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Abstract: Recently, a novel degree-based molecular structure descriptor, called Sombor index was introduced. Let \( G \) be a graph. Then, the Sombor index of \( G \) is defined as

\[
SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)}.
\]

In this paper, we give some lemmas that can be used to compare the Sombor indices between two graphs. With these lemmas, we determine the graph with maximum \( SO \) among all cacti with \( n \) vertices and \( k \) cut edges. Furthermore, the unique graph with maximum \( SO \) among all cacti with \( n \) vertices and \( p \) pendant vertices is characterized. In addition, we find the extremal graphs with respect to \( SO \) among all quasi-unicyclic graphs.

Keywords: topological index; vertex degree; Sombor index; cactus; quasi-unicyclic graph

1. Introduction

In this paper, we only consider simple undirected graphs. Let \( G = (V(G), E(G)) \) be a graph with \( n \) vertices and \( m \) edges. If \( m = n + k - 1 \), then \( G \) is called a \( k \)-cyclic graph. A 1-cyclic graph is usually called a unicyclic graph. The complement \( G^c \) of \( G \) is the graph with the vertex set \( V(G) \), and \( xy \in E(G^c) \iff xy \notin E(G) \). The degree of a vertex \( v \) in \( G \), denoted by \( d_G(v) \), is the number of edges incident with \( v \). A vertex of degree one is called a pendant vertex of \( G \), while the edge incident with a pendant vertex is known as a pendant edge. The vertex adjacent to a pendant vertex is usually called a support vertex. To subdivide an edge \( e \) is to delete \( e \), add a new vertex \( x \), and join \( x \) to the end-vertices of \( e \). Suppose \( D \subseteq E(G) \). Then, denote by \( G - D \) the graph obtained from \( G \) by deleting all the elements in \( D \). If \( D = \{e\} \), we write \( G - e \) for \( G - \{e\} \) for simplicity. For a connected graph \( G \), if \( G - e \) is disconnected, then \( e \) is called a cut edge. If \( D \subseteq E(G^c) \), denote by \( G + D \) the graph obtained from \( G \) by adding all of elements in \( D \) to the graph \( G \).

A graph invariant is a numerical quantity which is invariant under graph isomorphism. It is usually referred to as a topological index in chemical graph theory. It is shown that some topological indices can be used to reflect physico-chemical and biological properties of molecules in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) studies [1–3]. Among various topological indices, degree-based and distance-based topological indices have been extensively investigated (see in [4–7]).

In 2021, a novel degree-based topological index was introduced by I. Gutman in [8], called the Sombor index. It was inspired by the geometric interpretation of degree-radii of the edges and defined as

\[
SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)}
\]

for a graph \( G \). I. Gutman [8] also defined the reduced Sombor index as

\[
SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2}.
\]
Later, K. C. Das et al. [9] proposed the following index:

\[ \text{SO}^\dagger(G) = \sum_{u \in E(G)} \sqrt{(d_G(u) + 1)^2 + (d_G(v) + 1)^2}. \]

We name it as the increased Sombor index in this paper.

Recently, the Sombor index has received a lot of attention within mathematics and chemistry. For example, the chemical applicability of the Sombor index, especially the predictive and discriminative potentials was investigated in [10,11]. The results indicate that the Sombor index may be successfully applied for the modeling of thermodynamic properties of compounds and confirm the suitability of this new index in QSPR analysis. For more chemical applications, the readers may see in [12–14] for reference. K. C. Das et al. [15,16] obtained some lower and upper bounds on \( \text{SO} \) in terms of graph parameters. They also presented some relations between \( \text{SO} \) and the Zagreb indices. The relations between \( \text{SO} \) and other degree-based indices were examined in [17].

Graphs having maximum Sombor index among all connected \( k \)-cyclic graphs of order \( n \), where \( 1 \leq k \leq n-2 \), were investigated in [9,18]. R. Cruz et al. [19] characterized the extremal graphs with respect to \( \text{SO} \) over all (connected) chemical graphs, chemical trees, and hexagonal systems. H. Liu [20] determined the extremal graphs with maximum \( \text{SO} \) among all cacti with fixed number of cycles and perfect matchings.

N. Ghanbari et al. [21] studied this index for certain graphs and also examined the effects on \( \text{SO}(G) \) when \( G \) is modified by operations on vertex and edge of \( G \).

Inspired by these works, we establish some new extremal results of the Sombor index.

Recall that a connected graph is a cactus if any two of its cycles have at most one common vertex. A connected graph \( G \) is called a quasi-unicyclic graph if there is a vertex \( v \in V(G) \) such that \( G - v \) is unicyclic. Let \( G_1 \) and \( G_2 \) be two graphs with no vertices in common. The join of \( G_1 \) and \( G_2 \), denoted by \( G_1 \vee G_2 \), is the graph with \( V(G_1 \vee G_2) = V(G_1) \cup V(G_2) \) and \( E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{x_1x_2 : x_1 \in V(G_1), x_2 \in V(G_2)\} \). Let \( P_n, C_n \) and \( S_n \) be the path, cycle and the star with \( n \) vertices, respectively.

This paper is organized as follows. In Section 2, some lemmas are introduced to compare the Sombor indices between two graphs. As applications, in Section 3, the unique graph with maximum \( \text{SO} \) among all cacti with \( n \) vertices and \( k \) cut edges is determined. Furthermore, the unique graph with maximum \( \text{SO} \) among all cacti with \( n \) vertices and \( p \) pendant vertices is characterized. In Section 4, we present the minimum and maximum \( \text{SO} \) of quasi-unicyclic graphs.

### 2. Preliminaries

For convenience, let \( f(x, y) = \sqrt{x^2 + y^2} \), where \( x, y \geq 1 \). For \( f(x, y) \), we have the following result.

**Lemma 1** ([20,22]). Let \( h(x, y) \) be defined for \( x \geq 1, y \geq 1 \) as

\[ h(x, y) = f(x + 1, y) - f(x, y) = \sqrt{(x+1)^2 + y^2} - \sqrt{x^2 + y^2}. \]

Then, for any value of \( y \geq 1 \), \( h \) is increasing as a function of \( x \); for any value of \( x \geq 1 \), \( h \) is decreasing as a function of \( y \).

Let \( P = u_1 \cdots u_k \) be a path in a graph \( G \) with \( d_G(u) \geq 3, d_G(u_1) = \cdots = d_G(u_{k-1}) = 2 \) and \( d_G(u_k) = 1 \). Then, \( P \) is called a pendant path in \( G \) and \( u \) is called the origin of \( P \). In [23], B. Horoldagya et al. showed the following transformation.

**Lemma 2** ([23]). Let \( P \) and \( Q \) be two pendant paths with origins \( u \) and \( v \) in graph \( G \), respectively. Let \( x \) be a neighbor vertex of \( u \) who lies on \( P \) and \( y \) be the pendant vertex on \( Q \). Denote \( G' = (G - ux) + xy \). Then, \( \text{SO}(G) > \text{SO}(G') \).
Now, we introduce some new transformations which increase the Sombor index of a graph.

**Lemma 3.** Let $G$ be a graph and $e = uv$ an edge of $G$ with $N_G(u) \cap N_G(v) = \emptyset$. Let $G'$ be the graph obtained from $G$ by first deleting the edge $e$ and identifying $u$ with $v$, and then attaching a pendant vertex $w$ to the common vertex (see Figure 1). If $d_G(u) \geq 2$ and $d_G(v) \geq 2$, then $SO(G) < SO(G')$.

![Figure 1. Graphs G and G'.](image)

**Proof of Lemma 3.** Suppose $d_G(u) = p + 1$, $d_G(v) = q + 1$, $N_G(u) = \{v, u_1, u_2, \ldots, u_p\}$ and $N_G(v) = \{u, v_1, v_2, \ldots, v_q\}$. Then, $p, q \geq 1$. Therefore,

$$SO(G') - SO(G) = f(p + q + 1, 1) - f(p + 1, q + 1) + \sum_{i=1}^{p} [f(p + q + 1, d'_{G'}(u_i)) - f(p + 1, d_G(u_i))] + \sum_{i=1}^{q} [f(p + q + 1, d'_{G'}(v_i)) - f(q + 1, d_G(v_i))] > f(p + q + 1, 1) - f(p + 1, q + 1) > 0.$$

□

**Lemma 4.** Let $G$ be a graph and $G_{u,v}(p,q)$ the graph obtained from $G$ by attaching $p$ and $q$ pendant edges to $u$ and $v$, respectively, where $u, v \in V(G)$ and $p \geq q \geq 1$. Suppose $|N_G(u) \setminus \{v\}| = |N_G(v) \setminus \{u\}| = a$. Let $N_G(u) \setminus \{v\} = \{x_1, x_2, \ldots, x_a\}$ and $N_G(v) \setminus \{u\} = \{y_1, y_2, \ldots, y_a\}$. If $d_G(x_i) = d_G(y_i)$ for each $1 \leq i \leq a$, then $SO(G_{u,v}(p,q)) < SO(G_{u,v}(p + 1, q + 1))$.

**Proof of Lemma 4.** If $uv \in E(G)$, then by Lemma 1,

$$SO(G_{u,v}(p + 1, q - 1)) - SO(G_{u,v}(p,q)) = f(a + p + 2, a + q) - f(a + p + 1, a + q + 1) + \sum_{i=1}^{a} [f(a + p + 2, d_G(x_i)) - f(a + p + 1, d_G(x_i))] + \sum_{i=1}^{a} [f(a + q, d_G(y_i)) - f(a + q + 1, d_G(y_i))] + (p + 1)f(a + p + 2, 1) - pf(a + p + 1, 1) + (q - 1)f(a + q + 1, 1) - qf(a + q + 1, 1) > \sum_{i=1}^{a} [h(a + p + 1, d_G(x_i)) - h(a + q, d_G(y_i))] + f(a + p + 2, 1) - f(a + q, 1) + p[f(a + p + 2, 1) - f(a + p + 1, 1)] - q[f(a + q + 1, 1) - f(a + q, 1)] \
\geq f(a + p + 2, 1) - f(a + q, 1) + ph(a + p + 1, 1) - qh(a + q, 1) > 0.$$

Now, suppose $uv \notin E(G)$. Then $d_G(u) = d_G(v) = a$. Therefore,
Let \( G \) be a graph and \( C \) a 4-cycle in \( G \). Suppose \( N_G(v_1) \cap N_G(v_3) = \{v_2, v_4\} \). Let \( N_G(v_1) \setminus \{v_2, v_4\} = \{v_{11}, v_{12}, \ldots, v_{1n_1}\} \) and \( N_G(v_3) \setminus \{v_2, v_4\} = \{v_{31}, v_{32}, \ldots, v_{3n_3}\} \), where \( n_1 = d_G(v_1) - 2 > 0 \) and \( n_3 = d_G(v_3) - 2 > 0 \). Let \( G' = (G - \{v_1v_{11}, \ldots, v_1v_{1n_1}\}) + \{v_3v_{31}, \ldots, v_3v_{3n_3}\} \). Then, \( SO(G) < SO(G') \).

**Proof of Lemma 5.** Suppose \( d_G(v_2) = n_2 + 2 \) and \( d_G(v_4) = n_4 + 2 \), where \( n_2, n_4 \geq 0 \). By Lemma 1,

\[
SO(G') - SO(G) = \sum_{i=1}^{n_1} [f(n_1 + n_3 + 2, d_G(v_{1i})) - f(n_1 + 2, d_G(v_{1i}))] + \sum_{j=1}^{n_3} [f(n_3 + n_3 + 2, d_G(v_{3j})) - f(n_3 + 2, d_G(v_{3j}))] + f(n_1 + n_3 + 2, n_2 + 2) - f(n_3 + 2, n_2 + 2) - [f(n_1 + 2, n_2 + 2) - f(2, n_2 + 2)] + f(n_1 + n_3 + 2, n_4 + 2) - f(n_3 + 2, n_4 + 2) - [f(n_1 + 2, n_4 + 2) - f(2, n_4 + 2)] > f(n_1 + n_3 + 2, n_2 + 2) - f(n_3 + 2, n_2 + 2) - [f(n_1 + 2, n_2 + 2) - f(2, n_2 + 2)] + f(n_1 + n_3 + 2, n_4 + 2) - f(n_3 + 2, n_4 + 2) - [f(n_1 + 2, n_4 + 2) - f(2, n_4 + 2)] = \sum_{i=1}^{n_1+1} [h(n_3 + i, n_2 + 2) - h(i, n_2 + 2)] + \sum_{i=2}^{n_1+1} [h(n_3 + i, n_4 + 2) - h(i, n_4 + 2)] > 0.
\]

**Lemma 6.** Let \( G \) be a graph and \( C_3 = v_1v_2v_3v_1 \) be a 3-cycle in \( G \). Suppose \( N_G(v_1) \cap N_G(v_2) = \{v_3\} \). Let \( N_G(v_1) \setminus \{v_2, v_3\} = \{v_{11}, v_{12}, \ldots, v_{1n_1}\} \) and \( N_G(v_2) \setminus \{v_1, v_3\} = \{v_{21}, v_{22}, \ldots, v_{2n_2}\} \), where \( n_1 = d_G(v_1) - 2 > 0 \) and \( n_2 = d_G(v_2) - 2 > 0 \). Denote \( G' = (G - \{v_1v_{11}, \ldots, v_1v_{1n_1}\}) + \{v_2v_{21}, \ldots, v_2v_{2n_2}\} \). Then, \( SO(G) < SO(G') \).

**Proof of Lemma 6.** Suppose \( d_G(v_3) = n_3 + 2 \), where \( n_3 \geq 0 \). By Lemma 1,
we investigate the maximal values of the Sombor index over the sets $C_r$ (see Figure 2).

Let $G$ be the graph with maximum increased Sombor index among all unicyclic graphs.

**Theorem 1.**

pendant vertices such that no two of the new edges are adjacent, and then subdividing one

By considering the version of $SO$ in these lemmas.

Remark 1. By the definitions of $SO$ and $SO^+$, it is easy to see that Lemmas 3–6 also hold if we replace $SO$ with $SO^+$ in these lemmas.

By Remark 1, we easily get the following result which will be used later.

**Theorem 1.** Let $G$ be the graph with maximum increased Sombor index among all unicyclic graphs of order $n$. Then $G \cong C_3(n-3,0,0)$, where $C_3(n-3,0,0)$ is obtained from a 3-cycle $C_3$ by attaching $n-3$ pendant vertices to one vertex of $C_3$.

**Proof of Theorem 1.** By considering the version of $SO^+$ of Lemma 3, each cut edge of $G$ is pendant and the girth of $G$ is 3. Moreover, all pendant vertices are adjacent to one common vertex by Lemma 6. Therefore, $G \cong C_3(n-3,0,0)$.

3. Sombor Index of Cacti

Denote by $C^k_n$ the set of all cacti of order $n$ with $k$ cut edges, and $C(n,p)$ the set of all cacti of order $n$ with $p$ pendant vertices. Then, $0 \leq k \leq n-1$ and $k \neq n-2$. In this section, we investigate the maximal values of the Sombor index over the sets $C^k_n$ and $C(n,p)$.

Given two integers $k$ and $n$ with $0 \leq k \leq n-1$ and $k \neq n-2$, if $n-k$ is even, denote by $G_1$ the graph obtained from a star $S_{n-1}$ by first adding $\frac{n-k-2}{2}$ new edges between its pendant vertices such that no two of the new edges are adjacent, and then subdividing one new edge; if $n-k$ is odd, denote by $G_2$ the graph obtained from a star $S_n$ by adding $\frac{n-k-1}{2}$ new edges between its pendant vertices such that no two of the new edges are adjacent (see Figure 2).

![Figure 2. Graphs $G_1$ and $G_2$.](image)

The following theorem shows that the graph $S_n$ has maximum Sombor index over $C_{n-1}^n$. Therefore, we assume $k \neq n-1$ in the following.
Theorem 2 ([8]). For any tree $T$ of order $n$,
\[\text{SO}(P_n) \leq \text{SO}(T) \leq \text{SO}(S_n).\]
Equality holds if and only if $T \cong P_n$ or $T \cong S_n$.

Theorem 3. For graphs in $C^k_n$, where $0 \leq k \leq n - 3$,
(1) if $n - k$ is even, $G_1$ is the unique graph with maximum Sombor index;
(2) if $n - k$ is odd, $G_2$ is the unique graph with maximum Sombor index, where $G_1$ and $G_2$ are depicted in Figure 2.

Proof of Theorem 3. Let $G$ be the graph with maximum Sombor index in $C^k_n$. By Lemma 3, each cut edge of $G$ is pendant. We show that the following propositions hold for $G$. □

Proposition 1. Each cycle in $G$ is of length 3 or 4.

Proof of Proposition 1. Suppose to the contrary that $G$ has a cycle $C = v_1v_2\cdots v_tv_1$ of length $t \geq 5$. Without loss of generality, we assume that $d_G(v_1) = \max\{d_G(v_i)|1 \leq i \leq t\}$. Define $G' = (G - v_3v_4) + \{v_1v_3, v_1v_4\}$. Then, $G' \in C^k_n$ and
\[
\text{SO}(G') - \text{SO}(G) = f(d_{G'}(v_1), d_{G'}(v_3)) + f(d_{G'}(v_1), d_{G'}(v_4)) - f(d_G(v_1), d_G(v_3)) - f(d_G(v_1), d_G(v_4)) > 0,
\]
a contradiction to the choice of $G$. Therefore, Proposition 1 holds. □

Proposition 2. Each 4-cycle has at most one vertex of degree larger than 2 in $G$.

Proof of Proposition 2. Suppose there is a 4-cycle $C = v_1v_2v_3v_4$ containing at least two vertices of degree larger than 2. Since $G$ has maximum Sombor index, any two vertices of $C$ with degree larger than 2 must be adjacent by Lemma 5. Thus, $C$ contains exactly two adjacent vertices of degree 2. Without loss of generality, we assume that $d_G(v_1) = n_1 + 2 > 2, d_G(v_2) = n_2 + 2 > 2$ and $d_G(v_3) = d_G(v_4) = 2$. Suppose $N_G(v_1) \setminus \{v_2, v_4\} = \{v_1v_1, v_1v_2, \ldots, v_1v_{n_1}\}$ and $N_G(v_2) \setminus \{v_1, v_3\} = \{v_2v_1, v_2v_2, \ldots, v_2v_{n_2}\}$. Let $G' = (G - \{v_1v_2, v_1v_3, \ldots, v_1v_{n_2}\}) + \{v_1v_2, v_1v_3, \ldots, v_1v_{n_2}\}$. Then, $G' \in C^k_n$ and
\[
\text{SO}(G') - \text{SO}(G) > f(n_1 + n_2 + 2, 2) - f(n_1 + 2, n_2 + 2) + f(n_1 + n_2 + 2, 2) - f(n_1 + 2, 2) - [f(n_2 + 2, 2) - f(2, 2)]
\]
\[
= f(n_1 + n_2 + 2, 2) - f(n_1 + 2, n_2 + 2) + \sum_{i=2}^{n_2+1} \left[h(n_1 + i, 2) - h(i, 2)\right]
\]
\[
> 0,
\]
a contradiction.

By Lemma 6, each 3-cycle has at most one vertex of degree larger than 2. Combining it with Propositions 1 and 2, $G$ is obtained from $s$ copies of $C_4$ and $t$ copies of $C_3$ by first taking one vertex of each of them and fusing them together into a new common vertex $v$, and then attaching $k$ pendant vertices at $v$, where $3s + 2t + k + 1 = n$. Suppose $s \geq 2$. Then, there are at least two 4-cycles $C = v_1y_1z_1v$ and $C' = v_2y_2z_2v$. Let $G' = (G - \{x_1y_1, x_2y_2\}) + \{x_1z_2, y_1v, y_2v\}$. Then $G' \in C^k_n$ and $\text{SO}(G') - \text{SO}(G) > (6f(d_G(v) + 2, 2) + 3f(2, 2)) - (4f(d_G(v), 2) + 4f(2, 2)) > 0$, a contradiction. This implies $0 \leq s \leq 1$. Therefore, $s = 1$ if $n - k$ is even and $s = 0$ otherwise, i.e., $G \cong G_1$ if $n - k$ is even and $G \cong G_2$ otherwise. □
Next, we find the maximal graph with respect to the Sombor index among $C(n,p)$ with $n$ vertices and $p$ pendant vertices. As $S_{n-1}$ is the only graph with $n-1$ pendant vertices, we assume $0 \leq p \leq n-2$ in the following. Before we give our main result, we show a lemma.

**Lemma 7.** Let $G$ be a graph and $e = uv \in E(G)$ with $N_G(u) \cap N_G(v) = \emptyset$. Suppose $N_G(u) \setminus \{v\} = \{x_1, \ldots, x_t, w_1, \ldots, w_p\}$ and $N_G(v) \setminus \{u\} = \{y_1, \ldots, y_t, z_1, \ldots, z_q\}$, where $d(x_1) = \cdots = d(x_t) = 2$, $d(w_1) = \cdots = d(w_p) = 1$, $d(y_1) = \cdots = d(y_t) = 2$ and $d(z_1) = \cdots = d(z_q) = 1$. Suppose $s \geq 2$. Let $G'$ be obtained from $G$ by first deleting the edge $e$ and identifying $u$ with $v$, and then subdividing the edge $ux_1$. If $t + q \geq 2$, or $t = 0$ with $q = 1$, then $SO(G) < SO(G')$.

**Proof of Lemma 7.** By direct calculation, we get

$$SO(G') - SO(G) = (p + q)f(s + p + t + q, 1) - pf(s + p + 1, 1) - qf(t + q + 1, 1) + (s + t)f(s + p + t + q, 2) - sf(s + p + 1, 2) - tf(t + q + 1, 2) + f(2, 2) - f(t + q + 1, s + p + 1) \geq q[f(s + p + t + q, 1) - f(t + q + 1, 1)] + s[f(s + p + t + q, 2) - f(s + p + 1, 2)] + t[f(s + p + t + q, 2) - f(t + q + 1, 2)] - [f(t + q + 1, s + p + 1) - f(2, s + p + 1) + f(s + p + 1, 2) - f(2, 2, 2)] = q \sum_{i=2}^{s+p} h(t + q + i - 1, 1) + t \sum_{i=2}^{s+p} h(t + q + i - 1, 2) - \sum_{i=2}^{s+p} h(i, 2) + s[f(s + p + t + q, 2) - f(s + p + 1, 2)] - [f(t + q + 1, s + p + 1) - f(2, s + p + 1)] + \sum_{i=2}^{t+q} h(s + p + i - 1, 2) - \sum_{i=2}^{t+q} h(i, s + p + 1) > 0$$

We denote the right side of equation (1) by $A$. Then, by Lemma 1,

$$A > s[f(s + p + t + q, 2) - f(s + p + 1, 2)] - [f(t + q + 1, s + p + 1) - f(2, s + p + 1)] = \sum_{i=2}^{t+q} h(s + p + i - 1, 2) - \sum_{i=2}^{t+q} h(i, s + p + 1) > 0$$

if $t + q \geq 2$. Now, suppose $t = 0$ and $q = 1$. Then, $A = \sum_{i=2}^{t+q} [h(i, 1) - h(i, 2)] > 0$ by Lemma 1, which completes the proof. □

Denote by $DS_{p,q}$ the double star obtained from a star $S_{p+2}$ by attaching $q$ pendant vertices to one pendant vertex. Then $DS_{p,q}$ has $n = p + q + 2$ vertices.

**Theorem 4.** For graphs in $C(n,p)$, where $0 \leq p \leq n-2$ and $n \geq 5$,

(1) if $p = n-2$, $DS_{n-3,1}$ is the unique graph with maximum Sombor index;
(2) if $p \leq n-3$ and $n-p$ is even, $G_1$ is the unique graph with maximum Sombor index;
(3) if $p \leq n-3$ and $n-k$ is odd, $G_2$ is the unique graph with maximum Sombor index, where $G_1$ and $G_2$ are depicted in Figure 2.

**Proof of Theorem 4.** If $p = n-2$, then any graph in $C(n,p)$ is a double star. By Lemma 4, $DS_{n-3,1}$ is the unique graph with maximum Sombor index. Now suppose $p \leq n-3$. Let $G$ be the graph with maximum Sombor index in $C(n,p)$. Then, the following claims hold. □

**Claim 1.** $G$ must contain a cycle.


Proof of Claim 1. Suppose not. Then, $G$ is a tree. As $p \leq n - 3$, there are two non-pendant vertices $u$ and $v$ of $G$ with $uv \notin E(G)$. Let $G' = G + uv$. Then, $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$, a contradiction to the choice of $G$.

By the same argument as that of Theorem 3, each cycle in $G$ is of length 3 or 4. Moreover, each cycle of $G$ has at most one vertex of degree larger than 2. Let $T$ be the graph obtained from $G$ by deleting all vertices of degree 2 in each cycle. Then, $T$ is a tree. Let $d(T)$ be the diameter of $T$. \hfill $\square$

Claim 2. $d(T) \leq 3$.

Proof of Claim 2. Suppose $d(T) \geq 4$. Then there are two non-pendant vertices $u$ and $v$ of $T$ with $uv \notin E(T)$. Let $G' = G + uv$. Then $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$, a contradiction, which implies Claim 2 holds.

Similarly, we have \hfill $\square$

Claim 3. For any two cycles $C_1$ and $C_2$ in $G$, the length of the path connecting them is 0 or 1.

Proof of Claim 3. Suppose there are two cycles $C_1$ and $C_2$ such that the length of the path $P$ connecting them is larger than 1. Let $P = u_0u_1 \cdots u_l$, where $u_0 \in V(C_1)$ and $u_l \in V(C_2)$. Then $l > 1$. Define $G' = G + uu_0u_1$. Then $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$, a contradiction, which implies Claim 3 holds. \hfill $\square$

Claim 4. Any two cycles of $G$ have one common vertex.

Proof of Claim 4. Suppose there are two cycles $C_1$ and $C_2$ having no vertices in common. Then by Claim 3, the length of the path $P$ connecting them is 1. Suppose $P = u_1v_1$, where $u_1 \in V(C_1)$ and $v_1 \in V(C_2)$. As each cycle of $G$ has at most one vertex of degree larger than 2, $N_G(u_1) \cap N_G(v_1) = \emptyset$.

We show that for each vertex $w \in (N_G(u_1) \setminus \{v_1\}) \cup (N_G(v_1) \setminus \{u_1\})$, $d_G(w) \in \{1, 2\}$. Without loss of generality, suppose there is a vertex $w \in N_G(v_1) \setminus \{u_1\}$ with $d_G(w) \geq 3$. Then $w \in V(T)$. Let $G' = G + wu_1$. Then, $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$, a contradiction.

Now let $u_2 \in V(C_1) \cap N_G(u_1)$. Let $G'$ be obtained from $G$ by first deleting the edge $u_1v_1$ and identifying $u_1$ with $v_1$, and then subdividing the edge $u_1u_2$. Then $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$ by Lemma 7, a contradiction. Therefore, Claim 4 holds. \hfill $\square$

Claim 5. All pendant vertices in $G$ are adjacent to $u$, where $u$ is the common vertex of all cycles in $G$.

Proof of Claim 5. Suppose there is a support vertex $v \neq u$. Let $d_G(u, v)$ be the distance between $u$ and $v$ in $G$. Then $d_G(u, v) \in \{1, 2\}$ by Claim 2. If $d_G(u, v) = 2$, by letting $G' = G + uv$, we get $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$, a contradiction. Therefore, $d_G(u, v) = 1$.

Suppose for each vertex $w \in N_G(v) \setminus \{u\}$, $d_G(w) = 1$. Then by Claim 1, there are at least two vertices of degree 2 adjacent to $u$ except $v$. Let $u_1 \in N_G(u) \setminus \{v\}$ with $d_G(u_1) = 2$. Denote by $G'$ the graph obtained from $G$ by first deleting the edge $uv$ and identifying $u$ with $v$, and then subdividing the edge $u_1v_1$. Then $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$ by Lemma 7, a contradiction. Therefore, we may assume that there is a vertex $v_1 \in N_G(v) \setminus \{u\}$ with $d_G(v_1) \geq 2$. Let $G' = G + uv_1$. Then $G' \in \mathcal{C}(n, p)$ and $SO(G') > SO(G)$, a contradiction. This completes the proof of Claim 5.

By the same argument as that of Theorem 3, there is at most one 4-cycle in $G$. Therefore, $G$ is obtained from $s$ copies of $C_4$ and $t$ copies of $C_3$ by first taking one vertex of each of them and fusing them together into a new common vertex $u$, and then attaching $p$ pendant vertices at $u$, where $3s + 2t + p + 1 = n$ and $0 \leq s \leq 1$. Therefore, $s = 1$ if $n - p$ is even and $s = 0$ otherwise, i.e., $G \cong G_1$ if $n - p$ is even and $G \cong G_2$ otherwise. \hfill $\square$
4. Sombor Index of Quasi-Unicyclic Graphs

Let \( \mathcal{QU}(n) \) be the set of all quasi-unicyclic graphs of order \( n \). Denote by \( \infty(p, l, q) \) the graph obtained from two cycles \( C_p \) and \( C_q \) by connecting a vertex \( v \in V(C_p) \) and a vertex \( v \in V(C_q) \) by a path \( v_0v_1 \cdots v_l \) of length \( l \) (identifying \( u \) with \( v \) if \( l = 0 \), where \( v_0 = u \), \( v_l = v \) and \( p + q + l = n + 1 \). Let \( \Theta(s, t, r) \) be a union of three paths \( P_{s+1}, P_{t+1}, P_{r+1} \) resp. with common end vertices, where \( s + t + r + 1 = n, s \geq t \geq r \geq 1 \) and at most one of them is 1.

**Theorem 5.** Let \( G \in \mathcal{QU}(n) \) be the graph with minimum Sombor index, where \( n \geq 4 \). Then \( G \cong \Theta(s, t, 1) \) or \( \infty(p, l, q) \), and \( SO(G) = (2n - 5)/2 + 4/\sqrt{3} \).

**Proof of Theorem 5.** As \( G \in \mathcal{QU}(n) \), there is a vertex \( v_n \) in \( G \) such that \( G - v_n = H \) is a unicyclic graph. Let \( d_G(v_n) = k \). Then \( k \geq 2 \). As \( G \) has the minimum Sombor index, \( k = 2 \). Let \( N_G(v_n) = \{v_1, v_2\} \).

We first show that \( H \) has at most two pendant vertices. Suppose \( H \) has at least three pendant vertices. If \( \max\{d_H(v_1), d_H(v_2)\} \geq 2 \), then \( G \) has at least two pendant paths, say \( P = uu_1 \cdots u_4 \) and \( Q = ww_1 \cdots w_4 \), where \( d_G(u), d_G(w) \geq 3 \). Let \( G' = (G - uu_1) + u_1w_1 \). Then, \( G' \in \mathcal{QU}(n) \) and \( SO(G') < SO(G) \) by Lemma 2, a contradiction. Therefore, we may assume that \( d_H(v_1) = d_H(v_2) = 1 \). Then, there is a pendant path \( P = xx_1 \cdots x_l \) in \( G \), where \( d_G(x) = a \geq 3, d_G(x_1) = \cdots = d_G(x_{l - 1}) = 2 \) and \( d_G(x_l) = 1 \). Define \( G = (G - xx_1, v_1v_n) + \{v_1x_1, x_1v_n\} \). Then, \( G' \in \mathcal{QU}(n) \). By direct calculation, we get \( SO(G') - SO(G) < f(2, 2) - f(1, a) < 0 \) if \( l = 1 \), and

\[
SO(G') - SO(G) < 2f(2, 2) - (f(a, 2) + f(1, 2)) = f(2, 2) - f(1, 2) - [f(a, 2) - f(2, 2)] = h(1, 2) - \sum_{i=2}^{a-1} h(i, 2) < 0
\]

if \( l \geq 2 \). This contradicts to the definition of \( G \). Therefore, there are at most two pendant vertices in \( H \).

Now, we show that every pendant vertex in \( H \) is adjacent to \( v_n \) in \( G \). Suppose there is a pendant vertex \( v \) in \( H \) with \( v \not\in \{v_1, v_2\} \). Then there is one vertex in \( \{v_1, v_2\} \), say \( v_1 \), such that \( d_G(v_1) = a \geq 3 \). Let \( w \) be the neighbor of \( v \) in \( G \). Obviously, \( d_G(w) = b \geq 2 \). If \( w \not\in \{v_1, v_2\} \), \( G' = (G - wv_n) + wv_n \). Then, \( G' \in \mathcal{QU}(n) \) and \( SO(G') < SO(G) \) by Lemma 3, a contradiction. Therefore, \( w = v_1, v_2 \). Now, let \( G' = (G - v_nv_1) + v_nv \). Then, \( G' \in \mathcal{QU}(n) \) and

\[
SO(G') - SO(G) < f(2, 2) + f(2, b) - [f(2, a) + f(1, b)] = f(2, b) - f(1, b) - [f(a, 2) - f(2, 2)] = h(1, b) - \sum_{i=2}^{a-1} h(i, 2) < 0,
\]

a contradiction.

From the above, \( G \) is a bicyclic graph with no pendant vertices. i.e., \( G \cong \Theta(s, t, r) \) or \( \infty(p, l, q) \). By direct calculation, we have \( SO(\Theta(s, t, r)) = (n - 5)f(2, 2) + 6f(2, 3) \) if \( r \geq 2 \), \( SO(\Theta(s, t, r)) = (n - 4)f(2, 2) + 4f(2, 3) + f(3, 3) \) if \( r = 1 \), \( SO(\infty(p, l, q)) = (n - 3)f(2, 2) + 4f(2, 4) \) if \( l = 0 \), \( SO(\infty(p, l, q)) = (n - 4)f(2, 2) + 6f(2, 3) \) if \( l \geq 2 \) and \( SO(\infty(p, l, q)) = (n - 4)f(2, 2) + 4f(2, 3) + f(3, 3) \) if \( l = 1 \). Since \( (n - 3)f(2, 2) + 4f(2, 4) > (n - 5)f(2, 2) + 6f(2, 3) > (n - 4)f(2, 2) + 4f(2, 3) + f(3, 3) \), we get \( G \cong \Theta(s, t, 1) \) or \( \infty(p, 1, q) \), and \( SO(G) = (n - 4)f(2, 2) + 4f(2, 3) + f(3, 3) = (2n - 5)/2 + 4/\sqrt{3} \). □
Here, we recall some theory of majorization. A subset \( X \subseteq \mathbb{R}^n \) is a convex set if for any \( x, y \in X \) and any \( \lambda \) with \( 0 < \lambda < 1 \), \( \lambda x + (1 - \lambda) y \in X \). Let \( X \subseteq \mathbb{R}^n \) be a convex set. For a function \( f : X \to \mathbb{R} \), if for any \( x, y \in X \) and any \( \lambda \) with \( 0 < \lambda < 1 \), \( \lambda f(x) + (1 - \lambda) f(y) \leq f(\lambda x + (1 - \lambda) y) \), then \( f \) is called a convex function. If the inequality above is strict for all \( x, y \in X \) with \( x \neq y \), then \( f \) is a strictly convex function. Let \( I \) be an interval and \( f : I \to \mathbb{R} \) be a real twice-differentiable function on \( I \), then it is well-known that \( f \) is convex if and only if \( f''(x) \geq 0 \) for all \( x \in I \), and \( f \) is strictly convex if \( f''(x) > 0 \) for all \( x \in I \).

For each vector \( x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \), consider the decreasing rearrangement of it, i.e., we always assume that \( x_1 \geq x_2 \geq \cdots \geq x_n \). Then we have the following definition and majorization inequality.

**Definition 1** ([24]). For \( x, y \in \mathbb{R}^n \),

\[
\begin{aligned}
x \prec y \text{ if } & \begin{cases} 
\sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} y_i, & k = 1, 2, \ldots, n - 1, \\
\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i, 
\end{cases}
\end{aligned}
\]

When \( x \prec y \), \( x \) is said to be majorized by \( y \) (\( y \) majorizes \( x \)).

**Lemma 8** ([25]). Let \( I \subseteq \mathbb{R} \) be an interval and \( f : I \to \mathbb{R} \) a strictly convex function. Let \( c = (c_1, c_2, \ldots, c_n) \) and \( d = (d_1, d_2, \ldots, d_n) \) be two vectors in \( \mathbb{R}^n \) with \( c_i, d_i \in I \) for each \( i = 1, 2, \ldots, n \). If \( c \prec d \), then \( \sum_{i=1}^{n} f(c_i) \leq \sum_{i=1}^{n} f(d_i) \), with equality if and only if \( c = d \).

**Theorem 6.** Let \( G \in \mathcal{GU}(n) \). Then,

\[
\text{SO}(G) \leq 2(n - 4) \sqrt{(n - 1)^2 + 4 + 4(n - 1)^2 + 9 + (n + 2)\sqrt{2}},
\]

with equality if and only if \( G \cong C_3(n - 4, 0, 0) \cup K_1 \), where \( C_3(n - 4, 0, 0) \) is obtained from a 3-cycle \( C_3 \) by attaching \( n - 4 \) pendant vertices to one vertex of \( C_3 \).

**Proof of Theorem 6.** Let \( v_n \) be a vertex in \( G \) such that \( G - v_n = H \) is a unicyclic graph. Let \( V(H) = \{v_1, v_2, \ldots, v_{n-1}\} \) and \( d_G(v_n) = k \). Then, \( 2 \leq k \leq n - 1 \). By the definition of the Sombor index, we get

\[
\text{SO}(G) \leq \sum_{i=1}^{n-1} \sqrt{(n - 1)^2 + (d_H(v_i) + 1)^2} + \sum_{v_i \neq v_j \in E(H)} \sqrt{(d_H(v_i) + 1)^2 + (d_H(v_j) + 1)^2}.
\]

Moreover, the equality holds if and only if \( d_G(v_n) = n - 1 \). First we consider the maximum value of \( \sum_{v_i \neq v_j \in E(H)} \sqrt{(d_H(v_i) + 1)^2 + (d_H(v_j) + 1)^2} \). By Theorem 1,

\[
\sum_{v_i \neq v_j \in E(H)} \sqrt{(d_H(v_i) + 1)^2 + (d_H(v_j) + 1)^2} = \text{SO}^+(H) \leq \text{SO}^+(C_3(n - 4, 0, 0)),
\]

with equality if and only if \( H \cong C_3(n - 4, 0, 0) \).

Now, we calculate the maximum value of \( \sum_{i=1}^{n-1} \sqrt{(n - 1)^2 + (d_H(v_i) + 1)^2} \). Consider the function \( g(x) = \sqrt{(n - 1)^2 + (x + 1)^2}, \ 1 \leq x \leq n - 2 \).
Then, \( g''(x) = \frac{2(n-1)^2 + (x+1)^2}{2((n-1)^2 + (x+1)^2)^2} > 0 \), \( 1 \leq x \leq n - 2 \). Therefore, \( g(x) \) is strictly convex on \( 1 \leq x \leq n - 2 \). Note that \( H \) is a unicyclic graph and \( \sum_{i=1}^{n-1} d_H(v_i) = 2(n-1) \), by [26], the degree sequence \( d(H) = (d_H(v_1), (d_H(v_2), \ldots, (d_H(v_{n-1})) \) satisfies \( d(H) \prec (n-2, 2, 2, 1, \ldots, 1) \). By Lemma 8, \( \sum_{i=1}^{n-1} g((d_H(v_i))) \leq g(n-2) + 2g(2) + (n-4)g(1) \), that is,

\[
\sum_{i=1}^{n-1} \sqrt{(n-1)^2 + (d_H(v_i) + 1)^2} \\
\leq \sqrt{(n-1)^2 + (n-2+1)^2 + 2\sqrt{(n-1)^2 + (2+1)^2}} \\\n+ (n-4)\sqrt{(n-1)^2 + (1+1)^2} \\
= (n-1)\sqrt{2} + 2\sqrt{(n-1)^2 + 9} + (n-4)\sqrt{(n-1)^2 + 4}.
\]

Moreover, equality holds if and only if \( d(H) = (n-2, 2, 2, 1, \ldots, 1) \), i.e., \( H \cong C_3(n-4, 0, 0) \).

Based on the above,

\[
SO(G) \\
\leq (n-1)\sqrt{2} + 2\sqrt{(n-1)^2 + 9} + (n-4)\sqrt{(n-1)^2 + 4} \\
+ (n-4)\sqrt{(n-1)^2 + 2^2} + 2\sqrt{(n-1)^2 + 3^2} + \sqrt{3^2 + 3^2} \\
= 2(n-4)\sqrt{(n-1)^2 + 4} + 4\sqrt{(n-1)^2 + 9} + (n+2)\sqrt{2}.
\]

Moreover, the equality holds if and only if \( G \cong C_3(n-4, 0, 0) \lor K_1 \). \( \square \)

5. Conclusions

As graph invariants, topological indices are used for QSAR and QSPR studies. Therefore, it is very important to study the extremal graphs with respect to topological indices in chemical graph theory. Until now, many topological indices have been introduced and several of them have been found various applications. As a novel index, the Sombor index has received a lot of attention within mathematics and chemistry. In this paper, we give some transformations to compare the Sombor indices between two graphs. With these transformations, we present the maximum Sombor index among cacti \( C_d \) and \( \mathcal{C}(n, p) \). Moreover, the maximum and minimum Sombor index among all quasi-unicyclic graphs are characterized. It is interesting to consider the minimum Sombor index of cacti with some graph parameters. We will consider it for future study.

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