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Ordering Unicyclic Graphs with a Fixed Girth by Sombor Indices

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Abstract

The Sombor index indicated by the symbol $SO(G)$ is calculated by adding the contributions of each vertex to the total number of edges in G, while the reduced Sombor index $SO_{red}(G)$ refines this measure by discounting the contributions of pendant vertices, which have a degree of 1.

$$SO(G) = \sum_{xy \in E(G)} \sqrt{{d_x}^2 + {d_y}^2}$$

$$SO_{red}(G) = \sum_{xy \in E(G)} \sqrt{(d_x - 1)^2 + (d_y - 1)^2}$$

for a given vertex x in graph G, d_x corresponds to the degree of that vertex. Our focus centers on exploring the Sombor index and reduced Sombor index of unicyclic graphs, specifically addressing

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graphs with a predetermined girth. We determine the first four smallest Sombor index and reduced Sombor index values and identifying the corresponding graphs that achieve these extremes.

1 Introduction

In this research endeavor, we direct our attention to undirected and connected graphs denoted as $G = (V, E)$. For any vertex x in a graph G, has a degree d_x, indicating the number of directly connected vertices. We denote $N(x)$ as the set of vertices adjacent to x. If x and y are considered to be adjacent or neighbours, it can be written as $x \sim y$. Furthermore, $G - x$ indicates the graph obtained by eliminating a specific vertex x from the original graph and removing all edges connected to it. Moreover, a vertex with a degree of 1 is commonly referred to as a pendant vertex and any edge in graph G that is connected to a pendant vertex is known as a pendant edge. When we remove an edge xy from the graph or add an edge xy to it, we represent the resulting graphs as $G - xy$ and $G + xy$, respectively. The expression $A := B$ is employed to redesignate B as A.

In the realm of graph theory, numerous research studies have been devoted to investigating the Sombor index and its extremal properties in various graph classes. Gutman et al. [5] examined the problem of obtaining graphs with the maximum (or minimum) Sombor index values in trees and graphs with a specified order n, while Réti et al. [10] focused on connected graph classes like unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs of order n. Sun et al. [12] provided a characterization of extremal graphs with the maximum and minimum Sombor index values based on the domination number ($\gamma(G)$).

Zhou et al. [15] used a different approach, characterizing extremal trees and unicyclic graphs with the maximum and minimum Sombor index values, while considering the matching number as a relevant parameter. Similarly, in another study, Zhou et al. [14] explored extremal Sombor index within the same graph class, taking into account a given maximum degree. Das et al. [4] contributed to the field by establishing bounds on the Sombor index of trees considering order, number of pendant vertices and the independence number. They also provided characterizations of the graphs the maximum and minimum Sombor index values.

Aashtab et al. [1] discovered a fascinating property of the Sombor index. According to their findings, let G be a graph. If, for every other connected graph G' with the same number of vertices and edges, $SO(G) - SO(G') < 0$, then G is categorized as an almost regular graph. Making use of this significant property, Liu et al. [8] applied it to determine the smallest Sombor index of tricyclic and tetracyclic graphs.

Horoldagva et al. [7] established several lower and upper bounds for the Sombor index of connected graphs, considering various graph parameters, including the maximum degree. On the other hand, Das et al. [3] provided an upper bound for the Sombor index of connected graphs with a specified independence number. Zhang et al. [13] continued exploring extremal graphs concerning the Sombor index with specific parameters such as girth, chromatic number and matching number.

In addition, Liu et al. [9] derived various bounds for the reduced Sombor index, considering different graph characteristics and parameters. Also, they calculated the expected values related to the reduced Sombor index within random polyphenyl chains, as well as the bounds of reduced Sombor spectral radius and energy. Furthermore, their work included the determination of ordering the minimum of trees, chemical unicyclic graphs, chemical bicyclic graphs and chemical tricyclic graphs. Moreover, they explored the applications of the reduced Sombor index in analyzing octane isomers.

The Sombor index and reduced Sombor index are graph-theoretical parameters that measures the complexity and structural properties of a graph. It was introduced by Gutman [6] and has since garnered significant attention in the field of chemical graph theory and other related disciplines. The Sombor index and reduced Sombor index are denoted by $SO(G)$ and $SO_{red}(G)$ are formulated as

$$SO(G) = \sum_{xy \in E(G)} \sqrt{{d_x}^2 + {d_y}^2}$$

$$SO_{red}(G) = \sum_{xy \in E(G)} \sqrt{(d_x - 1)^2 + (d_y - 1)^2}.$$

Senthilkumar et al. [11] concentrate on the behavior of the maximum Sombor index with unicyclic graphs that have a fixed girth and very recently, Zhang et al. [13] and Chen and Zhu [2] independently identified the minimum Sombor index of unicyclic graphs characterized by a fixed girth. Inspired by the works, we order the minimum uniyclic graphs of a given girth κ $(3 \leq \kappa \leq n)$ by Sombor index and reduced Sombor index.

At this juncture, it is prudent to introduce certain notations and terminologies that will assume significance in the ensuing sections. The set $\mathbb{U}_n$ represents all unicyclic graphs that consist of at least five vertices. Subsequently, $\mathbb{U}_{n,\kappa}$ represents the subset of unicyclic graphs characterized by a fixed girth κ $(3 \leq \kappa \leq n)$ and a specific number of n vertices. Interestingly, the set $\mathbb{U}_n$ can be constructed as the amalgamation of $\mathbb{U}_{n,\kappa}$ sets for varying girth values, a succinct depiction being $\mathbb{U}_n = \bigcup_{\kappa=3}^{n} \mathbb{U}_{n,\kappa}$. Furthermore, $\mathbf{C}_n$ denotes the cycle on n vertices, it can be inferred that $\mathbb{U}_{n,n} = \mathbf{C}_n$. In a similar manner, $\mathcal{U}^1_{n,n-1}$ denotes the distinctive unicyclic graph with a girth $n-1$ and n vertices is concluded that $\mathbb{U}_{n,n-1} = \mathcal{U}^1_{n,n-1}$. The forthcoming discussions will focus exclusively on instances where $3 \leq \kappa \leq n-2$.

2 Investigating the smallest Sombor indices in $\mathbb{U}_{n,\kappa}$ graphs

This section delves into the analysis of the graphs within the set $\mathbb{U}_{n,\kappa}$, and aims to ascertain the first to fourth smallest values of the Sombor indices along with their corresponding extremal graphs. To facilitate this analysis, we commence by introducing several lemmas that will prove instrumental in our exploration.

Lemma 1. *Consider* $f(v) = \sqrt{a^2 + v^2} - \sqrt{b^2 + v^2}$, *where* $a > b \geq 1$ *and* $v \geq 1$. *This function exhibits a decreasing trend.*

Proof. Since we have for $v \geq 1$,

$$f'(v) = \frac{v}{\sqrt{a^2 + v^2}} - \frac{v}{\sqrt{b^2 + v^2}} < 0,$$

which is a decreasing function when $v \geq 1$ and $a > b \geq 1$. ■

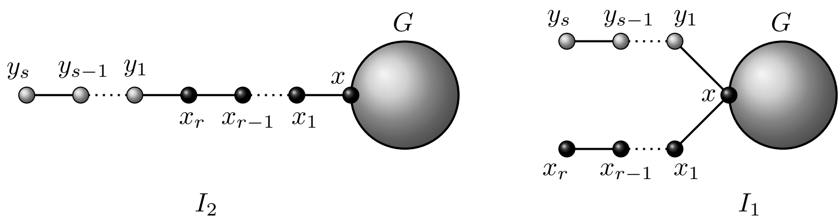

Figure 1. Graphs I_1 and I_2

Transformation 1: Consider a vertex x in a connected graph G that is not trivial. Create a new graph I_1 by connecting 2 pendant paths, U and V, to the vertex x in G. Where $U := xx_1...x_r$ and $V := xy_1...y_s(r \geq s \geq 1)$; I_2 be the graph created from I_1 by connecting an edge $x_r y_1$ and removing an edge xy_1. (Refer to Figure 1 for a visual representation of these graphs.)

Lemma 2. *Consider the graphs in Transformation 1 to be denoted by* I_1 *and* I_2. *Then* $SO(I_1) > SO(I_2)$ *and* $SO_{red}(I_1) > SO_{red}(I_2)$.

Proof. Let $d_{I_1}(x) = \alpha \geq 3$, and $N_G(x) = N_{I_1}(x) \setminus \{x_1, y_1\} = \{z_1, z_2, \ldots, z_{\alpha-2}\}$. Each vertex z_i (for $1 \leq i \leq \alpha - 2$) has a degree in I_1, denoted as $d_G(z_i) = d_{I_1}(z_i) = \alpha_i$. Lemma 1, states that for $a > b \geq 1$ and $v \geq 1$, $f(v)$ is decreasing. We intend to examine three scenarios, each with a different value for r and s.

Case (1): $r = s = 1$.

When $d_{I_1}(x_1) = d_{I_1}(y_1) = 1$. It follows that

$$
\begin{aligned}
& SO(I_1) - SO(I_2) \\
&= \sum_{i=1}^{\alpha-2} \sqrt{d_{I_1}^2(x) + d_{I_1}^2(z_i)} + \sqrt{d_{I_1}^2(x) + d_{I_1}^2(x_1)} + \sqrt{d_{I_1}^2(x) + d_{I_1}^2(y_1)} \\
&\quad - \sum_{i=1}^{\alpha-2} \sqrt{d_{I_2}^2(x) + d_{I_2}^2(z_i)} - \sqrt{d_{I_2}^2(x) + d_{I_2}^2(x_1)} - \sqrt{d_{I_2}^2(x_1) + d_{I_2}^2(y_1)} \\
&= \sum_{i=1}^{\alpha-2} \sqrt{\alpha^2 + {\alpha_i}^2} + 2\sqrt{\alpha^2 + 1^2} - \sum_{i=1}^{\alpha-2} \sqrt{(\alpha-1)^2 + {\alpha_i}^2} \\
&\quad - \sqrt{(\alpha-1)^2 + 2^2} - \sqrt{2^2 + 1^2} \\
&= \sum_{i=1}^{\alpha-2} \left(\sqrt{\alpha^2 + {\alpha_i}^2} - \sqrt{(\alpha-1)^2 + {\alpha_i}^2} \right) + 2\sqrt{\alpha^2 + 1} \\
&\quad - \sqrt{\alpha^2 - 2\alpha + 5} - \sqrt{5} \\
&> 2\sqrt{\alpha^2 + 1} - \sqrt{\alpha^2 - 2\alpha + 5} - \sqrt{5} > 0.
\end{aligned}
$$

Case (2) : $r > s = 1$.

When $d_{I_1}(x_1) = 2$ and $d_{I_1}(y_1) = 1$. It follows that

$$
\begin{aligned}
& SO(I_1) - SO(I_2) \\
&= \sum_{i=1}^{\alpha-2} \sqrt{d_{I_1}^2(x) + d_{I_1}^2(z_i)} + \sqrt{d_{I_1}^2(x) + d_{I_1}^2(x_1)} + \sqrt{d_{I_1}^2(x) + d_{I_1}^2(y_1)} \\
&\quad + \sqrt{d_{I_1}^2(x_{r-1}) + d_{I_1}^2(x_r)} - \sum_{i=1}^{\alpha-2} \sqrt{d_{I_2}^2(x) + d_{I_2}^2(z_i)} - \sqrt{d_{I_2}^2(x) + d_{I_2}^2(x_1)} \\
&\quad - \sqrt{d_{I_2}^2(x_r) + d_{I_2}^2(y_1)} - \sqrt{d_{I_2}^2(x_{r-1}) + d_{I_2}^2(x_r)} \\
&= \sum_{i=1}^{\alpha-2} \sqrt{\alpha^2 + {\alpha_i}^2} + \sqrt{\alpha^2 + 1^2} + \sqrt{\alpha^2 + 2^2} + \sqrt{2^2 + 1^2}
\end{aligned}
$$

$$
\begin{aligned}
&-\sum_{i=1}^{\alpha-2}\sqrt{(\alpha-1)^2+{\alpha_i}^2}-\sqrt{(\alpha-1)^2+2^2}-\sqrt{2^2+2^2}-\sqrt{2^2+1^2}\\
&=\left(\sum_{i=1}^{\alpha-2}\sqrt{\alpha^2+{\alpha_i}^2}-\sqrt{(\alpha-1)^2+{\alpha_i}^2}\right)+\sqrt{\alpha^2+1}+\sqrt{\alpha^2+4}\\
&-\sqrt{\alpha^2-2\alpha+5}-\sqrt{8}\\
&>\sqrt{\alpha^2+1}+\sqrt{\alpha^2+4}-\sqrt{\alpha^2-2\alpha+5}-\sqrt{8}>0.
\end{aligned}
$$

Case (3) : $r \geq s > 1$.
When $d_{I_1}(x_1) = d_{I_1}(y_1) = 2$. It follows that

$$
\begin{aligned}
&SO(I_1)-SO(I_2)\\
&=\sum_{i=1}^{\alpha-2}\sqrt{d^2_{I_1}(x)+d^2_{I_1}(z_i)}+\sqrt{d^2_{I_1}(x)+d^2_{I_1}(x_1)}+\sqrt{d^2_{I_1}(x)+d^2_{I_1}(y_1)}\\
&+\sqrt{d^2_{I_1}(x_r)+d^2_{I_1}(x_{r-1})}-\sum_{i=1}^{\alpha-2}\sqrt{d^2_{I_2}(x)+d^2_{I_2}(z_i)}-\sqrt{d^2_{I_2}(x)+d^2_{I_2}(x_1)}\\
&-\sqrt{d^2_{I_2}(x_r)+d^2_{I_2}(x_{r-1})}-\sqrt{d^2_{I_2}(x_r)+d^2_{I_2}(y_1)}\\
&=\sum_{i=1}^{\alpha-2}\sqrt{\alpha^2+{\alpha_i}^2}+2\sqrt{\alpha^2+2^2}+\sqrt{2^2+1^2}-\sum_{i=1}^{\alpha-2}\sqrt{(\alpha-1)^2+{\alpha_i}^2}\\
&-\sqrt{(\alpha-1)^2+2^2}-2\sqrt{2^2+2^2}\\
&=\sum_{i=1}^{\alpha-2}\left(\sqrt{\alpha^2+{\alpha_i}^2}-\sqrt{(\alpha-1)^2+{\alpha_i}^2}\right)+2\sqrt{\alpha^2+4}\\
&-\sqrt{\alpha^2-2\alpha+5}-2\sqrt{8}+\sqrt{5}\\
&>2\sqrt{\alpha^2+4}-\sqrt{\alpha^2-2\alpha+5}-2\sqrt{8}+\sqrt{5}>0.
\end{aligned}
$$

Hence $SO(I_1) > SO(I_2)$ and similarly $SO_{red}(I_1) > SO_{red}(I_2)$. This concludes the proof. ■

Transformation 2: Consider G be a non trivial connected graph. Choose two unique vertices x and y in G with $d_G(x), d_G(y) \geq 2$. Now, construct a graph H_1 by connecting 2 paths U and V, at x and y, respectively. These path can be represented as follows: $U := xx_1 \dots x_r$ and $V := yy_1 \dots y_s(r \geq$

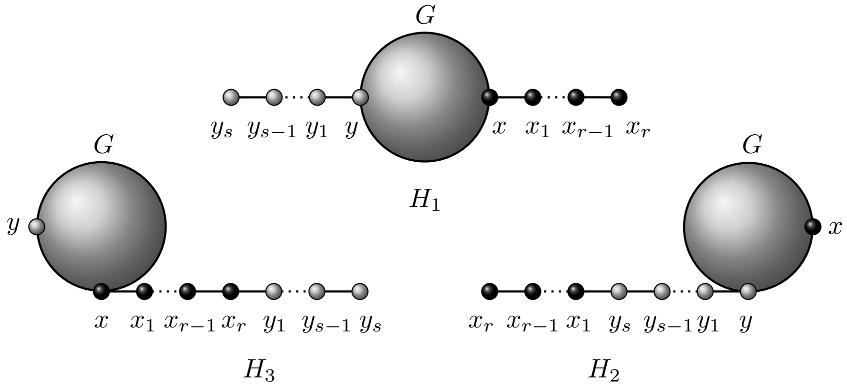

Figure 2. Graphs H_1, H_2 and H_3

$s \geq 1$). Let H_2 be the graph created from H_1 by connecting an edge $y_s x_1$ and removing xx_1 and H_3 be the graph created from H_1 by connecting an edge $x_r y_1$ and removing yy_1. (Refer to Figure 2 for visual representation of these graphs.)

Lemma 3. *Consider the graphs H_1, H_2 and H_3 in Transformation 2. Then*

$$SO(H_1) > \max\{SO(H_2), SO(H_3)\}$$
$$SO_{red}(H_1) > \max\{SO_{red}(H_2), SO_{red}(H_3)\}.$$

Proof. We can make the assumption that, with no loss of generality, $SO(H_3) \geq SO(H_2)$. Lemma 1, states that for $a > b \geq 1$ and $v \geq 1$, $f(v)$ is decreasing. Let $d_{H_1}(x) = \alpha \geq 3$ and $d_{H_1}(y) = \eta \geq 3$. Now, consider $N_G(y) = N_{H_1}(y) \setminus \{y_1\} = \{z_1, z_2, \ldots, z_{\eta-1}\}$. Each vertex z_i (for $1 \leq i \leq \eta - 1$) has a degree in H_1, denoted as $d_{H_1}(z_i) = \eta_i$. Furthermore, if the edge $xy \in E(H_1)$, then $z_1 = x$. We intend to examine three scenarios, each based on different values for r and s.

Case (1) : $r = s = 1$.

In this case, $d_{H_1}(x_1) = d_{H_1}(y_1) = 1$, it follows that

$$\begin{aligned}
&SO(H_1) - SO(H_3) \\
&= \sum_{i=1}^{\eta-1} \sqrt{d_{H_1}^2(y) + d_{H_1}^2(z_i)} + \sqrt{d_{H_1}^2(x) + d_{H_1}^2(x_1)} + \sqrt{d_{H_1}^2(y) + d_{H_1}^2(y_1)} \\
&- \sum_{i=1}^{\eta-1} \sqrt{d_{H_2}^2(y) + d_{H_2}^2(z_i)} - \sqrt{d_{H_2}^2(x) + d_{H_2}^2(x_1)} - \sqrt{d_{H_2}^2(x_1) + d_{H_2}^2(y_1)}
\end{aligned}$$

$$\begin{aligned}
&= \sum_{i=1}^{\eta-1} \sqrt{\eta^2 + {\eta_i}^2} + \sqrt{\eta^2 + 1^2} + \sqrt{\alpha^2 + 1^2} - \sum_{i=1}^{\eta-1} \sqrt{(\eta-1)^2 + {\eta_i}^2} \\
&- \sqrt{\alpha^2 + 2^2} - \sqrt{2^2 + 1^2} \\
&= \sum_{i=1}^{\eta-1} \left(\sqrt{\eta^2 + {\eta_i}^2} - \sqrt{(\eta-1)^2 + {\eta_i}^2} \right) + \sqrt{\eta^2 + 1} + \sqrt{\alpha^2 + 1} \\
&- \sqrt{\alpha^2 + 4} - \sqrt{5} \\
&> \sqrt{\eta^2 + 1} + \sqrt{\alpha^2 + 1} - \sqrt{\alpha^2 + 4} - \sqrt{5} > 0.
\end{aligned}$$

Case (2) : $r > s = 1$.

In this case, $d_{H_1}(x_1) = 2$ and $d_{H_1}(y_1) = 1$. It follows that

$$\begin{aligned}
&SO(H_1) - SO(H_3) \\
&= \sum_{i=1}^{\eta-1} \sqrt{d_{H_1}^2(y) + d_{H_1}^2(z_i)} + \sqrt{d_{H_1}^2(y) + d_{H_1}^2(y_1)} \\
&+ \sqrt{d_{H_1}^2(x_{r-1}) + d_{H_1}^2(x_r)} - \sum_{i=1}^{\eta-1} \sqrt{d_{H_2}^2(y) + d_{H_2}^2(z_i)} \\
&- \sqrt{d_{H_2}^2(x_{r-1}) + d_{H_2}^2(x_r)} - \sqrt{d_{H_2}^2(x_r) + d_{H_2}^2(y_1)} \\
&= \sum_{i=1}^{\eta-1} \sqrt{\eta^2 + {\eta_i}^2} + \sqrt{\eta^2 + 1^2} + \sqrt{2^2 + 1^2} \\
&- \sum_{i=1}^{\eta-1} \sqrt{(\eta-1)^2 + {\eta_i}^2} - \sqrt{2^2 + 2^2} - \sqrt{2^2 + 1^2}
\end{aligned}$$

$$= \sum_{i=1}^{\eta-1} \left(\sqrt{\eta^2 + {\eta_i}^2} - \sqrt{(\eta-1)^2 + {\eta_i}^2} \right) + \sqrt{\eta^2+1} - \sqrt{8}$$
$$> \sqrt{\eta^2+1} - \sqrt{8} > 0.$$

Case (3) : $r \geq s > 1$.
In this case, $d_{H_1}(x_1) = d_{H_1}(y_1) = 2$. It follows that

$$SO(H_1) - SO(H_3)$$
$$= \sum_{i=1}^{\eta-1} \sqrt{d^2_{H_1}(y) + d^2_{H_1}(z_i)} + \sqrt{d^2_{H_1}(y) + d^2_{H_1}(y_1)}$$
$$+ \sqrt{d^2_{H_1}(x_r) + d^2_{H_1}(x_{r-1})} - \sum_{i=1}^{\eta-1} \sqrt{d^2_{H_2}(y) + d^2_{H_2}(z_i)}$$

$$- \sqrt{d^2_{H_2}(x_r) + d^2_{H_2}(x_{r-1})} - \sqrt{d^2_{H_2}(x_r) + d^2_{H_2}(y_1)}$$
$$= \sum_{i=1}^{\eta-1} \sqrt{\eta^2 + {\eta_i}^2} + \sqrt{\eta^2 + 2^2} + 2\sqrt{2^2+1^2}$$
$$- \sum_{i=1}^{\eta-1} \sqrt{(\eta-1)^2 + {\eta_i}^2} - 2\sqrt{2^2+2^2} - \sqrt{2^2+1^2}$$
$$= \sum_{i=1}^{\eta-1} \left(\sqrt{\eta^2 + {\eta_i}^2} - \sqrt{(\eta-1)^2 + {\eta_i}^2} \right) + \sqrt{\eta^2+4} - 2\sqrt{8} + \sqrt{5}$$
$$> \sqrt{\eta^2+4} - 2\sqrt{8} + \sqrt{5} > 0.$$

Hence $SO(H_1) > SO(H_3)$ and similarly $SO_{red}(H_1) > SO_{red}(H_3)$.This concludes the proof. ■

The graph known as $\mathcal{U}_{n,\kappa}$ is referred to as a unicyclic graph comprising n vertices and girth of κ, with $3 \leq \kappa \leq n-1$. As can be seen in Figure 3, this graph is constructed by joining a vertex x to a cycle $\mathbf{C}_\kappa$ via a path that has a length of $n - \kappa$.

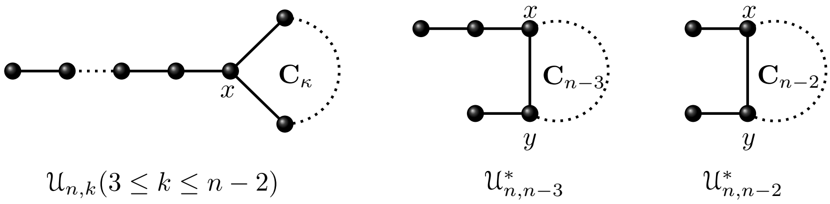

Figure 3. The set of graphs $\mathcal{U}_{n,\kappa}(3 \le \kappa \le n-2)$, $\mathcal{U}^*_{n,n-3}$ and $\mathcal{U}^*_{n,n-2}$.

Theorem 1. *Consider $G \in \mathbb{U}_{n,\kappa}$, when $3 \le \kappa \le n-2$. For such graphs, the following inequalities hold:*

$$SO(G) \ge (n-4)\sqrt{8} + 3\sqrt{13} + \sqrt{5},$$
$$SO_{red}(G) \ge (n-4)\sqrt{2} + 3\sqrt{5} + 1.$$

Equality is maintained, if and only if $G \cong \mathcal{U}_{n,\kappa}$.

Proof. Consider $\mathbf{C} := y_1y_2y_3\dots y_\kappa y_1$ be the cycle graph in G. It follows that there is at least one vertex in $\{y_1, y_2, \dots, y_\kappa\}$ of degree at least 3.

Assume to the contrary that at least two vertices in $\{y_1, y_2, \dots, y_\kappa\}$ have degree at least three. In accordance with Lemmas 2 and 3, we have $SO(G) > SO(\mathcal{U}_{n,\kappa})$, which is a contradiction. Thus, we may assume that the set $\{y_1, y_2, \dots, y_\kappa\}$ contains exactly one vertex of degree at least 3, say y_i. If $d(y_i) \ge 4$, based on Lemma 2 $SO(G) > SO(\mathcal{U}_{n,\kappa})$, which is also a contradiction. Hence $d(y_i) = 3$ and by Lemma 2, equality is true if and only if $G \cong \mathcal{U}_{n,\kappa}$ and that $SO(G) \ge SO(\mathcal{U}_{n,\kappa})$.
Consequently,

$$SO(\mathcal{U}_{n,\kappa}) = (n-4)\sqrt{8} + 3\sqrt{13} + \sqrt{5}.$$

In a similar way,

$$SO_{red}(\mathcal{U}_{n,\kappa}) = (n-4)\sqrt{2} + 3\sqrt{5} + 1.$$

The proof for Theorem 1 is now concluded. ∎

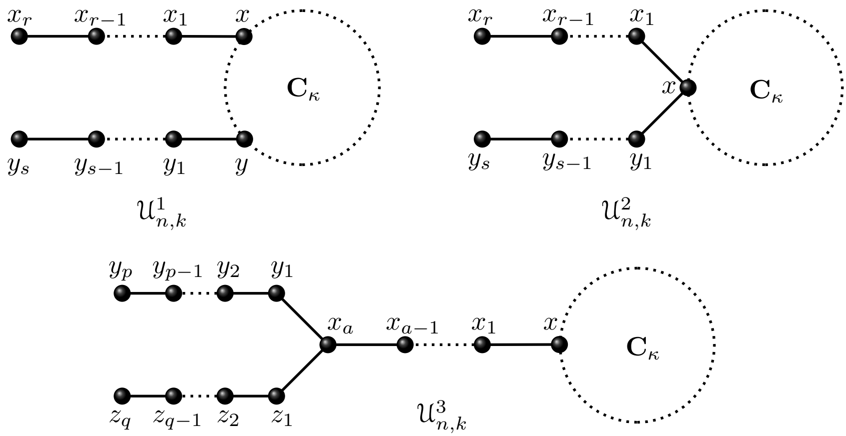

Figure 4. The sets of graphs $\mathcal{U}^1_{n,\kappa}$, $\mathcal{U}^2_{n,\kappa}(3 \leq \kappa \leq n-2)$ and $\mathcal{U}^3_{n,\kappa}$ $(3 \leq \kappa \leq n-3)$.

Under the assumption that for each $3 \leq \kappa \leq n-2$, it is possible to define 3 different collections of unicyclic graphs that have n vertices. In the cycle $\mathbf{C}_\kappa$, 2 paths with lengths r and s are connected to 2 distinct vertices x and y to produce the graphs $\mathcal{U}^1_{n,\kappa}$, where $(r \geq s \geq 1$ and $r+s = n-\kappa)$. In a cycle $\mathbf{C}_\kappa$, 2 paths with lengths r and s are connected to single vertex x to produce the graphs $\mathcal{U}^2_{n,\kappa}$, where $(r \geq s \geq 1$ and $r+s = n-\kappa)$.

A path with a length of a that connects a vertex x from $\mathbf{C}_\kappa$ to another vertex y, which is not a pendant vertex. There are two additional paths y_p and z_q where $(p, q \geq 1)$ and have combined length of $p+q = b$ that is connected to y. This arrangement creates graphs in $\mathcal{U}^3_{n,\kappa}$, where $(b \geq 2, a \geq 1$ and $a+b = n-\kappa)$. (Refer to Figure 4 for a visual representation of these graphs.)

Lemma 4. *Consider* $G \in \mathcal{U}^1_{n,\kappa} \cup \mathcal{U}^2_{n,\kappa}$ *when* $3 \leq \kappa \leq n-4$. *For such graphs, the following inequalities hold:*

$$SO(G) \geq (n-7)\sqrt{8} + 4\sqrt{13} + \sqrt{18} + 2\sqrt{5}$$
$$SO_{red}(G) \geq (n-7)\sqrt{2} + 4\sqrt{5} + \sqrt{8} + 2.$$

Equality is maintained, if and only if $G \in \mathcal{U}^1_{n,\kappa}$, *for the edge* xy *belongs to* *the graph G with* $r \geq s > 1$.

Proof. Suppose $G \in \mathcal{U}^1_{n,\kappa}$.
In the case where the edge xy belongs to the graph G, this implies that

$$SO(G) = \begin{cases} (n-6)\sqrt{8} + 3\sqrt{13} + \sqrt{18} + \sqrt{10} + \sqrt{5}, & when \ \ r > s = 1, \\ (n-7)\sqrt{8} + 4\sqrt{13} + \sqrt{18} + 2\sqrt{5}, & when \ \ r \geq s > 1. \end{cases}$$

and

$$SO_{red}(G) = \begin{cases} (n-6)\sqrt{2} + 3\sqrt{5} + \sqrt{8} + 3, & when \ \ r > s = 1, \\ (n-7)\sqrt{2} + 4\sqrt{5} + \sqrt{8} + 2, & when \ \ r \geq s > 1. \end{cases}$$

when $xy \notin E(G)$, then

$$SO(G) = \begin{cases} (n-7)\sqrt{8} + 5\sqrt{13} + \sqrt{10} + \sqrt{5}, & when \ \ r > s = 1, \\ (n-8)\sqrt{8} + 6\sqrt{13} + 2\sqrt{5}, & when \ \ r \geq s > 1. \end{cases}$$

and

$$SO_{red}(G) = \begin{cases} (n-7)\sqrt{2} + 5\sqrt{5} + 3, & when \ \ r > s = 1, \\ (n-8)\sqrt{2} + 6\sqrt{5} + 2, & when \ \ r \geq s > 1. \end{cases}$$

Given that $G \in \mathcal{U}^2_{n,\kappa}$. It follows that

$$SO(G) = \begin{cases} (n-5)\sqrt{8} + 3\sqrt{20} + \sqrt{17} + \sqrt{5}, & when \ \ r > s = 1, \\ (n-6)\sqrt{8} + 4\sqrt{20} + 2\sqrt{5}, & when \ \ r \geq s > 1. \end{cases}$$

and

$$SO_{red}(G) = \begin{cases} (n-5)\sqrt{2} + 3\sqrt{10} + 4, & when \ \ r > s = 1, \\ (n-6)\sqrt{2} + 4\sqrt{10} + 2, & when \ \ r \geq s > 1. \end{cases}$$

Since for Sombor index,

$$
\begin{aligned}
&(n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}<(n-8)\sqrt{8}+6\sqrt{13}+2\sqrt{5}\\
&<(n-6)\sqrt{8}+3\sqrt{13}+\sqrt{18}+\sqrt{10}+\sqrt{5}<(n-7)\sqrt{8}+5\sqrt{13}+\sqrt{10}+\sqrt{5}\\
&<(n-6)\sqrt{8}+4\sqrt{20}+2\sqrt{5}<(n-5)\sqrt{8}+3\sqrt{20}+\sqrt{17}+\sqrt{5}
\end{aligned}
$$

and for reduced Sombor index,

$$
\begin{aligned}
&(n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2<(n-6)\sqrt{2}+3\sqrt{5}+\sqrt{8}+3\\
&<(n-8)\sqrt{2}+6\sqrt{5}+2<(n-7)\sqrt{2}+5\sqrt{5}+3\\
&<(n-6)\sqrt{2}+4\sqrt{10}+2<(n-5)\sqrt{2}+3\sqrt{10}+4.
\end{aligned}
$$

Therefore, the aforementioned analysis confirms the validity of the assertions within the lemma, and thus, we can conclude the proof. ∎

Lemma 5. *Consider $G \in \mathfrak{U}^3_{n,\kappa}$ when $3 \le \kappa \le n-4$. For such graphs, the following inequalities hold:*

$$
\begin{aligned}
SO(G) &\ge (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5},\\
SO_{red}(G) &\ge (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2.
\end{aligned}
$$

Where equality is achieved only under the condition that the edge xy belongs to the graph G i.e., $a = 1$ and vertex $y \sim y_p$ and $y \sim z_q$, where $p > 1$ and $q > 1$.

Proof. Initially assume that $a = 1$. In this scenario, it can be deduced $b \ge 3$ and vertex $y \sim y_p$ and $y \sim z_q$ either $p = 1, q > 1$ or $q = 1, p > 1$. Hence,

$$
SO(G)=\begin{cases}(n-6)\sqrt{8}+3\sqrt{13}+\sqrt{18}+\sqrt{10}+\sqrt{5}, & \text{when } p=1 \text{ or } q=1,\\ (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}, & \text{when } p>1 \text{ and } q>1.\end{cases}
$$

and

$$
SO_{red}(G)=\begin{cases}(n-6)\sqrt{2}+3\sqrt{5}+\sqrt{8}+3, & \text{when } p=1 \text{ or } q=1,\\ (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2, & \text{when } p>1 \text{ and } q>1.\end{cases}
$$

Assume that $a > 1$. Then

$$SO(G) = \begin{cases} (n-6)\sqrt{8} + 4\sqrt{13} + 2\sqrt{10}, & \textit{when } p = 1 \textit{ and } q = 1, \\ (n-7)\sqrt{8} + 5\sqrt{13} + \sqrt{10} + \sqrt{5}, & \textit{when } p = 1 \textit{ or } q = 1, \\ (n-8)\sqrt{8} + 6\sqrt{13} + 2\sqrt{5}, & \textit{when } p > 1 \textit{ and } q > 1. \end{cases}$$

and

$$SO_{red}(G) = \begin{cases} (n-6)\sqrt{2} + 4\sqrt{5} + 4, & \textit{when } p = 1 \textit{ and } q = 1, \\ (n-7)\sqrt{2} + 5\sqrt{5} + 3, & \textit{when } p = 1 \textit{ or } q = 1, \\ (n-8)\sqrt{2} + 6\sqrt{5} + 2, & \textit{when } p > 1 \textit{ and } q > 1. \end{cases}$$

For Sombor index,

$$\begin{aligned} &(n-7)\sqrt{8} + 4\sqrt{13} + \sqrt{18} + 2\sqrt{5} < (n-8)\sqrt{8} + 6\sqrt{13} + 2\sqrt{5} \\ &< (n-6)\sqrt{8} + 3\sqrt{13} + \sqrt{18} + \sqrt{10} + \sqrt{5} < (n-7)\sqrt{8} + 5\sqrt{13} + \sqrt{10} + \sqrt{5} \\ &< (n-6)\sqrt{8} + 4\sqrt{13} + 2\sqrt{10}. \end{aligned}$$

and for reduced Sombor index,

$$\begin{aligned} &(n-7)\sqrt{2} + 4\sqrt{5} + \sqrt{8} + 2 < (n-6)\sqrt{2} + 3\sqrt{5} + \sqrt{8} + 3 \\ &< (n-8)\sqrt{2} + 6\sqrt{5} + 2 < (n-7)\sqrt{2} + 5\sqrt{5} + 3 \\ &< (n-6)\sqrt{2} + 4\sqrt{5} + 4. \end{aligned}$$

The lemma is true as a result. ■

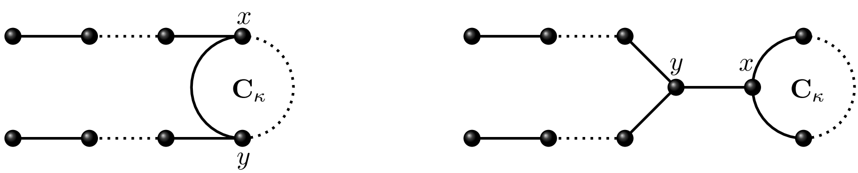

Figure 5. Two categories of graphs in the set $\mathcal{U}^*_{n,\kappa}$ $(3 \leq \kappa \leq n-4)$

Unicyclic graphs that have a girth $(3 \leq \kappa \leq n-4)$ with n vertices, are denoted as $\mathcal{U}^*_{n,\kappa}$. These graphs are constructed in two distinct manner: firstly, by connecting 2 paths, each with a minimum length of two, to 2 adjacent vertices, denoted as x, y of the cycle $\mathbf{C}_\kappa$; secondly, by establishing an edge that connects one vertex, denoted as x in $\mathbf{C}_\kappa$ to another vertex, denoted as y, which is part of a path with a length of $n-\kappa-1$. Figure 5 provides a visual representation of the fact that, y is placed in such a way that it is not adjacent to any of the pendant vertices. It is apparent that the set $\mathcal{U}^*_{n,\kappa} \subseteq \mathcal{U}^1_{n,\kappa} \cup \mathcal{U}^3_{n,\kappa}$. $SO(\mathcal{U}^*_{n,\kappa}) = (n-7)\sqrt{8} + 4\sqrt{13} + \sqrt{18} + 2\sqrt{5}$ and $SO_{red}(G) \geq (n-7)\sqrt{2} + 4\sqrt{5} + \sqrt{8} + 2$. To elaborate further, when $\kappa = n-3$, the $\mathcal{U}^*_{n,n-3}$ graph is created by the attachment of a path with a length of 2 along with an additional edge (pendant edge) that connects 2 neighboring vertices, denoted as x and y within the cycle $\mathbf{C}_{n-3}$. In a similar manner, when $\kappa = n-2$, it is possible to create the $\mathcal{U}^*_{n,n-2}$ graph by connecting 2 additional edges (pendant edges) to 2 neighboring vertices, denoted as x and y of the cycle $\mathbf{C}_{n-2}$. This process is portrayed in Figure 3. We are able to ascertain the second-smallest Sombor indices for the graphs within the $\mathbb{U}_{n,\kappa}$ set by employing reasoning analogous to that utilized in the proof of Theorem 1.

Theorem 2. *Consider $G \in \mathbb{U}_{n,\kappa}$ and $G \ncong \mathcal{U}_{n,\kappa}$. The following inequalities apply for such graphs:*
(1) If $3 \leq \kappa \leq n-4$, then

$$SO(G) \geq (n-7)\sqrt{8} + 4\sqrt{13} + \sqrt{18} + 2\sqrt{5}$$
$$SO_{red}(G) \geq (n-7)\sqrt{2} + 4\sqrt{5} + \sqrt{8} + 2.$$

Equality is maintained, if and only if $G \in \mathcal{U}^*_{n,\kappa}$.
(2) If $\kappa = n-3$, then

$$SO(G) \geq (n-6)\sqrt{8} + 3\sqrt{13} + \sqrt{18} + \sqrt{10} + \sqrt{5}$$
$$SO_{red}(G) \geq (n-6)\sqrt{2} + 3\sqrt{5} + \sqrt{8} + 3.$$

Equality is maintained, if and only if $G \cong \mathcal{U}^*_{n,n-3}$.
(3) If $\kappa = n-2$, then

$$SO(G) \geq (n-5)\sqrt{8} + 2\sqrt{13} + \sqrt{18} + 2\sqrt{10}$$
$$SO(G) \geq (n-5)\sqrt{2} + 2\sqrt{5} + \sqrt{8} + 4.$$

Equality is maintained, if and only if $G \cong \mathfrak{U}^*_{n,n-2}$.

Proof. Consider a unique cycle $\mathbf{C}$ in G, represented as $\mathbf{C} := y_1y_2...y_\kappa y_1$, then a cycle with atleast a degree of three must formed by atleast one vertex from the set $\{y_1, y_2, ...y_\kappa\}$.

If the length of the cycle $\mathbf{C}$ in the graph G is $3 \leq \kappa \leq n-4$ and if at least three of the vertices in the set $\{y_1, y_2, ...y_\kappa\}$ have a degree of at least three. Using Lemmas 2, 3 and 4, it can determine that there is a graph $G_1 \in \mathfrak{U}^1_{n,\kappa}$ satisfies that $SO(G) > SO(G_1) \geq (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}$ and $SO_{red}(G) > SO_{red}(G_1) \geq (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2$. If there are exactly 2 vertices in $\{y_1, y_2, ...y_\kappa\}$ that have at least a degree of 3, then Lemmas 2 and 4 indicate that there is a graph $G_2 \in \mathfrak{U}^1_{n,\kappa}$ such that $SO(G) \geq SO(G_2) \geq (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}$ and $SO_{red}(G) > SO_{red}(G_2) \geq (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2$, in the case where equality is maintained, if and only if $G \in \mathfrak{U}^1_{n,\kappa} \cap \mathfrak{U}^*_{n,\kappa}$.

According to Lemmas 2 and 4, if there is a vertex y_i in the set of vertices $\{y_1, y_2, ...y_\kappa\}$ that have a degree of at least three and $d(y_i) \geq 5$, then it implies the existence of a graph $G_3 \in \mathfrak{U}^2_{n,\kappa}$ such that $SO(G) > SO(G_3) > (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}$ and $SO_{red}(G) > SO_{red}(G_3) \geq (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2$. In a similar way, if $d(y_i) = 4$,then there must be a graph $G_4 \in \mathfrak{U}^2_{n,\kappa}$ such that $SO(G) > SO(G_4) > (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}$ and $SO_{red}(G) > SO_{red}(G_4) \geq (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2$.

As a result, we can reason that $d(y_i) = 3$. Due to the fact $G \ncong \mathfrak{U}_{n,\kappa}$. To maintain the existence of the cycle $\mathbf{C}$ at least one vertex outside the cycle must have at least a degree of 3; otherwise, the cycle cannot exist. If there are at least two vertices outside of the cycle $\mathbf{C}$ that each have a degree of at least three, then we can utilize the Lemmas 2 and 5 to conclude that there is a graph $G_5 \in \mathfrak{U}^3_{n,\kappa}$ such that $SO(G) > SO(G_5) > (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}$ and $SO_{red}(G) > SO_{red}(G_5) \geq (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2$.

As a consequence of this, we are able to make the assumption that, there exists one vertex that have a degree of at least three outside the cycle $\mathbf{C}$, which suggests that $G \in \mathfrak{U}^3_{n,\kappa}$ set. Then by utilizing Lemma 5, we can deduce that $SO(G) > (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}$ and $SO_{red}(G) \geq (n-7)\sqrt{2}+4\sqrt{5}+\sqrt{8}+2$.

Equality is maintained, if and only if $G \in \mathfrak{U}^*_{n,\kappa}$. Because $\mathfrak{U}^*_{n,\kappa} \subseteq$

$\mathcal{U}^1_{n,\kappa} \cup \mathcal{U}^3_{n,\kappa}$, the assertion (1) in the theorem must be true. When applied to the scenarios in which $\kappa = n-2$ or $\kappa = n-3$, similar arguments demonstrate that assertions (2) and (3) are also true. As a result, the theorem can be demonstrated. ■

Since

$$SO(\mathcal{U}_{n,n-1}) = (n-3)\sqrt{8} + 2\sqrt{13} + \sqrt{10}$$

and

$$SO_{red}(\mathcal{U}_{n,n-1}) = (n-3)\sqrt{2} + 2\sqrt{5} + 2.$$

For the cycle $\mathbf{C}_n$, $SO(\mathbf{C}_n) = n\sqrt{8}$ and $SO_{red}(\mathbf{C}_n) = n\sqrt{2}$. The following conclusions can be drawn by using Theorem 1 and Theorem 2 in a straightforward manner.

Corollary 1. *Let the graphs specified above be $\mathcal{U}_{n,\kappa}$ and $\mathcal{U}^*_{n,\kappa}$.*
(1) If $n = 5$, then
$SO(\mathcal{U}^*_{5,3}) > SO(\mathcal{U}_{5,4}) > SO(\mathcal{U}_{5,3}) > SO(\boldsymbol{C}_5)$.
(2) If $n = 6$, then
$SO(\mathcal{U}^*_{6,4}) > SO(\mathcal{U}^*_{6,3}) > SO(\mathcal{U}_{6,5}) > SO(\mathcal{U}_{6,4}) > SO(\boldsymbol{C}_6)$.
(3) If $n \geq 7$, then
$SO(\mathcal{U}^*_{n,n-2}) > SO(\mathcal{U}^*_{n,n-3}) > SO(\mathcal{U}^*_{n,n-4}) = ... = SO(\mathcal{U}^*_{n,3})$
$> SO(\mathcal{U}_{n,n-1}) > SO(\mathcal{U}_{n,3}) = ... = SO(\mathcal{U}_{n,n-2}) > SO(\boldsymbol{C}_n)$.

Corollary 2. *Let the graphs specified above be $\mathcal{U}_{n,\kappa}$ and $\mathcal{U}^*_{n,\kappa}$.*
(1) If $n = 5$, then
$SO_{red}(\mathcal{U}^*_{5,3}) > SO_{red}(\mathcal{U}_{5,4}) > SO_{red}(\mathcal{U}_{5,3}) > SO_{red}(\boldsymbol{C}_5)$.
(2) If $n = 6$, then
$SO_{red}(\mathcal{U}^*_{6,4}) > SO_{red}(\mathcal{U}^*_{6,3}) > SO_{red}(\mathcal{U}_{6,5}) > SO_{red}(\mathcal{U}_{6,4}) > SO_{red}(\boldsymbol{C}_6)$.
(3) If $n \geq 7$, then
$SO_{red}(\mathcal{U}^*_{n,n-2}) > SO_{red}(\mathcal{U}^*_{n,n-3}) = SO_{red}(\mathcal{U}^*_{n,n-4}) = ... = SO_{red}(\mathcal{U}^*_{n,3})$
$> SO_{red}(\mathcal{U}_{n,n-1}) > SO_{red}(\mathcal{U}_{n,3}) = ... = SO_{red}(\mathcal{U}_{n,n-2}) > SO_{red}(\boldsymbol{C}_n)$.

3 Conclusion

By employing Theorem 1 and 2, and Corollary 1 and 2 we can further deduce the following conclusions: the unique graphs in the $\mathcal{U}_{n,\kappa}$ set with $(3 \leq \kappa \leq n-2)$, that have the second-smallest Sombor indices, and the unique graphs in the set $\mathcal{U}_{n,n-1}$ that have the third-smallest Sombor indices are in the set $\mathbb{U}_n$. Additionally, the graphs in $\mathcal{U}^*_{5,3}$ have the fourth-smallest Sombor indices out of all graphs in $\mathbb{U}_5$, and the graphs in $\mathcal{U}^*_{6,3}$ have the fourth-smallest Sombor indices out of all graphs in $\mathbb{U}_6$. Finally, for $n \geq 7$, the $\mathcal{U}^*_{n,\kappa}$ graph set with $(3 \leq \kappa \leq n-4)$ possess the fourth-smallest Sombor indices out of all graphs in $\mathbb{U}_n$.

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