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Article

Some Extremal Graphs with Respect to Sombor Index

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Abstract: Let G be a graph with set of vertices $V(G)$ ($|V(G)| = n$) and edge set $E(G)$. Very recently, a new degree-based molecular structure descriptor, called Sombor index is denoted by $SO(G)$ and is defined as $SO = SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2}$, where $d_G(v_i)$ is the degree of the vertex v_i in G. In this paper we present some lower and upper bounds on the Sombor index of graph G in terms of graph parameters (clique number, chromatic number, number of pendant vertices, etc.) and characterize the extremal graphs.

Keywords: graph; Sombor index; chromatic number; clique number

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1. Introduction

Let $G = (V, E)$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. If the vertices v_i and v_j are adjacent, we write $v_iv_j \in E(G)$. For $i \in \{1, 2, \ldots, n\}$, let $d_G(v_i)$ be the degree of the vertex v_i. The *maximum degree* of a graph G will be denoted by Δ. A vertex v_i of degree 1 is called a *pendant vertex* (also known as *leaf*), the edge incident with a pendant vertex is called a *pendant edge*. For any two nonadjacent vertices v_i and v_j of a graph G, we let $G + v_iv_j$ be the graph obtained from G by adding the edge v_iv_j. For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v_i\}$ and $E' = \{v_iv_j\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v_i$ and $G - v_iv_j$ for short, respectively. The *chromatic number* of a graph G, denoted by $\chi(G)$, is the minimum number of colors such that vertices of G can be colored with these colors in order that no two adjacent vertices have the same color. A *clique* of graph G is a subset V_0 of $V(G)$ such that in $G[V_0]$, the subgraph of G induced by V_0, any two vertices are adjacent. The *clique number* of G, denoted by $\omega(G)$, is the number of vertices in a largest clique of G. For two vertex-disjoint graphs G_1 and G_2, we denote by $G_1 \bigcup G_2$ the graph which consists of two components G_1 and G_2. As usual, P_n, C_n, $K_{1,n-1}$ and $K_{p,q}$ $(p + q = n)$, denote, respectively, the path, the cycle, the star and the complete bipartite graph on n vertices. Other undefined notations and terminology on the graph theory can be found in [1].

A topological descriptor is a numerical descriptor of the topology of a molecule. These topological descriptors are used for predicting the physico-chemical and/or biological properties of molecules in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies [2,3]. In the literature, several degree- and distance-based topological descriptors were proposed and studied by some researchers [4–17]. Very recently, a new degree-based molecular structure descriptor was introduced, the Sombor index is denoted by $SO(G)$ and is defined as follows [18]:

$$SO = SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2}. \tag{1}$$

Many fundamental mathematical properties such as lower and upper bounds can be found in, e.g., [3,10,18–26]. This topological index was motivated by the geometric interpretation of the degree radius of an edge v_iv_j, which is the distance from the origin to the ordered pair $(d_G(v_i), d_G(v_j))$.

Denote by $\mathcal{W}(n, \omega)$ the set of connected graphs of order n with clique number ω. The long kite graph $Ki_{n,\omega}$ (see, Figure 1) is a graph of order n obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between a vertex from the clique and an endpoint from the path. In particular, for $\omega = n$, $Ki_{n,\omega} \cong K_n$. Let $G \cong Ki_{n,\omega}$. For $\omega \le n-2$, we have

$$\begin{aligned}
&\sum_{\substack{v_iv_j \in E(G) \\ v_i, v_j \in V(K_\omega)}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\
&= \binom{\omega-1}{2} \sqrt{(\omega-1)^2 + (\omega-1)^2} + (\omega-1)\sqrt{\omega^2 + (\omega-1)^2} \\
&= \binom{\omega-1}{2} \sqrt{2}\,(\omega-1) + (\omega-1)\sqrt{2\omega^2 - 2\omega + 1},
\end{aligned}$$

$$\sum_{\substack{v_iv_j \in E(G) \\ v_i, v_j \in V(G - V(K_\omega))}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} = (n-\omega-2)\sqrt{8} + \sqrt{5}$$

and hence

$$\begin{aligned}
SO(Ki_{n,\omega}) &= \sum_{\substack{v_iv_j \in E(G) \\ v_i, v_j \in V(K_\omega)}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} + \sum_{\substack{v_iv_j \in E(G) \\ v_i, v_j \in V(G - V(K_\omega))}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\
&\quad + \sqrt{\omega^2 + 4} \\
&= \binom{\omega-1}{2} \sqrt{2}\,(\omega-1) + (\omega-1)\sqrt{2\omega^2 - 2\omega + 1} + \sqrt{\omega^2 + 4} \\
&\quad + (n-\omega-2)\sqrt{8} + \sqrt{5}.
\end{aligned}$$

In this paper, we present a lower bound on SO of graph G in terms of n and clique number ω, and characterize the extremal graphs.

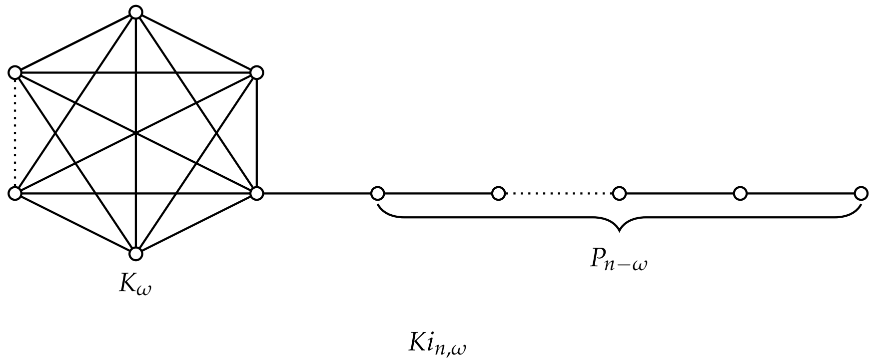


Figure 1. The long kite graph $Ki_{n,\omega}$.

Theorem 1. *Let $G \in \mathcal{W}(n, \omega)$. Then $SO(G) \ge SO(Ki_{n,\omega})$ with equality holding if and only if $G \cong Ki_{n,\omega}$.*

Corollary 1. [18] *Let G be a connected graph of order n. Then $SO(G) \ge SO(P_n)$ with equality holding if and only if $G \cong P_n$.*

Proof of Corollary 1. Let ω be the clique number of graph G. Then $\omega \geq 2$. Therefore one can easily see that

$$SO(G) \geq SO(Ki_{n,\omega}) \geq SO(Ki_{n,\omega-1}) \geq \cdots \geq SO(Ki_{n,3}) \geq SO(Ki_{n,2}) = SO(P_n).$$

hence we obtain the required result. □

Let $\mathcal{X}(n,k)$ be the set of connected graphs of order n with chromatic number k. Recall that the Turán graph $T_n(k)$ is a complete k-partite graph of order n whose partition sets differ in size by at most 1. When $k = n$, the only graph in $\mathcal{X}(n,k)$ is K_n. So, we now assume that $n = kq + r$ where $0 \leq r < k$, i.e., $q = \left\lfloor \frac{n}{k} \right\rfloor$ in $\mathcal{X}(n,k)$. We now give an upper bound on SO of graph G in terms of n and chromatic number k, and characterize the extremal graphs.

Theorem 2. *For any graph $G \in \mathcal{X}(n,k)$, we have*

$$SO(G) \leq r\,(k-r) \left\lfloor \frac{n}{k} \right\rfloor \left\lceil \frac{n}{k} \right\rceil \sqrt{\left(n - \left\lfloor \frac{n}{k} \right\rfloor\right)^2 + \left(n - \left\lceil \frac{n}{k} \right\rceil\right)^2} + \sqrt{2}\binom{r}{2} \left\lceil \frac{n}{k} \right\rceil^2 \left(n - \left\lceil \frac{n}{k} \right\rceil\right) + \sqrt{2}\binom{k-r}{2} \left\lfloor \frac{n}{k} \right\rfloor^2 \left(n - \left\lfloor \frac{n}{k} \right\rfloor\right)$$

with equality holding if and only if $G \cong T_n(k)$.

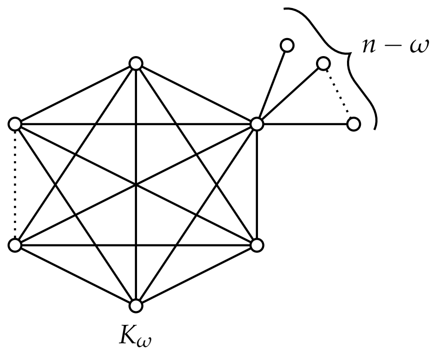
Recall that a short kite graph Ki_n^{ω} obtained by adding $n-\omega$ pendant vertices to the unique vertex of clique K_ω; see Figure 2. Let $G \cong Ki_n^{n-p}$. We have

$$\begin{aligned}\sum_{\substack{v_iv_j \in E(G)\\ v_i, v_j \in V(K_\omega)}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} &= \frac{(n-p-1)(n-p-2)}{2}\sqrt{(n-p-1)^2 + (n-p-1)^2} \\ &\quad + (n-p-1)\sqrt{(n-1)^2 + (n-p-1)^2} \\ &= \frac{(n-p-1)(n-p-2)}{\sqrt{2}}(n-p-1) \\ &\quad + (n-p-1)\sqrt{(n-1)^2 + (n-p-1)^2}\end{aligned}$$

and hence

$$\begin{aligned}SO(Ki_n^{n-p}) &= \sum_{\substack{v_iv_j \in E(G)\\ v_i, v_j \in V(K_\omega)}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} + \sum_{\substack{v_iv_j \in E(G), v_i \in V(K_\omega)\\ v_j \in V(G - V(K_\omega))}} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\ &= p\sqrt{(n-1)^2 + 1} + \frac{(n-p-1)(n-p-2)}{\sqrt{2}}(n-p-1) \\ &\quad + (n-p-1)\sqrt{(n-1)^2 + (n-p-1)^2}.\end{aligned}$$

Finally we give an upper bound on Sombor index in terms of n, p pendant vertices, and characterize the extremal graphs.



Ki_n^{ω}

Figure 2. The short kite graph Ki_n^{ω}.

Theorem 3. *Let G be a graph of order n with p pendant vertices. Then*

$$SO(G) \leq SO(Ki_n^{n-p}) \tag{2}$$

with equality holding if and only if $G \cong Ki_n^{n-p}$.

2. Preliminaries

From the definition of Sombor index, we have

Lemma 1. *Let G be a graph. Then* $SO(G) > SO(G-e)$, *where e is any edge in G.*

Lemma 2. [18] *Let T be a tree of order n. Then* $SO(T) \geq (n-3)\sqrt{8} + 2\sqrt{5}$ *with equality if and only if* $T \cong P_n$.

Lemma 3. [10] *Let T be a tree of order n* (>4) *with* $T \ncong P_n$. *Then* $SO(T) > (n-1)\sqrt{8}$.

In [10], the following two sets are defined:

$$A = \{v_i v_j \in E(G) : d_G(v_i) = 2 > 1 = d_G(v_j)\},$$
$$D = \{v_i v_j \in E(G) : d_G(v_i) \geq 3,\, d_G(v_j) \geq 2 \text{ or } d_G(v_i) \geq 4,\, d_G(v_j) = 1\}.$$

The following result has been proved in [10].

Lemma 4. [10] *Let T* $(\ncong P_n)$ *be a tree of order n. Then* $|D| \geq |A|$.

3. Proofs

Proof of Theorem 1. For $\omega = n$, we have $G \cong K_n$ and hence the equality holds. For $\omega = n-1$, $Ki_{n,n-1}$ is a subgraph of G as $G \in \mathcal{W}(n,\omega)$. Hence by Lemma 1, we obtain

$$SO(G) \geq SO(Ki_{n,n-1}) = \binom{n-2}{2}\sqrt{2}\,(n-2) + (n-2)\sqrt{2n^2-6n+5} + \sqrt{n^2-2n+2}$$

with equality if and only if $G \cong Ki_{n,n-1}$. For $\omega = 2$, we have $G \cong T_n$ or T_n is a subgraph of G, where T_n is a tree of order n. By Lemmas 1 and 2, we have $SO(G) \geq SO(T_n) \geq (n-3)\sqrt{8} + 2\sqrt{5}$. Moreover, $SO(G) = (n-3)\sqrt{8} + 2\sqrt{5}$ if and only if $G \cong P_n$.

Otherwise, $3 \leq \omega \leq n-2$. Since the clique number of G is ω, we can assume that a clique of G is $S(G) = \{v_1, v_2, \ldots, v_\omega\}$. Let H be a connected graph with $H \subseteq G$ such that $V(H) = V(G)$ and $H - E(K_\omega) \cong T_1 \cup T_2 \cup \cdots \cup T_\omega$, where $T_1, T_2, \ldots, T_\omega$ are the trees with $v_i \in V(T_i)$, $|V(T_i)| = n_i$ $(1 \leq i \leq \omega)$, $n_1 \geq n_2 \geq \cdots \geq n_\omega$ and $n_1 + n_2 + \cdots + n_\omega = n$. Moreover, $S(G) = S(H)$. By Lemma 1, we have $SO(G) \geq SO(H)$ with equality if and only if $G \cong H$. For $1 \le i \le \omega$, we have $v_i \in V(T_i)$ and $d_H(v_i) = d_{T_i}(v_i) + \omega - 1$. Moreover, $d_H(v_i) = d_T(v_i)$ for $\omega + 1 \le i \le n$ and $T \in \{T_1, \ldots, T_\omega\}$. Thus, we have

$$\begin{aligned} SO(G) &= \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\ &\ge \sum_{v_iv_j \in E(H)} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} \\ &= \sum_{v_iv_j \in E(K_\omega)} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} + \sum_{\substack{v_iv_j \in E(H), v_i \in V(G - V(K_\omega)), \\ v_j \in V(K_\omega) \text{ or } v_j \in V(G - V(K_\omega))}} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} \\ &= \sum_{v_iv_j \in E(K_\omega)} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} + \sum_{k=1}^{\omega} \sum_{v_iv_j \in E(T_k)} \sqrt{d_H(v_i)^2 + d_H(v_j)^2}. \end{aligned} \tag{3}$$

Claim 1. For $2 \le i \le \omega$, $\sum_{v_kv_\ell \in E(T_i)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2} \ge (n_i - 1)\sqrt{8}$ with equality if and only if $n_i = 1$.

Proof of Claim 1. Let

$$A_i = \sum_{v_kv_\ell \in E(T_i)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2}, \quad 2 \le i \le \omega.$$

For $n_i = 1$ $(2 \le i \le \omega)$, then $A_i = (n_i - 1)\sqrt{8} = 0$, the equality holds in **Claim 1**. For $n_i = 2$ $(2 \le i \le \omega)$, then

$$A_i = \sqrt{\omega^2 + 1} > (n_i - 1)\sqrt{8}$$

as $\omega \ge 3$, the inequality strictly holds in **Claim 1**. Otherwise, $n_i \ge 3$. First we assume that $T_i \cong P_{n_i}$. Thus, we have $d_{T_i}(v_i) = 1$ or $d_{T_i}(v_i) = 2$. When $d_{T_i}(v_i) = 1$, we obtain

$$A_i = \sqrt{\omega^2 + 4} + (n_i - 3)\sqrt{8} + \sqrt{5} > (n_i - 1)\sqrt{8}$$

as $\omega \ge 3$ and $\sqrt{13} + \sqrt{5} > 2\sqrt{8}$. When $d_{T_i}(v_i) = 2$, we obtain

$$\begin{aligned} & A_i = \sqrt{\omega^2 + 4} + \sqrt{\omega^2 + 1} + (n_i - 4)\sqrt{8} + \sqrt{5} > (n_i - 1)\sqrt{8} \\ \text{or} \quad & A_i = 2\sqrt{\omega^2 + 4} + (n_i - 5)\sqrt{8} + 2\sqrt{5} > (n_i - 1)\sqrt{8} \end{aligned}$$

as $\omega \ge 3$ and $\sqrt{13} + \sqrt{5} > 2\sqrt{8}$.
Next we assume that $T_i \ncong P_{n_i}$. Since $d_H(v_i) > d_{T_i}(v_i)$ $(2 \le i \le \omega)$ with Lemma 3, we obtain

$$A_i > \sum_{v_kv_\ell \in E(T_i)} \sqrt{d_{T_i}(v_k)^2 + d_{T_i}(v_\ell)^2} > (n_i - 1)\sqrt{8}.$$

Claim 1 is proved. □

Claim 2.

$$\sum_{v_kv_\ell \in E(T_1)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2} \ge \begin{cases} \sqrt{\omega^2 + 1} & \text{if } n_1 = 2, \\ \sqrt{\omega^2 + 4} + (n_1 - 3)\sqrt{8} + \sqrt{5} & \text{if } n_1 \ge 3 \end{cases}$$

with equality if and only if $T_1 \cong P_{n_1}$ with $d_{T_1}(v_1) = 1$.

Proof of Claim 2. Let

$$A_1 = \sum_{v_kv_\ell \in E(T_1)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2}.$$

Since $\omega \leq n-2$ and $n_1 \geq n_i$ $(2 \leq i \leq \omega)$, we have $n_1 \geq 2$. For $n_1 = 2$, we have $A_1 = \sqrt{\omega^2+1}$, the equality holds in **Claim 2**. Otherwise, $n_1 \geq 3$. We have $v_1 \in V(T_1)$. First we assume that $T_1 \cong P_{n_1}$. Thus, we have $d_{T_1}(v_1) = 1$ or $d_{T_1}(v_1) = 2$. If $d_{T_1}(v_1) = 1$, then we obtain

$$A_1 = \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5}.$$

The equality holds in **Claim 2**. Otherwise, $d_{T_1}(v_1) = 2$. We consider two cases:

Case 1. $n_1 = 3$. In this case

$$A_1 = 2\sqrt{(\omega+1)^2+1} > \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5}$$

as $\omega \geq 3$.

Case 2. $n_1 \geq 4$. We obtain

$$\begin{aligned} A_1 &= \sqrt{(\omega+1)^2+4} + \sqrt{(\omega+1)^2+1} + (n_1-4)\sqrt{8} + \sqrt{5} \\ &> \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5} \\ \text{or } A_1 &= 2\sqrt{(\omega+1)^2+4} + (n_1-5)\sqrt{8} + 2\sqrt{5} > \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5} \end{aligned}$$

as $\omega \geq 3$ and $\sqrt{20} + \sqrt{5} > 2\sqrt{8}$.

Next we assume that $T_1 \ncong P_{n_1}$. Then $n_1 \geq 4$. If $n_1 = 4$, then $T_1 \cong K_{1,3}$ and one can easily check that $A_1 > \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5}$. Otherwise, $n_1 \geq 5$. We consider the following two cases:

Case 3. $d_{T_1}(v_1) = 1$. Let v_r be a vertex adjacent to v_1 in tree T_1. Then $d_{T_1}(v_r) \geq 2$ as $n_1 \geq 5$. First suppose that $T_1 - v_1 \cong P_{n_1-1}$. Then $d_{T_1}(v_r) = 3$. One can easily see that

$$\begin{aligned} A_1 &= \sqrt{(d_{T_1}(v_1)+\omega-1)^2+9} + \sum_{v_k v_\ell \in E(T_1-v_1)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2} \\ &= \sqrt{\omega^2+9} + \sum_{v_k v_\ell \in E(T_1-v_1)} \sqrt{d_{T_1}(v_k)^2 + d_{T_1}(v_\ell)^2} \\ &> \sqrt{\omega^2+9} + \sqrt{13} + (n_1-4)\sqrt{8} + \sqrt{5} > \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5} \end{aligned}$$

as $\sqrt{13} + \sqrt{5} > 2\sqrt{8}$.

Next suppose that $T_1 - v_1 \ncong P_{n_1-1}$. In this case $d_{T_1}(v_r) \geq 2$. Since $T_1 - v_1$ is a tree of order $n_1 - 1$, by Lemma 3, we obtain

$$\begin{aligned} A_1 &= \sqrt{(d_{T_1}(v_1)+\omega-1)^2+d_{T_1}(v_r)^2} + \sum_{v_k v_\ell \in E(T_1-v_1)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2} \\ &\geq \sqrt{\omega^2+4} + \sum_{v_k v_\ell \in E(T_1-v_1)} \sqrt{d_{T_1}(v_k)^2 + d_{T_1}(v_\ell)^2} \\ &> \sqrt{\omega^2+4} + \sum_{v_k v_\ell \in E(T_1-v_1)} \sqrt{d_{T_1-v_1}(v_k)^2 + d_{T_1-v_1}(v_\ell)^2} \\ &> \sqrt{\omega^2+4} + (n_1-2)\sqrt{8} > \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5}. \end{aligned}$$

Case 4. $d_{T_1}(v_1) \geq 2$. For $d_{T_1}(v_1) = n_1 - 1$, one can easily check that $A_1 > \sqrt{\omega^2+4} + (n_1-3)\sqrt{8} + \sqrt{5}$. So now we have $d_{T_1}(v_1) \leq n_1 - 2$. Since $n_1 \geq 5$ and T_1 is a tree, $T_1 - v_1 = \ell K_1 \cup T_1^1 \cup T_1^2 \cup \cdots \cup T_1^k$ $(\ell \geq 0, k \geq 1)$, (say), where T_1^i $(1 \leq i \leq k)$ is a tree of order n_1^i $(= |V(T_1^i)| \geq 2)$ with $\sum_{i=1}^{k} n_1^i = n_1 - \ell - 1$. Thus, we have $d_H(v_1) =$

$d_{T_1}(v_1) + \omega - 1 = \omega + k + \ell - 1$. Let v_r be a vertex in T_1^i such that $v_1 v_r \in E(T_1)$, where $1 \le i \le k$. We now prove that

$$\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} \ge (n_1^i - 2)\sqrt{8} + \sqrt{5}. \tag{3}$$

First we assume that $T_1^i \ncong P_{n_1^i}$. Then by Lemma 3, $SO(T_1') > (n_1^i - 1)\sqrt{8}$. We obtain

$$\begin{aligned}\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} &> \sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1^i}(v_j)^2 + d_{T_1^i}(v_\ell)^2} \\ &= SO(T_1^i) \\ &> (n_1^i - 1)\sqrt{8} > (n_1^i - 2)\sqrt{8} + \sqrt{5}.\end{aligned}$$

the result strictly holds in (3).

Next we assume that $T_1^i \cong P_{n_1^i}$. For $d_{T_1^i}(v_r) = 1$, we have $d_{T_1}(v_r) = d_{T_1^i}(v_r) + 1 = 2$, $d_{T_1}(v_k) = d_{T_1^i}(v_k)$ for $v_k \in V(T_1^i - v_r)$, and hence we obtain

$$\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} = (n_1^i - 2)\sqrt{8} + \sqrt{5}.$$

The equality holds in (3). Otherwise, $d_{T_1^i}(v_r) = 2$. In this case $d_{T_1}(v_r) = d_{T_1^i}(v_r) + 1 = 3$ and $d_{T_1}(v_k) = d_{T_1^i}(v_k)$ for $v_k \in V(T_1^i - v_r)$. If $2 \le n_1^i \le 3$, then one can easily check that the result holds in (3). Otherwise, $n_1^i \ge 4$. We obtain

$$\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} = 2\sqrt{13} + 2\sqrt{5} + (n_1^i - 5)\sqrt{8}$$

or

$$\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} = \sqrt{13} + \sqrt{10} + 2\sqrt{5} + (n_1^i - 5)\sqrt{8}.$$

One can easily check that

$$\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} > (n_1^i - 2)\sqrt{8} + \sqrt{5} \text{ as } \sqrt{13} + \sqrt{5} > 2\sqrt{8}.$$

Again the result holds in (3).

Using the result in (3), we obtain

$$\begin{aligned} A_1 = & \sum_{v_k v_\ell \in E(T_1)} \sqrt{d_H(v_k)^2 + d_H(v_\ell)^2} \\ = & \sum_{v_i : v_1 v_i \in E(T_1)} \sqrt{d_H(v_1)^2 + d_H(v_i)^2} + \textstyle\sum_{i=1}^k \displaystyle\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_H(v_j)^2 + d_H(v_\ell)^2} \\ = & \ \ell\sqrt{d_H(v_1)^2 + 1} + \sum_{\substack{v_i : v_1 v_i \in E(T_1) \\ d_{T_1}(v_i) \ge 2}} \sqrt{d_H(v_1)^2 + d_H(v_i)^2} \\ & + \textstyle\sum_{i=1}^k \displaystyle\sum_{v_j v_\ell \in E(T_1^i)} \sqrt{d_{T_1}(v_j)^2 + d_{T_1}(v_\ell)^2} \\ \ge & \ \ell\sqrt{d_H(v_1)^2 + 1} + k\sqrt{d_H(v_1)^2 + 4} + \textstyle\sum_{i=1}^k \left[(n_1^i - 2)\sqrt{8} + \sqrt{5}\right] \\ = & \ \ell\sqrt{(\omega + k + \ell - 1)^2 + 1} + k\sqrt{(\omega + k + \ell - 1)^2 + 4} \\ & + (n_1 - 1 - \ell - 2k)\sqrt{8} + k\sqrt{5}. \end{aligned} \tag{5}$$

If $\ell \geq 1$, then from (5), we obtain

$$\begin{aligned}A_1 &> \sqrt{\omega^2+4} + (\ell-1)\sqrt{(\omega+k+\ell-1)^2+1} + k\sqrt{(\omega+k+\ell-1)^2+4} \\ &\quad + (n_1-1-\ell-2k)\sqrt{8} + k\sqrt{5} \\ &\geq \sqrt{\omega^2+4} + \sqrt{5} + (n_1-1-2k)\sqrt{8} + (k-1)(\sqrt{13}+\sqrt{5}) \\ &> \sqrt{\omega^2+4} + \sqrt{5} + (n_1-3)\sqrt{8}\end{aligned}$$

as $\sqrt{13}+\sqrt{5} > 2\sqrt{8}$. Otherwise, $\ell = 0$. In this case $k \geq 2$. From (5), we obtain

$$\begin{aligned}A_1 &\geq k\sqrt{(\omega+k-1)^2+4} + (n_1-1-2k)\sqrt{8} + k\sqrt{5} \\ &> \sqrt{\omega^2+4} + \sqrt{5} + (n_1-1-2k)\sqrt{8} + (k-1)(\sqrt{13}+\sqrt{5}) \\ &> \sqrt{\omega^2+4} + \sqrt{5} + (n_1-3)\sqrt{8}\end{aligned}$$

as $\sqrt{13}+\sqrt{5} > 2\sqrt{8}$. **Claim 2** is proved. □

Using **Claim 1** and **Claim 2**, we obtain

$$\sum_{k=1}^{\omega} \sum_{v_iv_j \in E(T_k)} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} \geq \sqrt{\omega^2+4} + (n-\omega-2)\sqrt{8} + \sqrt{5}$$

with equality if and only if $n_2 = \cdots = n_\omega = 1$ and $T_1 \cong P_{n_1}$ with $d_{T_1}(v_1) = 1$, i.e., $G \cong Ki_{n,\omega}$.

Since $n \geq \omega + 2$, we have $d_H(v_1) \geq \omega$ and $d_H(v_i) \geq \omega - 1$ $(2 \leq i \leq \omega)$. Using the above result in (3), we obtain

$$\begin{aligned}SO(G) &\geq \sum_{i=2}^{\omega} \sqrt{d_H(v_1)^2 + d_H(v_i)^2} + \sum_{\substack{v_iv_j \in E(K_\omega) \\ 2 \leq i < j \leq \omega}} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} \\ &\quad + \sum_{k=1}^{\omega} \sum_{v_iv_j \in E(T_k)} \sqrt{d_H(v_i)^2 + d_H(v_j)^2} \\ &\geq (\omega-1)\sqrt{2\omega^2-2\omega+1} + \binom{\omega-1}{2}\sqrt{2}(\omega-1) + \sqrt{\omega^2+4} \\ &\quad + (n-\omega-2)\sqrt{8} + \sqrt{5} \\ &= SO(Ki_{n,\omega}).\end{aligned}$$

This completes the proof of the theorem. □

Let $n_1, n_2, \ldots, n_k$ be positive integers with $\sum\limits_{i=1}^{k} n_i = n$. Denote by $K_{n_1,n_2,\ldots,n_k}$ a complete k-partite graph of order n whose partition sets are of size $n_1, n_2, \ldots, n_k$, respectively. We will determine the extremal graph in $\mathcal{X}(n,k)$ with respect to Sombor index of graphs G. For this we first prove a related lemma below.

Lemma 5. *Let $K_{n_1,n_2,\ldots,n_k}$ be a graph defined as above with $n_i - n_j \geq 2$ for $i < j$. Then*

$$SO(K_{n_1,n_2,\ldots,n_i,\ldots,n_j,\ldots,n_k}) < SO(K_{n_1,n_2,\ldots,n_i-1,\ldots,n_j+1,\ldots,n_k}).$$

Proof. Without loss of generality, we can assume that $n_1 - n_2 \geq 2$. This lemma will be proved if we can prove the following:

$$SO(K_{n_1, n_2, \dots, n_k}) < SO(K_{n_1-1, n_2+1, \dots, n_k}).$$

By the definition of Sombor index, we obtain

$$\begin{aligned} SO(K_{n_1, n_2, \dots, n_k}) &= \sum_{1 \leq i < j \leq k} n_i\, n_j \sqrt{(n-n_i)^2 + (n-n_j)^2} \\ &= \sum_{3 \leq i < j \leq k} n_i\, n_j \sqrt{(n-n_i)^2 + (n-n_j)^2} + n_1\, n_2 \sqrt{(n-n_1)^2 + (n-n_2)^2} \\ &\quad + n_1 \sum_{i=3}^{k} n_i \sqrt{(n-n_1)^2 + (n-n_i)^2} + n_2 \sum_{i=3}^{k} n_i \sqrt{(n-n_2)^2 + (n-n_i)^2}. \end{aligned}$$

Then, in view of the fact that $n_1 - 1 \geq n_2 + 1$, we obtain

$$\begin{aligned} & SO(K_{n_1-1, n_2+1, n_3, \dots, n_k}) - SO(K_{n_1, n_2, n_3, \dots, n_k}) \\ &= (n_1-1)\,(n_2+1) \sqrt{(n-n_1+1)^2 + (n-n_2-1)^2} - n_1\, n_2 \sqrt{(n-n_1)^2 + (n-n_2)^2} \\ &\quad + (n_1-1) \sum_{i=3}^{k} n_i \sqrt{(n-n_1+1)^2 + (n-n_i)^2} - n_1 \sum_{i=3}^{k} n_i \sqrt{(n-n_1)^2 + (n-n_i)^2} \\ &\quad + (n_2+1) \sum_{i=3}^{k} n_i \sqrt{(n-n_2-1)^2 + (n-n_i)^2} - n_2 \sum_{i=3}^{k} n_i \sqrt{(n-n_2)^2 + (n-n_i)^2} \\ &= (n_1 n_2 + n_1 - n_2 - 1) \sqrt{(n-n_1+1)^2 + (n-n_2-1)^2} - n_1\, n_2 \sqrt{(n-n_1)^2 + (n-n_2)^2} \\ &\quad + n_1 \sum_{i=3}^{k} n_i \left[\sqrt{(n-n_1+1)^2 + (n-n_i)^2} - \sqrt{(n-n_1)^2 + (n-n_i)^2} \right] \\ &\quad - n_2 \sum_{i=3}^{k} n_i \left[\sqrt{(n-n_2)^2 + (n-n_i)^2} - \sqrt{(n-n_2-1)^2 + (n-n_i)^2} \right] \\ &\quad + \sum_{i=3}^{k} n_i \left[\sqrt{(n-n_2-1)^2 + (n-n_i)^2} - \sqrt{(n-n_1+1)^2 + (n-n_i)^2} \right]. \end{aligned} \tag{6}$$

Claim 3.

$$(n_1 n_2 + n_1 - n_2 - 1) \sqrt{(n-n_1+1)^2 + (n-n_2-1)^2} > n_1\, n_2 \sqrt{(n-n_1)^2 + (n-n_2)^2}.$$

Proof of Claim 3. Since $n_1 \geq n_2 + 2$, we have

$$(n-n_2-1)^2 \geq (n_1-1)^2 \geq (n_1-1)\,(n_2+1) = n_1\, n_2 + n_1 - n_2 - 1 > n_1\, n_2,$$

that is,

$$(n-n_1+1)^2 + (n-n_2-1)^2 > n_1\, n_2,$$

that is,

$$\frac{2(n_1-n_2-1)}{n_1\, n_2} > \frac{2(n_1-n_2-1)}{(n-n_1+1)^2 + (n-n_2-1)^2},$$

that is,

$$1 + \frac{2(n_1-n_2-1)}{n_1\, n_2} > \frac{(n-n_1)^2 + (n-n_2)^2}{(n-n_1+1)^2 + (n-n_2-1)^2},$$

that is,

$$\left(1 + \frac{n_1-n_2-1}{n_1\, n_2}\right)^2 > \frac{(n-n_1)^2 + (n-n_2)^2}{(n-n_1+1)^2 + (n-n_2-1)^2},$$

which finishes the proof of **Claim 3**. □

Claim 4. For $3 \le i \le k$,

$$n_1\left[\sqrt{(n-n_1+1)^2+(n-n_i)^2}-\sqrt{(n-n_1)^2+(n-n_i)^2}\right]$$
$$> n_2\left[\sqrt{(n-n_2)^2+(n-n_i)^2}-\sqrt{(n-n_2-1)^2+(n-n_i)^2}\right].$$

Proof of Claim 4. Since $n_1 - n_2 \ge 2$, we have

$$2(n_1-n_2)(n-n_1-n_2)+n_1+n_2>0, \text{ that is, } n_1\left[2(n-n_1)+1\right]>n_2\left[2(n-n_2)-1\right].$$

Moreover,

$$\sqrt{(n-n_1+1)^2+(n-n_i)^2} \le \sqrt{(n-n_2-1)^2+(n-n_i)^2}$$

and

$$\sqrt{(n-n_1)^2+(n-n_i)^2} < \sqrt{(n-n_2)^2+(n-n_i)^2},$$

that is,

$$\sqrt{(n-n_1+1)^2+(n-n_i)^2}+\sqrt{(n-n_1)^2+(n-n_i)^2}$$
$$< \sqrt{(n-n_2-1)^2+(n-n_i)^2}+\sqrt{(n-n_2)^2+(n-n_i)^2}.$$

From the above results, we obtain

$$\frac{n_1\left[2(n-n_1)+1\right]}{\sqrt{(n-n_1+1)^2+(n-n_i)^2}+\sqrt{(n-n_1)^2+(n-n_i)^2}}$$
$$> \frac{n_2\left[2(n-n_2)-1\right]}{\sqrt{(n-n_2)^2+(n-n_i)^2}+\sqrt{(n-n_2-1)^2+(n-n_i)^2}},$$

that is,

$$\frac{n_1\left[(n-n_1+1)^2+(n-n_i)^2-(n-n_1)^2-(n-n_i)^2\right]}{\sqrt{(n-n_1+1)^2+(n-n_i)^2}+\sqrt{(n-n_1)^2+(n-n_i)^2}}$$
$$> \frac{n_2\left[(n-n_2)^2+(n-n_i)^2-(n-n_2-1)^2-(n-n_i)^2\right]}{\sqrt{(n-n_2)^2+(n-n_i)^2}+\sqrt{(n-n_2-1)^2+(n-n_i)^2}},$$

which finishes the proof of **Claim 4**. □

Since $n_1 \ge n_2 + 2$, we have $n - n_2 - 1 \ge n - n_1 + 1$ and hence

$$\sqrt{(n-n_2-1)^2+(n-n_i)^2} \ge \sqrt{(n-n_1+1)^2+(n-n_i)^2}$$

for $3 \le i \le k$. Using the above result with **Claims 3** and **4**, from (6), we obtain

$$SO(K_{n_1-1,n_2+1,n_3,\dots,n_k}) > SO(K_{n_1,n_2,n_3,\dots,n_k}).$$

This completes the proof of the lemma. □

We are now ready to proof of Theorem 2.

Proof of Theorem 2. From the definition of chromatic number, any graph G from $\mathcal{X}(n,k)$ has k color classes each of which is an independent set. Suppose that these k classes have order $n_1, n_2, \ldots, n_k$, respectively. By Lemma 1, we obtain $SO(G) \le SO(K_{n_1,n_2,\ldots,n_k})$ with equality holding if and only if $G \cong K_{n_1,n_2,\ldots,n_k}$. We now apply Lemma 5 several times (if needed) and we obtain $SO(K_{n_1,n_2,\ldots,n_k}) \le SO(T_n(k))$ with equality holding if and only if $G \cong T_n(k)$. From the above two results with

$$SO(T_n(k)) = r\,(k-r)\left\lfloor \frac{n}{k} \right\rfloor \left\lceil \frac{n}{k} \right\rceil \sqrt{\left(n - \left\lfloor \frac{n}{k} \right\rfloor\right)^2 + \left(n - \left\lceil \frac{n}{k} \right\rceil\right)^2} + \sqrt{2}\binom{r}{2}\left\lceil \frac{n}{k} \right\rceil^2 \left(n - \left\lceil \frac{n}{k} \right\rceil\right) + \sqrt{2}\binom{k-r}{2}\left\lfloor \frac{n}{k} \right\rfloor^2 \left(n - \left\lfloor \frac{n}{k} \right\rfloor\right),$$

we obtain the required result. This finishes the proof of this theorem. □

Proof of Theorem 3. Let $S = \{v_{n-p+1}, v_{n-p+2}, \ldots, v_n\}$ $(|S| = p)$ be the set of pendant vertices in G. Let $H_{n,\underbrace{n_1,\ldots,\,n_{n-p}}}$ be a graph obtained from G such that any two vertices v_i and v_j $(v_i,\, v_j \in V(G)\backslash S,\, v_iv_j \notin E(G))$ join by an edge, where n_i $(\ge 0,\, 1 \le i \le n-p)$ is the number of pendant vertices adjacent to the vertex v_i and $n_1 \ge n_2 \ge \cdots \ge n_{n-p}$, $n_1 + n_2 + \cdots + n_{n-p} = p$. Then by Lemma 1, one can easily see that $SO(G) \le SO(H_{n,\underbrace{n_1,\ldots,\,n_{n-p}}})$. If $H_{n,\underbrace{n_1,\ldots,\,n_{n-p}}} \cong Ki_n^{n-p}$, then the equality holds in (2). Otherwise, $H_{n,\underbrace{n_1,\ldots,\,n_{n-p}}} \ncong Ki_n^{n-p}$. Let $H_{n,\underbrace{n_1+1,\, n_2-1,\ldots,\,n_{n-p}}} \cong H_1$, $H_{n,\underbrace{n_1,\, n_2,\ldots,\,n_{n-p}}} \cong H_2$. Since $n_1 \ge n_2$, we obtain

$$\begin{aligned}
& SO(H_1) - SO(H_2) \\
&= \sum_{\substack{v_k: v_1v_k \in E(H_1) \\ d_{H_1}(v_k)=1}} \sqrt{d_{H_1}(v_1)^2 + 1} + \sum_{\substack{v_k: v_1v_k \in E(H_1) \\ d_{H_1}(v_k)>1}} \sqrt{d_{H_1}(v_1)^2 + d_{H_1}(v_k)^2} \\
&+ \sum_{\substack{v_k: v_2v_k \in E(H_1) \\ d_{H_1}(v_k)=1}} \sqrt{d_{H_1}(v_2)^2 + 1} + \sum_{\substack{v_k: v_2v_k \in E(H_1) \\ d_{H_1}(v_k)>1}} \sqrt{d_{H_1}(v_1)^2 + d_{H_1}(v_k)^2} \\
&- \sum_{\substack{v_k: v_1v_k \in E(H_2) \\ d_{H_2}(v_k)=1}} \sqrt{d_{H_2}(v_1)^2 + 1} - \sum_{\substack{v_k: v_1v_k \in E(H_2) \\ d_{H_2}(v_k)>1}} \sqrt{d_{H_2}(v_1)^2 + d_{H_2}(v_k)^2} \\
&- \sum_{\substack{v_k: v_2v_k \in E(H_2) \\ d_{H_2}(v_k)=1}} \sqrt{d_{H_2}(v_2)^2 + 1} - \sum_{\substack{v_k: v_2v_k \in E(H_2) \\ d_{H_2}(v_k)>1}} \sqrt{d_{H_2}(v_2)^2 + d_{H_2}(v_k)^2} \\
&= (n_1+1)\sqrt{(n+n_1-p)^2+1} + \sum_{i=3}^{n-p} \sqrt{(n+n_1-p)^2 + (n+n_i-p-1)^2} \\
&+ (n_2-1)\sqrt{(n+n_2-p-2)^2+1} + \sum_{i=3}^{n-p} \sqrt{(n+n_2-p-2)^2 + (n+n_i-p-1)^2} \\
&- n_1\sqrt{(n+n_1-p-1)^2+1} - \sum_{i=3}^{n-p} \sqrt{(n+n_1-p-1)^2 + (n+n_i-p-1)^2} \\
&- n_2\sqrt{(n+n_2-p-1)^2+1} - \sum_{i=3}^{n-p} \sqrt{(n+n_2-p-1)^2 + (n+n_i-p-1)^2} \\
&+ \sqrt{(n+n_1-p)^2 + (n+n_2-p-2)^2} - \sqrt{(n+n_1-p-1)^2 + (n+n_2-p-1)^2}.
\end{aligned} \tag{7}$$

Claim 5. $n_1\sqrt{a^2+1} + n_2\sqrt{(b-1)^2+1} > n_1\sqrt{(a-1)^2+1} + n_2\sqrt{b^2+1}$, where $a = n + n_1 - p$ and $b = n + n_2 - p - 1$.

Proof of Claim 5. First we assume that $n_1 = n_2$. Thus, we have $a = b + 1$. In this case we have to prove that

$$\sqrt{(b+1)^2+1} + \sqrt{(b-1)^2+1} > \sqrt{b^2+1} + \sqrt{b^2+1},$$

that is,

$$\sqrt{(b+1)^2+1} - \sqrt{b^2+1} > \sqrt{b^2+1} - \sqrt{(b-1)^2+1},$$

that is,

$$2b + \sqrt{b^2+1}\,\sqrt{(b-1)^2+1} > \sqrt{b^2+1}\,\sqrt{(b+1)^2+1},$$

that is,

$$\sqrt{b^2+1}\,\sqrt{(b-1)^2+1} > b^2 - b + 1,$$

after squaring both sides, one can easily check that the above result is true. Hence the **Claim 5** is true for $n_1 = n_2$.

Next we assume that $n_1 \geq n_2 + 1$. In this case we have to prove that

$$n_1\left(\sqrt{a^2+1} - \sqrt{(a-1)^2+1}\right) > n_2\left(\sqrt{b^2+1} - \sqrt{(b-1)^2+1}\right).$$

One can easily see that

$$\sqrt{b^2+1} - \sqrt{(b-1)^2+1} < 1.$$

Using this, from the above, we have to prove that

$$\frac{n_1}{n_2} > \frac{1}{\sqrt{a^2+1} - \sqrt{(a-1)^2+1}},$$

that is,

$$\sqrt{a^2+1} > \sqrt{(a-1)^2+1} + \frac{n_2}{n_2+1},$$

that is,

$$2a - 1 > \frac{2n_2}{n_2+1}\sqrt{(a-1)^2+1} + \left(\frac{n_2}{n_2+1}\right)^2,$$

that is,

$$2a - 2 > \frac{2n_2}{n_2+1}\sqrt{(a-1)^2+1},$$

that is,

$$(a-1)^2\,(n_2+1)^2 > n_2^2\Big((a-1)^2+1\Big),$$

that is,

$$(a-1)^2\,(2n_2+1) > n_2^2,$$

which is always true as $a \geq n_1 + 1 \geq n_2 + 2$. This completes the proof of **Claim 5**. □

Claim 6. $\sqrt{(r+1)^2+t^2} + \sqrt{(s-1)^2+t^2} > \sqrt{r^2+t^2} + \sqrt{s^2+t^2}$, where $r = n + n_1 - p - 1$, $s = n + n_2 - p - 1$ and $t = n + n_i - p - 1$.

Proof of Claim 6. We have to prove that

$$\sqrt{(r+1)^2+t^2} - \sqrt{s^2+t^2} > \sqrt{r^2+t^2} - \sqrt{(s-1)^2+t^2},$$

that is,

$$(r+1)^2+t^2+s^2+t^2-2\sqrt{(r+1)^2+t^2}\,\sqrt{s^2+t^2}$$
$$> r^2+t^2+(s-1)^2+t^2-2\sqrt{r^2+t^2}\,\sqrt{(s-1)^2+t^2},$$

that is,

$$\left(r+s+\sqrt{r^2+t^2}\,\sqrt{(s-1)^2+t^2}\right)^2 > \left((r+1)^2+t^2\right)(s^2+t^2),$$

that is,

$$\sqrt{r^2+t^2}\,\sqrt{(s-1)^2+t^2} > r(s-1)+t^2,$$

that is,

$$(r-s+1)^2 > 0,$$

which is true always. This completes the proof of **Claim 6**. □

Claim 7. $\sqrt{(n+n_1-p)^2+(n+n_2-p-2)^2} > \sqrt{(n+n_1-p-1)^2+(n+n_2-p-1)^2}$.

Proof of Claim 7. We have to prove that

$$(n+n_1-p)^2+(n+n_2-p-2)^2 > (n+n_1-p-1)^2+(n+n_2-p-1)^2,$$

that is,

$$2(n+n_1-p) > 2(n+n_2-p)-2,$$

that is,

$$n_1-n_2+1>0,$$

which is true always. This completes the proof of **Claim 7**. □

By **Claim 5**, we obtain

$$\begin{aligned}&(n_1+1)\sqrt{a^2+1}+(n_2-1)\sqrt{(b-1)^2+1}-n_1\sqrt{(a-1)^2+1}-n_2\sqrt{b^2+1}\\ &=n_1\sqrt{a^2+1}+n_2\sqrt{(b-1)^2+1}-n_1\sqrt{(a-1)^2+1}-n_2\sqrt{b^2+1}\\ &\qquad+\sqrt{a^2+1}-\sqrt{(b-1)^2+1}\\ &>\sqrt{a^2+1}-\sqrt{(b-1)^2+1}>0.\end{aligned} \tag{8}$$

By **Claim 6**, we obtain

$$\begin{aligned}&\sum_{i=3}^{n-p}\Bigg[\sqrt{(n+n_1-p)^2+(n+n_i-p-1)^2}+\sqrt{(n+n_2-p-2)^2+(n+n_i-p-1)^2}\\ &-\sqrt{(n+n_1-p-1)^2+(n+n_i-p-1)^2}-\sqrt{(n+n_2-p-1)^2+(n+n_i-p-1)^2}\Bigg]\\ &>0.\end{aligned} \tag{9}$$

Using (8), (9) with **Claim 7** in (7), we obtain $SO(H_1) > SO(H_2)$. Using this result several times (if needed), we obtain

$$SO(H_{n,\underbrace{n_1,\,n_2,\ldots,\,n_{n-p}}}) < SO(H_{n,\underbrace{n_1+1,\,n_2-1,\ldots,\,n_{n-p}}}) < \cdots < SO(Ki_n^{n-p}).$$

as $H_{n,\underbrace{n_1,\ldots,\,n_{n-p}}} \ncong Ki_n^{n-p}$. Hence

$$SO(G) \le SO(H_{n,\underbrace{n_1,\ldots,\,n_{n-p}}}) < SO(Ki_n^{n-p}).$$

This completes the proof of the theorem. □

4. Conclusions

Sombor index was used to model entropy and enthalpy of vaporization of alkanes with satisfactory prediction potential, indicating that this topological index may be used successfully on modeling thermodynamic properties of compounds. In this paper we presented some lower and upper bounds on the Sombor index of graph G in terms of graph parameters (clique number, chromatic number, number of pendant vertices, etc.) and characterize the extremal graphs. Here we pose two related problems.

Problem 1. Characterize the maximal graph with respect to Sombor index among all connected graphs of order n with clique number ω.

Problem 2. Characterize the minimal graph with respect to Sombor index among all connected graphs of order n with p pendant vertices.

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