\right] \\
& + \left[f(p_1+4,p_2+4) - f(p_1+5,p_2+3)\right] \\
& + \left[f(p_1+4,q_1+2) - f(p_1+5,q_1+2)\right] \\
& - \left[f(p_2+3,q_1+2) - f(p_2+4,q_1+2)\right] \\
& + \left[f(p_1+4,q_2+2) - f(p_1+5,q_2+2)\right] \\
& - \left[f(p_2+3,q_2+2) - f(p_2+4,q_2+2)\right] \\
& + \left[f(p_1+4,q_3+2) - f(p_1+5,q_3+2)\right] \\
& - \left[f(p_2+3,q_3+2) - f(p_2+4,q_3+2)\right] \\
= \quad & \left[p_1\varphi(p_1+4,1) - p_2\varphi(p_2+3,1)\right] + \left[f(p_2+3,1) - f(p_1+5,1)\right] \\
& + \left[f(p_1+4,p_2+4) - f(p_1+5,p_2+3)\right] \\
& + \left[\varphi(p_1+4,q_1+2) - \varphi(p_2+3,q_1+2)\right] \\
& + \left[\varphi(p_1+4,q_2+2) - \varphi(p_2+3,q_2+2)\right] \\
& + \left[\varphi(p_1+4,q_3+2) - \varphi(p_2+3,q_3+2)\right]
\end{aligned}$$

Since $p_1 \geq p_2$, using Lemma 3.1 we have that

$$\begin{aligned}
\Delta_1 < \quad & f(p_1+4,p_2+4) - f(p_1+5,p_2+3) \\
= \quad & \sqrt{p_1^2+p_2^2+8p_1+8p_2+32} - \sqrt{p_1^2+p_2^2+10p_1+6p_2+34} < 0
\end{aligned}$$

By the same way, we can deduce the following inequalities (2) and (3).

(2) For any values of $q_1 \geq q_2 \geq 1$,

$$SO(T_{14}(n, p_1, 0, q_1, q_2, q_3)) < SO(T_{14}(n, p_1, 0, q_1+1, q_2-1, q_3))$$

(3) For any values of $p_1 \geq q_1 \geq 1$,

$$SO(T_{14}(n, p_1, 0, q_1, 0, 0)) < SO(T_{14}(n, p_1+1, 0, q_1-1, 0, 0))$$

(4) For any values of $q_1 \geq p_1 + 1$,

$$SO(T_{14}(n, p_1, 0, q_1, 0, 0)) < SO(T_{14}(n, p_1-1, 0, q_1+1, 0, 0))$$

$$\begin{aligned}
\Delta_2 = \;& SO(T_{14}(n, p_1, 0, q_1, 0, 0)) - SO(T_{14}(n, p_1-1, 0, q_1+1, 0, 0)) \\
= \;& q_1 \left[f(q_1+2, 1) - f(q_1+3, 1)\right] - p_1 \left[f(p_1+3, 1) - f(p_1+4, 1)\right] \\
& + \left[f(p_1+3, 1) - f(q_1+3, 1)\right] + 2\left[f(p_1+4, 2) - f(p_1+3, 2)\right] \\
& + \left[f(q_1+2, 4) - f(q_1+3, 4)\right] - \left[f(p_1+3, 4) - f(p_1+4, 4)\right] \\
& + \left[f(p_1+4, q_1+2) - f(p_1+3, q_1+3)\right] \\
= \;& \left[q_1 \varphi(q_1+2, 1) - p_1 \varphi(p_1+3, 1)\right] + \left[f(p_1+3, 1) - f(q_1+3, 1)\right] \\
& + 2\left[f(p_1+4, 2) - f(p_1+3, 2)\right] + \left[\varphi(q_1+2, 4) - \varphi(p_1+3, 4)\right] \\
& + \left[f(p_1+4, q_1+2) - f(p_1+3, q_1+3)\right]
\end{aligned}$$

Since $q_1 \geq p_1 + 1$, using Lemma 3.1 we have that

$$\begin{aligned}
q_1 \varphi(q_1+2, 1) - p_1 \varphi(p_1+3, 1) & \leq (p_1+1)\varphi(p_1+3, 1) - p_1 \varphi(p_1+3, 1) \\
& = \varphi(p_1+3, 1) \\
& = f(p_1+3, 1) - f(p_1+4, 1)
\end{aligned}$$

$$2[f(p_1+4, 2) - f(p_1+3, 2)] < 2[f(p_1+4, 1) - f(p_1+3, 1)]$$

$$\varphi(q_1+2, 4) - \varphi(p_1+3, 4) \leq 0$$

Thus, we can get that

$$\begin{aligned}
\Delta_2 < \;& \left[f(p_1+3, 1) - f(p_1+4, 1)\right] + \left[f(p_1+3, 1) - f(q_1+3, 1)\right] \\
& + 2\left[f(p_1+4, 1) - f(p_1+3, 1)\right] \\
& + \left[f(p_1+4, q_1+2) - f(p_1+3, q_1+3)\right]
\end{aligned}$$

$$< f(p_1+4,q_1+2)-f(p_1+3,q_1+3)$$
$$= \sqrt{p_1^2+q_1^2+8p_1+4q_1+20}-\sqrt{p_1^2+q_1^2+6p_1+6q_1+18}\leq 0$$

Using iteratively inequalities (1), (2), (3) and (4), we conclude that the graph of the form $T_{14}(n,p_1,p_2,q_1,q_2,q_3)$ with maximum value of the Sombor index is $T_{14}(n,n-5,0,0,0,0)$ or $T_{14}(n,0,0,n-5,0,0)$. (see $Figure.10$)

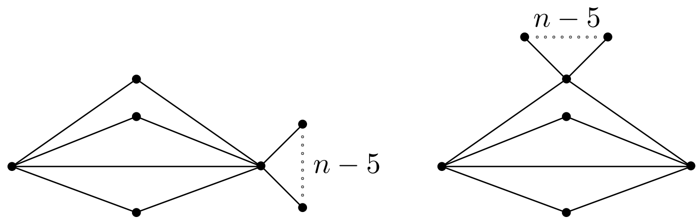


Figure 10. $T_{14}(n,n-5,0,0,0,0)$(left) and $T_{14}(n,0,0,n-5,0,0)$(right).

$$SO(T_{14}(n,n-5,0,0,0,0)) = (n-5)\sqrt{(n-1)^2+1}+3\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+16}+3\sqrt{20}$$

$$SO(T_{14}(n,0,0,n-5,0,0) = (n-5)\sqrt{(n-3)^2+1}+2\sqrt{(n-3)^2+16} + \sqrt{32}+4\sqrt{20}$$

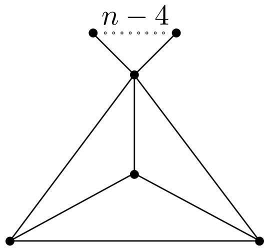
It is easy to see that $SO(T_{14}(n,0,0,n-5,0,0)) < SO(T_{14}(n,n-5,0,0,0,0))$.

■

By using the method similar to the proof of Lemma 3.6, we can have the following Lemma 3.7.

Lemma 3.7. *Let $n\geq 4$. For any values of $q_1,q_2,q_3,q_4\geq 0$ and $q_1+q_2+q_3+q_4=n-4$. We have that*

$$SO(T_{15}(n,q_1,q_2,q_3,q_4) < SO(T_{15}(n,n-4,0,0,0))$$



$T_{15}(n, n-4, 0, 0, 0)$

Figure 11. Graph used in Lemma 3.7 and Lemma 3.8.

Lemma 3.8. *Let $n \geq 5$. We have that*

$$SO(T_{14}(n, n-5, 0, 0, 0, 0)) > SO(T_{15}(n, n-4, 0, 0, 0))$$

Proof. For any values of $n \geq 5$,

$$\begin{aligned}\Delta_3 &= SO(T_{14}(n, n-5, 0, 0, 0, 0)) - SO(T_{15}(n, n-4, 0, 0, 0)) \\ &= 3\left[\sqrt{(n-1)^2+4} - \sqrt{(n-1)^2+9}\right] + 3\sqrt{20} - 3\sqrt{18} \\ &+ \left[\sqrt{(n-1)^2+16} - \sqrt{(n-1)^2+1}\right]\end{aligned}$$

Consider a function $f(n) = 3\left[\sqrt{(n-1)^2+4} - \sqrt{(n-1)^2+9}\right]$, where $n \geq 5$. By Lemma 3.1, $f(n)$ is strictly increasing for $n \geq 5$.

When $n \geq 12$, $f(n) \geq f(12) = 3\sqrt{125} - 3\sqrt{130}$, then $\Delta_3 > 3\sqrt{125} - 3\sqrt{130} + 3\sqrt{20} - 3\sqrt{18} > 0$.

When $5 \leq n \leq 11$, by simple calculations, we have that $\Delta_3 > 0$.

Hence, we can obtain that $SO(T_{14}(n, n-5, 0, 0, 0, 0)) > SO(T_{15}(n, n-4, 0, 0, 0))$. ■

From Lemma 3.4 – 3.8, we can get the following theorem.

Theorem 3.9. *Let $G \in \mathcal{G}_{n,3}$ and $n \geq 5$. Then*

$$SO(G) \leq (n-5)\sqrt{(n-1)^2+1} + 3\sqrt{(n-1)^2+4} + \sqrt{(n-1)^2+16} + 3\sqrt{20}$$

with equality if and only if G is isomorphic to the graph $T_{14}(n, n-5, 0, 0, 0, 0)$.

***Acknowledgment*:** The authors are grateful to the anonymous reviewers for their careful reading and helpful comments. This work is supported by the Natural Science Foundation of Xinjiang Province (No.2021D01C069) and the National Natural Science Foundation of China (grant number 12161085).

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