

## On extremal trees for the minimum Sombor index with fixed total domination number

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**Abstract:** The Sombor index of a graph  $G$  is a degree-based graph structure descriptor, defined as  $SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$ , in which  $d(x)$  is the degree of the vertex  $x \in V(G)$ , for  $x = u, v$ . In this paper, we find a sharp lower bound of the Sombor index in trees with fixed total domination number and we characterize the extremal trees. More precisely, given any tree  $T$  with order  $n$  and total domination number  $\gamma_t$ , we prove that  $SO(T) \geq \left(2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2}\right)(n - 2\gamma_t) + 4\sqrt{2}\gamma_t + 2\sqrt{5} - 6\sqrt{2}$ . This lower bound improves, in many cases, the known lower bounds given with the order and with the order and the domination number of the tree.

**Keywords:** Sombor index, total domination number, tree.

**AMS Subject classification:**

## 1. Introduction

Topological indices are numerical invariants that can be applied in describing molecular structures and have an essential role in the different sciences. Ivan Gutman in

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2021 [14] introduced a new topological index, namely the Sombor index, which is defined by

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

The study of the topological indices has shown the correlation between chemical compounds and their physico-chemical properties [12]. In particular, the discriminant and prediction potential of the Sombor index for chemical graphs were shown in [23], and it indicates that this descriptor may be successfully applied to model thermodynamic properties of compounds. Sombor index was used in that work to model the entropy and enthalpy of vaporization of alkanes. The importance of the Sombor index and its high accuracy in predicting physico-chemical properties was also studied in [11]. Some mathematical properties and results of the Sombor index of graphs can be found in [7–9, 13, 19, 21, 22], and other of its applications can be found in [20, 23].

The relationships between the Sombor index and other topological indices have been recently studied in the literature [9, 13]. Das et al. [9] obtained relations between the Sombor index and Zagreb indices of graphs, and Filipovski [13] obtained some relations between the Sombor index and some degree-based topological indices such as Zagreb indices, Forgotten index and Randić index. However, a topic which is generating more interest is to find relationships between topological indices and some well-known parameters in the graph [1–3, 5, 6, 16, 18, 19, 24, 25]. In [3, 5, 6, 24], authors determined lower and upper bounds for the geometric-arithmetic, Randić, Zagreb and Sombor index of a tree (a graph without cycles), respectively, in terms of the domination number and size of the tree. In [2, 4, 18], authors gave bounds for the Randić, Geometric-Arithmetic index and Zagreb index of a tree, respectively, in terms of the total domination number and size of the tree. In [1], the authors did the same with the Zagreb index and the Roman domination number. In [19], the extremal trees which attain the maximum and minimum Sombor index among all trees with given degree sequence were investigated. In [16], authors gave extremal trees for the Sombor index with a given diameter. The relation between energy and the Sombor index of a graph was studied in [25]. The minimum Sombor index of trees with given number of pendant vertices has been given in [17]. Very recently, Wang et al. [26] discussed the extremal problem of the bipartite graphs with a given diameter for the Sombor index. The authors determined the largest, second-largest and smallest Sombor indices of bipartite graphs with a given diameter.

In this work, we focus on finding a new lower bound for the Sombor index of trees using the number of vertices and the total domination number. Moreover, we characterize the extremal trees for this lower bound. As we show with some remarks after the main theorem, the bound presented in this work improves the ones obtained in [10, 24], in many cases. Throughout this paper, we suppose that  $G$  is a simple graph consisting with vertex set  $V(G)$  and edge set  $E(G)$ . A total dominating

set  $D$  of a graph  $G$  is a subset of  $V(G)$  such that each vertex in  $V(G)$  is adjacent to at least one vertex in  $D$ . The total domination number  $\gamma_t(G)$  is the minimum cardinality among all total dominating sets of  $G$ . For more information about the total domination number we refer to [15]. The neighbourhood set of a vertex  $u \in V(G)$  is the set of all vertices adjacent to  $u$  and it is denoted by  $N(u)$ . The closed neighbourhood of the vertex  $u$  is  $N[u] = N(u) \cup \{u\}$ . We consider  $|N(u)| = d(u)$ , which is the degree of the vertex  $u$ . A vertex is called a leaf if its degree is equal to 1, and it is called a support vertex if it is adjacent to a leaf. The diameter of a tree (a connected acyclic undirected graph) is the largest path between two leaves. Given a vertex  $v \in V(G)$ , the graph  $G - \{v\}$  is the graph whose vertex set is  $V(G) \setminus \{v\}$  and edge set is  $E(G) \setminus \{vu : u \in N(v)\}$ . Given an edge  $e \in E(G)$ , the graph  $G - \{e\}$  is the graph whose vertex set is  $V(G)$  and edge set is  $E(G) \setminus \{e\}$ . Given  $k$  vertices  $v_1, \dots, v_k$  or edges  $e_1, \dots, e_k$ , we consider  $G - \{v_1, \dots, v_k\} = (G - \{v_1, \dots, v_{k-1}\}) - \{v_k\}$  or  $G - \{e_1, \dots, e_k\} = (G - \{e_1, \dots, e_{k-1}\}) - \{e_k\}$ .

## 2. Lower Bound for the Sombor index of trees in terms of the total domination number

Sun and Du in [24] found extremal trees for the Sombor index with a given domination number. In this section, we provide a new lower bound for the Sombor index of trees in terms of the number of vertices and the total domination number. For that, we present here two lemmas we will use in the proof of the main theorem. All inequalities involving one variable functions presented in the proof of the main theorem have been checked with Mathematica program.

**Lemma 1.** [24] Consider  $h_c(x) = \sqrt{x^2 + (c+1)^2} - \sqrt{x^2 + c^2}$  for  $x \geq 1$  and any positive number  $c$ . Then  $h_c(x)$  is decreasing function for  $x$ .

**Lemma 2.** [24] Let  $x \geq 1$  and  $\varphi_c(x) = \sqrt{x^2 + c^2} - \sqrt{(x-1)^2 + c^2}$  for a positive number  $c$ . Then  $\varphi_c(x)$  is a increasing function for  $x$ .

**Theorem 1.** Let  $T$  be a tree of order  $n$  with total domination number  $\gamma_t$ . Then

$$SO(T) \geq \left(2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2}\right) (n - 2\gamma_t) + 4\sqrt{2}\gamma_t + 2\sqrt{5} - 6\sqrt{2}. \quad (2.1)$$

*Proof.* To simplify the computations, we define

$$f(n, \gamma_t) = \left(2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2}\right) (n - 2\gamma_t) + 4\sqrt{2}\gamma_t + 2\sqrt{5} - 6\sqrt{2}.$$

If  $n = 3$ , then  $SO(P_3) = 2\sqrt{5} > f(3, 2)$ . If  $n = 4$ , then  $SO(P_4) = 2\sqrt{5} + 2\sqrt{2} = f(4, 2)$  and  $SO(S_4) = 3\sqrt{10} > f(4, 2)$ . Therefore, we suppose that  $n \geq 5$  and that the result

is satisfied for any tree  $T$  such that  $|V(T)| = n - 1$ , and we will prove that it holds for any tree  $T$  with  $n$  vertices. In order to make the proof easier to read, we first present some claims.

**Claim 1.** Let  $v$  be a support vertex such that  $N(v) = \{u_1, \dots, u_i\}$ ,  $d(u_s) = 1$  for every  $s \in \{1, \dots, i - 1\}$  and  $d(u_i) = j \geq 2$ . If  $i \geq 4$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 1.* If we consider  $T_1 = T - \{u_1\}$ , we have  $\gamma_t(T_1) = \gamma_t$  and, by Lemma 2,

$$\begin{aligned}
 SO(T) &= SO(T_1) + \sqrt{i^2 + 1} + (i - 2) \left( \sqrt{i^2 + 1} - \sqrt{(i - 1)^2 + 1} \right) \\
 &\quad + \left( \sqrt{i^2 + j^2} - \sqrt{(i - 1)^2 + j^2} \right) \\
 &\geq f(n - 1, \gamma_t) + \sqrt{i^2 + 1} + (i - 2) \left( \sqrt{i^2 + 1} - \sqrt{(i - 1)^2 + 1} \right) \\
 &\quad + \left( \sqrt{i^2 + j^2} - \sqrt{(i - 1)^2 + j^2} \right) \\
 &= f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{i^2 + 1} \\
 &\quad + (i - 2) \left( \sqrt{i^2 + 1} - \sqrt{(i - 1)^2 + 1} \right) + \left( \sqrt{i^2 + j^2} - \sqrt{(i - 1)^2 + j^2} \right) \\
 &\geq f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{17} + 2(\sqrt{17} - \sqrt{10}) \\
 &\quad + \left( \sqrt{16 + j^2} - \sqrt{9 + j^2} \right).
 \end{aligned}$$

Since

$$- \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{17} + 2(\sqrt{17} - \sqrt{10}) + \left( \sqrt{16 + j^2} - \sqrt{9 + j^2} \right) > 0,$$

for every  $j \geq 2$ , we conclude that  $SO(T) > f(n, \gamma_t)$ .

**Claim 2.** Let  $v$  be a support vertex such that  $N(v) = \{u_1, u_2, u_3\}$ ,  $d(u_1) = d(u_2) = 1$  and  $d(u_3) = j \geq 2$ . If  $j \leq 5$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 2.* If we take again  $T_1 = T - \{u_1\}$  and we use the computation done in the proof of Claim 1 and Lemma 1, we get

$$\begin{aligned}
 SO(T) &\geq f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + 2\sqrt{10} - \sqrt{5} + \sqrt{9 + j^2} - \sqrt{4 + j^2} \\
 &> f(n, \gamma_t),
 \end{aligned}$$

for every  $j \leq 5$ .

**Claim 3.** Let  $v$  be a support vertex such that  $N(v) = \{u_1, u_2, u_3\}$ ,  $d(u_1) = d(u_2) = 1$  and  $d(u_3) = j \geq 2$ . If there exists a minimum total dominating set  $D$  in  $T$  such that  $|D \cap N(u_3)| \geq 2$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 3.* If we take  $T_2 = T - \{u_1, u_2\}$ , we have  $\gamma_t(T_2) = \gamma_t - 1$  and

$$\begin{aligned} SO(T) &= SO(T_2) + 2\sqrt{10} + \sqrt{j^2 + 9} - \sqrt{j^2 + 1} \\ &\geq f(n - 2, \gamma_t - 1) + 2\sqrt{10} + \sqrt{j^2 + 9} - \sqrt{j^2 + 1} \\ &= f(n, \gamma_t) - 4\sqrt{2} + 2\sqrt{10} + \sqrt{j^2 + 9} - \sqrt{j^2 + 1} \\ &> f(n, \gamma_t) - 4\sqrt{2} + 2\sqrt{10} > f(n, \gamma_t). \end{aligned}$$

**Claim 4.** Let  $v$  be a support vertex such that  $N(v) = \{u_1, u_2, u_3\}$ ,  $d(u_1) = d(u_2) = 1$  and  $d(u_3) = j \geq 3$ . If  $N(u_3) = \{v, w_1, \dots, w_{j-1}\}$  and  $d(w_i) = 1$  for every  $i \in \{1, \dots, j - 2\}$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 4.* By Claim 2 we can assume that  $j \geq 6$ . If we take  $T_1 = T - \{w_1\}$ , we have  $\gamma_t(T_1) = \gamma_t$  and

$$\begin{aligned} SO(T) &= SO(T_1) + \left(\sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9}\right) + \sqrt{j^2 + 1} \\ &\quad + (j-3)\left(\sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1}\right) + \left(\sqrt{j^2 + d(w_{j-1})^2} - \sqrt{(j-1)^2 + d(w_{j-1})^2}\right) \\ &\geq f(n, \gamma_t) - \left(2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2}\right) + \left(\sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9}\right) + \sqrt{j^2 + 1} \\ &\quad + (j-3)\left(\sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1}\right) + \left(\sqrt{j^2 + d(w_{j-1})^2} - \sqrt{(j-1)^2 + d(w_{j-1})^2}\right). \end{aligned}$$

Using Lemma 2,  $\sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9} \geq \sqrt{45} - \sqrt{34}$ ,  $\sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1} \geq \sqrt{37} - \sqrt{26}$  and  $\sqrt{j^2 + d(w_{j-1})^2} - \sqrt{(j-1)^2 + d(w_{j-1})^2} > 0$ , then

$$\begin{aligned} SO(T) &> f(n, \gamma_t) - \left(2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2}\right) + \sqrt{45} - \sqrt{34} + \sqrt{37} + 3(\sqrt{37} - \sqrt{26}) \\ &> f(n, \gamma_t). \end{aligned}$$

**Claim 5.** Let  $v$  be a support vertex such that  $N(v) = \{u_1, u_2\}$  and  $d(u_2) = j \geq 2$ . If there exists a minimum total dominating set  $D$  in  $T$  such that  $|D \cap N(u_2)| \geq 2$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 5.* If we take  $T_1 = T - \{u_1\}$  and we have  $\gamma_t(T_1) = \gamma_t - 1$ . Thus, we obtain

$$\begin{aligned}
 SO(T) &= SO(T_1) + \sqrt{5} + \sqrt{j^2 + 4} - \sqrt{j^2 + 1} \\
 &\geq f(n-1, \gamma_t - 1) + \sqrt{5} + \sqrt{j^2 + 4} - \sqrt{j^2 + 1} \\
 &= f(n, \gamma_t) + 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} - 4\sqrt{2} + \sqrt{5} + \sqrt{j^2 + 4} - \sqrt{j^2 + 1} \\
 &> f(n, \gamma_t).
 \end{aligned}$$

**Claim 6.** Let  $v$  be a support vertex such that  $N(v) = \{u_1, u_2\}$  and  $d(u_2) = j \geq 4$ . If  $N(u_2) = \{v, w_1, \dots, w_{j-1}\}$  and  $d(w_i) = 1$  for every  $i \in \{1, \dots, j-2\}$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 6.* If we take  $T_1 = T - \{w_1\}$ , we have

$$\begin{aligned}
 SO(T) &= SO(T_1) + \sqrt{j^2 + 1} + (j-3) \left( \sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1} \right) + \sqrt{j^2 + d(w_{j-1})^2} \\
 &\quad - \sqrt{(j-1)^2 + d(w_{j-1})^2} + \sqrt{j^2 + 4} - \sqrt{(j-1)^2 + 4} \\
 &\geq f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{j^2 + 1} + (j-3) \left( \sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1} \right) \\
 &\quad + \sqrt{j^2 + d(w_{j-1})^2} - \sqrt{(j-1)^2 + d(w_{j-1})^2} + \sqrt{j^2 + 4} - \sqrt{(j-1)^2 + 4}.
 \end{aligned}$$

It can be checked that

$$\begin{aligned}
 & - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{j^2 + 1} + (j-3) \left( \sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1} \right) \\
 & \quad + \sqrt{j^2 + 4} - \sqrt{(j-1)^2 + 4} > 0,
 \end{aligned}$$

for every  $j \geq 4$ , so we have that  $SO(T) > f(n, \gamma_t)$ .

**Claim 7.** If  $v_1, v_2, v_3, v_4, w$  are five vertices in  $T$  such that  $d(v_1) = d(w) = 1$ ,  $N(v_2) = \{v_1, v_3\}$ ,  $N(v_3) = \{v_2, v_4, w\}$  and  $d(v_4) = 2$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 7.* If we take  $T_1 = T - \{w\}$  we have

$$\begin{aligned}
 SO(T) &= SO(T_1) + 2\sqrt{13} - 2\sqrt{8} + \sqrt{10} \\
 &\geq f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + 2\sqrt{13} - 4\sqrt{2} + \sqrt{10} \\
 &> f(n, \gamma_t).
 \end{aligned}$$

**Claim 8.** Let  $v_1, v_2, v_3, v_4, w$  be five vertices in  $T$  such that  $d(v_1) = d(w) = 1$ ,  $N(v_2) = \{v_1, v_3\}$ ,  $N(v_3) = \{v_2, v_4, w\}$  and  $d(v_4) \geq 2$ . If  $|N(v_4) \cap D| \geq 2$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 8.* Let  $N(v_4) = \{v_3, v_5, z_1, \dots, z_{j-2}\}$ . If we take  $T_4 = T - \{v_1, v_2, v_3, w\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_4) + \sqrt{5} + \sqrt{10} + \sqrt{13} + \sqrt{j^2 + 9} + \left( \sqrt{j^2 + d(v_5)^2} - \sqrt{(j-1)^2 + d(v_5)^2} \right) \\ &\quad + \sum_{i=1}^{j-2} \left( \sqrt{j^2 + d(z_i)^2} - \sqrt{(j-1)^2 + d(z_i)^2} \right) \\ &> f(n-4, \gamma_t-2) + \sqrt{5} + \sqrt{10} + \sqrt{13} + \sqrt{j^2 + 9} \\ &= f(n, \gamma_t) - 8\sqrt{2} + \sqrt{5} + \sqrt{10} + \sqrt{13} + \sqrt{j^2 + 9} > f(n, \gamma_t), \end{aligned}$$

for every  $j \geq 2$ .

**Claim 9.** Let  $v_1, v_2, v_3, v_4$  be four vertices in  $T$  such that  $d(v_1) = 1$ ,  $N(v_2) = \{v_1, v_3\}$ ,  $N(v_3) = \{v_2, v_4\}$  and  $d(v_4) \geq 2$ . If  $|N(v_4) \cap D| \geq 2$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 9.* Let  $N(v_4) = \{v_3, v_5, z_1, \dots, z_{j-1}\}$ . If we take  $T_3 = T - \{v_1, v_2, v_3\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_3) + \sqrt{5} + \sqrt{8} + \sqrt{j^2 + 4} + \left( \sqrt{j^2 + d(v_5)^2} - \sqrt{(j-1)^2 + d(v_5)^2} \right) \\ &\quad + \sum_{i=1}^{j-2} \left( \sqrt{j^2 + d(z_i)^2} - \sqrt{(j-1)^2 + d(z_i)^2} \right) \\ &> f(n-3, \gamma_t-2) + \sqrt{5} + 2\sqrt{2} + \sqrt{j^2 + 4} \\ &= f(n, \gamma_t) + 2\sqrt{13} + 2\sqrt{5} - \frac{19\sqrt{2}}{2} + \sqrt{j^2 + 4} > f(n, \gamma_t), \end{aligned}$$

for every  $j \geq 2$ .

**Claim 10.** Let  $P = v_1 v_2 v_3 v_4 v_5$  be a path with five vertices in  $T$  such that  $d(v_1) = 1$ ,  $d(v_2) = d(v_3) = d(v_4) = 2$  and  $d(v_5) = j \geq 2$ . If  $j \geq 3$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 10.* Since we can assume that  $v_4 \notin D$ , if  $N(v_5) = \{v_4, w_1, w_2, \dots, w_{j-1}\}$  and we take  $T_4 = T - \{v_1, v_2, v_3, v_4\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_4) + \sqrt{5} + 2\sqrt{8} + \sqrt{j^2 + 4} + \sum_{i=1}^{j-1} \left( \sqrt{j^2 + d(w_i)^2} - \sqrt{(j-1)^2 + d(w_i)^2} \right) \\ &\geq f(n-4, \gamma_t-2) + \sqrt{5} + 4\sqrt{2} + \sqrt{j^2 + 4} + \sum_{i=1}^{j-1} \left( \sqrt{j^2 + d(w_i)^2} - \sqrt{(j-1)^2 + d(w_i)^2} \right) \\ &= f(n, \gamma_t) + \sqrt{5} - 4\sqrt{2} + \sqrt{j^2 + 4} + \sum_{i=1}^{j-1} \left( \sqrt{j^2 + d(w_i)^2} - \sqrt{(j-1)^2 + d(w_i)^2} \right). \end{aligned}$$

Since  $\sqrt{5} - 4\sqrt{2} + \sqrt{j^2 + 4} > 0$  for every  $j \geq 3$ , we have that  $SO(T) > f(n, \gamma_t)$ .

**Claim 11.** If  $P = v_1v_2v_3v_4v_5v_6$  is a path with six vertices in  $T$  such that  $d(v_1) = 1$ ,  $d(v_2) = d(v_3) = d(v_4) = d(v_5) = d(v_6) = 2$ , then  $SO(T) \geq f(n, \gamma_t)$ .

*Proof of Claim 11.* Using the computations done in the proof of Claim 10 with  $j = 2$  and  $T_4 = T - \{v_1, v_2, v_3, v_4\}$  we have

$$SO(T) \geq f(n, \gamma_t) + \sqrt{5} - 2\sqrt{2} + \sqrt{4 + d(v_6)^2} - \sqrt{1 + d(v_6)^2} = f(n, \gamma_t).$$

**Claim 12.** Let  $P = v_1v_2v_3v_4v_5v_6v_7$  be a path with seven vertices in  $T$  such that  $d(v_1) = 1$ ,  $d(v_2) = d(v_3) = d(v_4) = d(v_5) = 2$  and  $d(v_6) = j \geq 2$ . If  $j \geq 4$ ,  $N(v_6) = \{v_5, v_7, z_1, \dots, z_{j-2}\}$  and  $d(z_i) \leq 3$  for every  $i \in \{1, \dots, j-2\}$ , then  $SO(T) > f(n, \gamma_t)$ .

*Proof of Claim 12.* If we take  $T_5 = T - \{v_1, v_2, v_3, v_4, v_5\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_5) + \sqrt{5} + 3\sqrt{8} + \sqrt{4 + j^2} + \sqrt{j^2 + d(v_7)^2} - \sqrt{(j-1)^2 + d(v_7)^2} \\ &\quad + \sum_{i=1}^{j-2} \left( \sqrt{j^2 + d(z_i)^2} - \sqrt{(j-1)^2 + d(z_i)^2} \right) \\ &\geq f(n-5, \gamma_t-2) + \sqrt{5} + 6\sqrt{2} + \sqrt{4 + j^2} + \sqrt{j^2 + d(v_7)^2} - \sqrt{(j-1)^2 + d(v_7)^2} \\ &\quad + \sum_{i=1}^{j-2} \left( \sqrt{j^2 + d(z_i)^2} - \sqrt{(j-1)^2 + d(z_i)^2} \right) \\ &= f(n, \gamma_t) - 2\sqrt{13} + \frac{7\sqrt{2}}{2} - 2\sqrt{2} + \sqrt{4 + j^2} + \sqrt{j^2 + d(v_7)^2} - \sqrt{(j-1)^2 + d(v_7)^2} \\ &\quad + \sum_{i=1}^{j-2} \left( \sqrt{j^2 + d(z_i)^2} - \sqrt{(j-1)^2 + d(z_i)^2} \right). \end{aligned}$$

By Lemma 1, we know that

$$\sqrt{j^2 + d(z_i)^2} - \sqrt{(j-1)^2 + d(z_i)^2} \geq \sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9},$$

thus

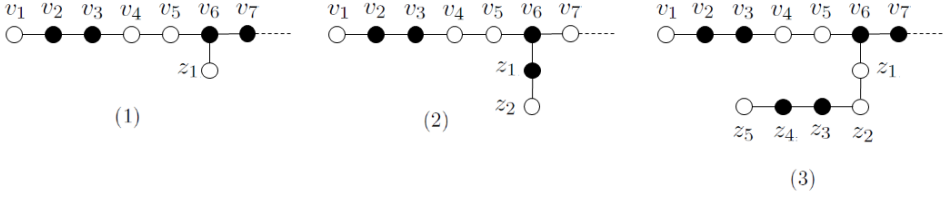
$$SO(T) > f(n, \gamma_t) - 2\sqrt{13} + \frac{3\sqrt{2}}{2} + \sqrt{4 + j^2} + (j-2) \left( \sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9} \right).$$

It can be checked that

$$-2\sqrt{13} + \frac{3\sqrt{2}}{2} + \sqrt{4 + j^2} + (j-2) \left( \sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9} \right) > 0$$

for every  $j \geq 4$ , so  $SO(T) > f(n, \gamma_t)$ .

Now, we take the longest path  $P = v_1 v_2 \dots v_{d+1}$  in  $T$ , whose length is equal to the diameter  $d$  of the tree. Since  $SO(P_5) > f(5, 3)$ ,  $SO(P_6) > f(6, 4)$  and  $SO(P_7) > f(7, 4)$ , by Claims 1-12 we can assume that  $d \geq 7$ ,  $d(v_2) = d(v_3) = d(v_4) = d(v_5) = 2$  and  $d(v_6) = 3$ . Moreover,  $v_6 \in D$  and, if  $N(v_6) = \{v_5, v_7, z_1\}$ , then, by Claims 1-12,  $d(z_1) \leq 2$  and the only three possibilities are shown in Figure 1, where black vertices represent vertices which can be considered in  $D$ .



**Figure 1.** The three cases left to prove after Claims 1-12

In these three cases, if we take  $T_5 = T - \{v_1, v_2, v_3, v_4, v_5\}$ , using Lemma 1 and the computation done in the proof of Claim 12, we have

$$\begin{aligned}
 SO(T) &\geq f(n, \gamma_t) - \sqrt{13} + \frac{3\sqrt{2}}{2} + \sqrt{9 + d(v_7)^2} - \sqrt{4 + d(v_7)^2} + \sqrt{9 + d(z_1)^2} - \sqrt{4 + d(z_1)^2}. \\
 &\geq f(n, \gamma_t) - \sqrt{13} + \frac{3\sqrt{2}}{2} + \sqrt{9 + d(v_7)^2} - \sqrt{4 + d(v_7)^2} + \sqrt{13} - 2\sqrt{2} \\
 &= f(n, \gamma_t) - \frac{\sqrt{2}}{2} + \sqrt{9 + d(v_7)^2} - \sqrt{4 + d(v_7)^2} \\
 &> f(n, \gamma_t),
 \end{aligned}$$

for  $d(v_7) = 2$ . Therefore, we suppose that  $d(v_7) \geq 3$  and we study the three cases separately.

*Case 1.* We suppose that  $N(v_6) = \{v_5, v_7, z_1\}$  and  $d(z_1) = 1$ , and we distinguish two new cases.

*Case 1.1.* We suppose that  $d(v_7) = 3$ . In such a case, if we take  $T_1 = T - \{z_1\}$  we have

$$\begin{aligned}
 SO(T) &= SO(T_1) + \sqrt{13} - \sqrt{8} + \sqrt{18} - \sqrt{13} + \sqrt{10} \geq f(n-1, \gamma_t) + \sqrt{2} + \sqrt{10} \\
 &= f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{2} + \sqrt{10} \\
 &= f(n, \gamma_t) - 2\sqrt{13} - \sqrt{5} + \frac{9\sqrt{2}}{2} + \sqrt{10} > f(n, \gamma_t).
 \end{aligned}$$

*Case 1.2.* We suppose that  $d(v_7) \geq 4$ . If there exists  $x \in D \cap (N(v_7) \setminus \{v_6\})$ , we can take  $T_6 = T - \{v_1, v_2, v_3, v_4, v_5, z_1\}$  to have

$$\begin{aligned} SO(T) &= SO(T_6) + \sqrt{5} + 3\sqrt{8} + \sqrt{13} + \sqrt{10} + \left( \sqrt{d(v_7)^2 + 9} - \sqrt{d(v_7)^2 + 1} \right) \\ &\geq f(n-6, \gamma_t - 3) + \sqrt{5} + 6\sqrt{2} + \sqrt{13} + \sqrt{10} + \left( \sqrt{d(v_7)^2 + 9} - \sqrt{d(v_7)^2 + 1} \right) \\ &= f(n, \gamma_t) + \sqrt{5} - 6\sqrt{2} + \sqrt{13} + \sqrt{10} + \left( \sqrt{d(v_7)^2 + 9} - \sqrt{d(v_7)^2 + 1} \right) \\ &> f(n, \gamma_t). \end{aligned}$$

Therefore, we suppose that  $D \cap N(v_7) = \{v_6\}$ . But, in this case, by Claims 1-12, if  $N(v_7) = \{v_6, v_8, x_1, \dots, x_{j-2}\}$ , we have that  $d(x_i) = 1$  for every  $i \in \{1, 2, \dots, j-2\}$ . If we take  $T_1 = T - \{x_1\}$ , by Lemma 2 we have

$$\begin{aligned} SO(T) &= SO(T_1) + \sqrt{j^2 + 1} + \left( \sqrt{j^2 + d(v_8)^2} - \sqrt{(j-1)^2 + d(v_8)^2} \right) \\ &\quad + \left( \sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9} \right) + (j-3) \left( \sqrt{j^2 + 1} - \sqrt{(j-1)^2 + 1} \right) \\ &\geq f(n-1, \gamma_t) + \sqrt{17} + \left( \sqrt{16 + d(v_8)^2} - \sqrt{9 + d(v_8)^2} \right) + 5 - \sqrt{18} + \sqrt{17} - \sqrt{10} \\ &\geq f(n, \gamma_t) - 2\sqrt{13} - \sqrt{5} + \frac{\sqrt{2}}{2} + 2\sqrt{17} + 5 - \sqrt{10} + \sqrt{16 + d(v_8)^2} - \sqrt{9 + d(v_8)^2} \\ &> f(n, \gamma_t). \end{aligned}$$

*Case 2.* We suppose that  $N(v_6) = \{v_5, v_7, z_1\}$ ,  $N(z_1) = \{v_6, z_2\}$  and  $d(z_2) = 1$ . If we denote  $N(v_7) = \{v_6, v_8, x_1, x_2, \dots, x_{j-2}\}$ , by Claims 1-12, we know that  $d(x_i) \leq 3$  for  $1 \leq i \leq j-2$ . We distinguish two cases.

*Case 2.1.* We suppose that there exists  $x \in D \cap (N(v_7) \setminus \{v_6\})$ . If we take  $T' = T - \{v_6, v_7\}$ , which has two disjoint components  $T_1$  and  $T_2$  containing the vertex  $v_6$  and  $v_7$ , respectively, using Lemmas 1 and 2, we have

$$\begin{aligned} SO(T) &= SO(T_1) + SO(T_2) + 2\sqrt{13} - 2\sqrt{8} + \sqrt{j^2 + 9} + \left( \sqrt{j^2 + d(v_8)^2} - \sqrt{(j-1)^2 + d(v_8)^2} \right) \\ &\quad + \sum_{i=1}^{j-2} \left( \sqrt{j^2 + d(x_i)^2} - \sqrt{(j-1)^2 + d(x_i)^2} \right) \\ &\geq f(n, \gamma_t) + 2\sqrt{5} - 6\sqrt{2} + 2\sqrt{13} - 4\sqrt{2} + 3\sqrt{2} + \left( \sqrt{j^2 + d(v_8)^2} - \sqrt{(j-1)^2 + d(v_8)^2} \right) \\ &\quad + (j-2) \left( \sqrt{j^2 + 9} - \sqrt{(j-1)^2 + 9} \right) \\ &\geq f(n, \gamma_t) + 2\sqrt{5} - 7\sqrt{2} + 2\sqrt{13} + \left( \sqrt{j^2 + d(v_8)^2} - \sqrt{(j-1)^2 + d(v_8)^2} \right) + 3\sqrt{2} - \sqrt{13} \\ &> f(n, \gamma_t) + 2\sqrt{5} - 4\sqrt{2} + \sqrt{13} > f(n, \gamma_t). \end{aligned}$$

*Case 2.2.* We suppose that  $N(v_7) \cap D = \{v_6\}$ . Firstly, let us see that  $v_7$  belongs to  $D$ . If  $d(x_1) = 1$ , it is clear that  $v_7$  must belong to  $D$ . If  $d(x_1) \geq 2$ , then, by

Claims 1-12,  $d(v_7) = 3$ ,  $d(x_1) = 2$  and there exist four vertices  $w_2, w_3, w_4$  and  $w_5$  such that  $x_1, w_2, w_3, w_4, w_5$  is a path,  $d(w_2) = d(w_3) = d(w_4) = 2$  and  $d(w_5) = 1$ . Consequently,  $v_7 \in D$ , and, if we take  $T_6 = T - \{v_1, v_2, v_3, v_4, z_1, z_2\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_6) + \sqrt{5} + 2\sqrt{13} + 6\sqrt{2} + \sqrt{j^2 + 9} - \sqrt{j^2 + 4} \\ &> f(n - 6, \gamma_t - 3) + \sqrt{5} + 2\sqrt{13} + 6\sqrt{2} \\ &= f(n, \gamma_t) + \sqrt{5} + 2\sqrt{13} - 6\sqrt{2} > f(n, \gamma_t). \end{aligned}$$

*Case 3.* We suppose that  $N(v_6) = \{v_5, v_7, z_1\}$  and there exist four vertices  $z_2, z_3, z_4, z_5$  such that  $P = z_1 z_2 z_3 z_4 z_5$  is a path,  $d(z_1) = d(z_2) = d(z_3) = d(z_4) = 2$  and  $d(z_5) = 1$ . If we denote  $N(v_7) = \{v_6, v_8, x_1, x_2, \dots, x_{j-2}\}$ , by Claims 1-12, we know that  $d(x_i) \leq 3$  for  $1 \leq i \leq j - 2$ . We distinguish two cases.

*Case 3.1.* We suppose that there exists  $x \in D \cap (N(v_7) \setminus \{v_6\})$ . If we take  $T_{10} = T - \{v_1, v_2, v_3, v_4, v_5, z_1, z_2, z_3, z_4, z_5\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_{10}) + 2\sqrt{5} + 2\sqrt{13} + 12\sqrt{2} + \sqrt{j^2 + 9} - \sqrt{j^2 + 1} \\ &\geq f(n - 10, \gamma_t - 5) + 2\sqrt{5} + 2\sqrt{13} + 12\sqrt{2} + \sqrt{j^2 + 9} - \sqrt{j^2 + 1} \\ &> f(n, \gamma_t) + 2\sqrt{5} + 2\sqrt{13} - 8\sqrt{2} > f(n, \gamma_t). \end{aligned}$$

*Case 3.2.* We suppose that  $N(v_7) \cap D = \{v_6\}$  and we distinguish two new cases.

*Case 3.2.1.* We suppose that  $d(x_i) = 1$  for every  $i \in \{1, 2, \dots, j - 2\}$ . If  $j \geq 4$  and we take  $T_1 = T - \{x_1\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_1) + \sqrt{j^2 + 1} + \left( \sqrt{j^2 + d(v_8)^2} - \sqrt{(j - 1)^2 + d(v_8)^2} \right) \\ &\quad + \left( \sqrt{j^2 + 9} - \sqrt{(j - 1)^2 + 9} \right) + (j - 3) \left( \sqrt{j^2 + 1} - \sqrt{(j - 1)^2 + 1} \right) \\ &> f(n - 1, \gamma_t) + \sqrt{j^2 + 1} + \left( \sqrt{j^2 + 9} - \sqrt{(j - 1)^2 + 9} \right) \\ &\quad + (j - 3) \left( \sqrt{j^2 + 1} - \sqrt{(j - 1)^2 + 1} \right) \\ &= f(n, \gamma_t) - \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + \sqrt{j^2 + 1} \\ &\quad + \left( \sqrt{j^2 + 9} - \sqrt{(j - 1)^2 + 9} \right) + (j - 3) \left( \sqrt{j^2 + 1} - \sqrt{(j - 1)^2 + 1} \right) \\ &> f(n, \gamma_t), \end{aligned}$$

for  $j \geq 4$ . Therefore, we suppose that  $N(v_7) = \{v_6, v_8, x_1\}$  with  $d(x_1) = 1$  and we study two new cases.

*Case 3.2.1.1.* We suppose  $d(v_8) \leq 3$ . Then, if we take  $T_6 = T - \{z_1, z_2, z_3, z_4, z_5, x_1\}$  we have

$$\begin{aligned} SO(T) &= SO(T_6) + \sqrt{5} + 2\sqrt{13} + 5\sqrt{2} + \sqrt{10} + \left( \sqrt{d(v_8)^2 + 9} - \sqrt{d(v_8)^2 + 4} \right) \\ &\geq f(n - 6, \gamma_t - 2) + \sqrt{5} + 2\sqrt{13} + 5\sqrt{2} + \sqrt{10} + \left( \sqrt{d(v_8)^2 + 9} - \sqrt{d(v_8)^2 + 4} \right) \\ &= f(n, \gamma_t) - \sqrt{5} - 2\sqrt{13} + 4\sqrt{2} + \sqrt{10} + \left( \sqrt{d(v_8)^2 + 9} - \sqrt{d(v_8)^2 + 4} \right) \\ &> f(n, \gamma_t), \end{aligned}$$

for every  $d(v_8) \leq 3$ .

*Case 3.2.1.2.* We suppose  $d(v_8) = p \geq 4$ . We denote  $N(v_8) = \{v_7, v_9, b_1, b_2, \dots, b_{p-2}\}$ , where, since  $v_8 \notin D$ ,  $d(b_l) \geq 2$  for every  $1 \leq l \leq p - 2$ . If there exists a minimum total dominating set  $D$  in  $T$  such that  $|D \cap N(v_8)| \geq 2$ , we take  $T' = T - \{v_7 v_8\}$  and using Lemmas 1 and 2, we have

$$\begin{aligned} SO(T) &= SO(T_1) + SO(T_2) + \sqrt{10} + 3\sqrt{2} - \sqrt{5} - \sqrt{13} + \sqrt{p^2 + 9} \\ &\quad + \left( \sqrt{p^2 + d(v_9)^2} - \sqrt{(p-1)^2 + d(v_9)^2} \right) + \sum_{i=1}^{p-2} \left( \sqrt{p^2 + d(b_i)^2} - \sqrt{(p-1)^2 + d(b_i)^2} \right) \\ &\geq f(n, \gamma_t) + 2\sqrt{5} - 6\sqrt{2} + \sqrt{10} + 3\sqrt{2} - \sqrt{5} - \sqrt{13} + 5 \\ &\quad + \left( \sqrt{16 + d(v_9)^2} - \sqrt{9 + d(v_9)^2} \right) + \sum_{i=1}^{p-2} \left( \sqrt{p^2 + d(b_i)^2} - \sqrt{(p-1)^2 + d(b_i)^2} \right) \\ &> f(n, \gamma_t) + \sqrt{5} - 3\sqrt{2} + \sqrt{10} - \sqrt{13} + 5 > f(n, \gamma_t). \end{aligned}$$

Therefore, we suppose that  $D \cap N(v_8) = \{v_7\}$  for any minimum total dominating set  $D$  in  $T$ . In such a case, by Claims 1-12, any path starting in  $v_8$  and containing the edge  $v_8 b_i$  ( $1 \leq i \leq p - 2$ ) must have length six or seven, but, in such a case, also by Claims 1-12,  $D \cap N(v_8) \neq \{v_7\}$ , a contradiction.

*Case 3.2.2.* We suppose that  $d(x_1) \geq 2$ . In such a case, by Claims 1-12, the path starting in  $v_7$  and containing the edge  $v_7 x_1$  must have length five or six. If it has length six, then  $N(v_7) \cap D \neq \{v_6\}$ , so it has length five,  $d(v_7) = 3$  and, if  $P = v_7 x_1 x'_2 x'_3 x'_4 x'_5$  is this path, it holds that  $d(x_1) = d(x'_2) = d(x'_3) = d(x'_4) = 2$  and  $d(x'_5) = 1$ . We distinguish two new cases.

*Case 3.2.2.1.* We suppose that there exists a minimum total dominating set  $D$  in  $T$  such that  $|D \cap N(v_8)| \geq 2$ . If we denote  $N(v_8) = \{v_7, v_9, b_1, \dots, b_{p-2}\}$  and we take  $T' = T - \{v_7 v_8\}$ , we have

$$\begin{aligned} SO(T) &= SO(T_1) + SO(T_2) + \sqrt{2} + \sqrt{p^2 + 9} + \left( \sqrt{p^2 + d(v_9)^2} - \sqrt{(p-1)^2 + d(v_9)^2} \right) \\ &\quad + \sum_{i=1}^{p-2} \left( \sqrt{p^2 + d(b_i)^2} - \sqrt{(p-1)^2 + d(b_i)^2} \right) \end{aligned}$$

$$\begin{aligned}
&> f(n, \gamma_t) + 2\sqrt{5} - 5\sqrt{2} + \sqrt{13} + \left( \sqrt{p^2 + d(v_9)^2} - \sqrt{(p-1)^2 + d(v_9)^2} \right) \\
&> f(n, \gamma_t) + 2\sqrt{5} - 5\sqrt{2} + \sqrt{13} > f(n, \gamma_t).
\end{aligned}$$

*Case 3.2.2.2.* We suppose that  $D \cap (N(v_8) \setminus \{v_7\}) = \emptyset$  for any minimum total dominating set  $D$ . As we saw before, if  $N(v_8) = \{v_7, v_9, b_1, \dots, b_{p-2}\}$ , any path starting in  $v_8$  and containing the edge  $v_8 b_i$  ( $1 \leq i \leq p-2$ ) must have length at least six, but, since  $v_8 \notin D$ , we get a contradiction. Consequently,  $d(v_8) = 2$ . We take  $T' = T - \{z_1, z_2, z_3, z_4, z_5, x_1, x'_2, x'_3, x'_4, x'_5\}$  and we have that

$$\begin{aligned}
SO(T) &= SO(T') + 9\sqrt{2} + 4\sqrt{13} + 2\sqrt{5} \\
&\geq f(n-10, \gamma_t - 4) + 9\sqrt{2} + 4\sqrt{13} + 2\sqrt{5} \\
&= f(n, \gamma_t) - 2 \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) - 16\sqrt{2} + 9\sqrt{2} + 4\sqrt{13} + 2\sqrt{5} \\
&= f(n, \gamma_t).
\end{aligned}$$

This completes the result.  $\square$

**Remark 1.** Das and Gutman in [10] presented a lower bound on Sombor index of trees in terms of the order. The lower bound of Sombor index for any tree  $T \not\cong P_n$  of order  $n \geq 7$ , is as follows [10, Theorem 3]

$$SO(T) \geq 3\sqrt{5} + 3\sqrt{13} + (n-7)\sqrt{8}.$$

For any  $n \geq 7$  and  $\gamma_t < \frac{n-2}{2}$ , since  $f(n, \gamma_t)$  is a decreasing function on  $\gamma_t$ , we have

$$\begin{aligned}
SO(T) &\geq f(n, \gamma_t) > f\left(n, \frac{n-2}{2}\right) = 2 \left( 2\sqrt{13} + \sqrt{5} - \frac{7\sqrt{2}}{2} \right) + 2(n-2)\sqrt{2} + 2\sqrt{5} - 6\sqrt{2} \\
&= 4\sqrt{5} + 4\sqrt{13} - 3\sqrt{2} + (n-7)\sqrt{8} > 3\sqrt{5} + 3\sqrt{13} + (n-7)\sqrt{8}.
\end{aligned}$$

Therefore, for any tree  $T$ , different from a path and such that  $\gamma_t(T) < \frac{n-2}{2}$ , the lower bound of Theorem 1 is bigger than the lower bound in [10, Theorem 3].

**Remark 2.** The maximum and minimum Sombor indices of trees with a given domination number were presented in [24, Theorem 3.2]. They proposed the following lower bound in terms of the domination number and the order of  $T$ .

$$\begin{aligned}
SO(T) &\geq (3\sqrt{13} + \sqrt{5} - 6\sqrt{2})n + (24\sqrt{2} - 3\sqrt{5} - 9\sqrt{13})\gamma + 2\sqrt{5} - 6\sqrt{2} \\
&= (3\sqrt{13} + \sqrt{5} - 6\sqrt{2})(n - 3\gamma) + 6\sqrt{2}\gamma + 2\sqrt{5} - 6\sqrt{2} = h(n, \gamma).
\end{aligned}$$

Let us show that, if  $\frac{2n}{11} \leq \gamma \leq \gamma_t \leq \frac{10\gamma}{7}$ , then  $f(n, \gamma_t) > h(n, \gamma)$ . If  $\gamma_t \leq \frac{10\gamma}{7}$ , since  $f(n, \gamma_t)$  is a decreasing function on  $\gamma_t$ , we have

$$(2\sqrt{13} + \sqrt{5} - \frac{7}{2}\sqrt{2})(n - 2\gamma_t) + 4\sqrt{2}\gamma_t \geq (2\sqrt{13} + \sqrt{5} - \frac{7}{2}\sqrt{2}) \left( n - \frac{20\gamma}{7} \right) + \frac{40\sqrt{2}\gamma}{7},$$

and

$$(2\sqrt{13} + \sqrt{5} - \frac{7}{2}\sqrt{2}) \left( n - \frac{20\gamma}{7} \right) + \frac{40\sqrt{2}\gamma}{7} > (3\sqrt{13} + \sqrt{5} - 6\sqrt{2})(n - 3\gamma) + 6\sqrt{2}\gamma,$$

if and only if

$$\left( \frac{23\sqrt{13} + \sqrt{5} - 58\sqrt{2}}{7} \right) \gamma > \left( \sqrt{13} - \frac{5\sqrt{2}}{2} \right) n.$$

Since  $\frac{23\sqrt{13} + \sqrt{5} - 58\sqrt{2}}{7} > \frac{11}{25}$  and  $\sqrt{13} - \frac{5\sqrt{2}}{2} < \frac{2}{25}$ , the inequality is satisfied when  $11\gamma \geq 2n$ , it means,  $\gamma \geq \frac{2n}{11}$ . Therefore,  $f(n, \gamma_t) > h(n, \gamma)$  when  $\frac{2n}{11} \leq \gamma \leq \gamma_t \leq \frac{10\gamma}{7}$ . That is satisfied, for instance, in the path  $P_{13}$  with 13 vertices, where  $\gamma(P_{13}) = 5$  and  $\gamma_t(P_{13}) = 7$ .

### 3. Extremal trees for the minimum Sombor index with fixed total domination number

We characterize extremal trees achieving the lower bound in Theorem 1. To do this, we describe a family of trees  $\mathfrak{T}$  that is defined recursively. We take the path of order  $4q$  for each integer  $q \geq 1$  in  $\mathfrak{T}$  and we make new trees in this family as follows. For a tree  $T \in \mathfrak{T}$ , if there is an edge  $xy \in E(T)$  such that  $d(x) = 2 = d(y)$ , neither  $x$  nor  $y$  is a support vertex and there is a minimum total dominating set  $D$  in the tree  $T$  such that  $x, y \in D$ , and we take two arbitrary paths  $P_1 = x_1x_2 \dots x_{4q+1}$  and  $P_2 = y_1y_2 \dots y_{4q'+1}$ , with  $q, q' \geq 1$ , the new tree  $T'$  with vertex set  $V(T) \cup V(P_1) \cup V(P_2)$  and edge set  $E(T) \cup E(P_1) \cup E(P_2) \cup \{xx_1, yy_1\}$ , belongs to  $\mathfrak{T}$ .

**Theorem 2.** *Let  $T$  be a tree of order  $n$  with total domination number  $\gamma_t$ . Then,*

$$SO(T) = \left( 2\sqrt{13} + \sqrt{5} - \frac{7}{2}\sqrt{2} \right) (n - 2\gamma_t) + 4\sqrt{2}\gamma_t + 2\sqrt{5} - 6\sqrt{2},$$

if and only if  $T \in \mathfrak{T}$ .

*Proof.* Let  $n_i$  be the number of vertices with degree  $i$ . For any tree  $T \in \mathfrak{T}$  of order  $n$  and a total domination number  $\gamma_t$ , we have

$$n_1 + n_2 + n_3 = n, \quad n_1 + 2n_2 + 3n_3 = 2(n - 1), \quad \gamma_t = 2n_3 + \frac{n - 5n_3}{2} = \frac{n - n_3}{2}.$$

Therefore, we get  $n_1 = n - 2\gamma_t + 2$ ,  $n_2 = 4\gamma_t - n - 2$  and  $n_3 = n - 2\gamma_t$ . Finally, by the definition of the Sombor index and the structure of trees  $T \in \mathfrak{T}$ , we conclude that

$$\begin{aligned} SO(T) &= 2n_3\sqrt{4+9} + n_1\sqrt{1+4} + \frac{n_3\sqrt{9+9}}{2} + \left( n - 1 - 2n_3 - n_1 - \frac{n_3}{2} \right) \sqrt{4+4} \\ &= 2\sqrt{13}(n - 2\gamma_t) + \sqrt{5}(n - 2\gamma_t + 2) + \frac{3}{2}\sqrt{2}(n - 2\gamma_t) + 2\sqrt{2} \left( -3 + 2\gamma_t - \frac{5}{2}(n - 2\gamma_t) \right) \\ &= \left( 2\sqrt{13} + \sqrt{5} - \frac{7}{2}\sqrt{2} \right) (n - 2\gamma_t) + 4\sqrt{2}\gamma_t + 2\sqrt{5} - 6\sqrt{2}. \end{aligned}$$

Now, using again the function

$$f(n, \gamma_t) = (2\sqrt{13} + \sqrt{5} - \frac{7}{2}\sqrt{2})(n - 2\gamma_t) + 4\sqrt{2}\gamma_t + 2\sqrt{5} - 6\sqrt{2},$$

let us see that, if  $T$  is a tree with order  $n$ , total domination number  $\gamma_t$  and  $SO(T) = f(n, \gamma_t)$ , then  $T \in \mathfrak{T}$ . By absurdum, we suppose that there exists a tree  $T$  such that  $SO(T) = f(n, \gamma_t)$  and  $T \notin \mathfrak{T}$ , and we take the tree  $T$  satisfying that with the minimum number of vertices. If we take the longest path  $v_1, v_2, \dots, v_{d+1}$  in  $T$ , whose length is equal to the diameter  $d$  of the tree, by Claims 1-12 and looking at the proof of Theorem 1, we know that we can have the situation given in Claim 11 or Case 3.2.2.2. If  $d(v_1) = 1$ ,  $d(v_2) = d(v_3) = d(v_4) = d(v_5) = d(v_6) = 2$ , and we take  $T_4 = T - \{v_1, v_2, v_3, v_4\}$ , we have

$$f(n, \gamma_t) = SO(T) = SO(T_4) + 8\sqrt{8} \geq f(n - 4, \gamma_t - 2) + 8\sqrt{8} = f(n, \gamma_t).$$

Therefore,  $SO(T_4) = f(n - 4, \gamma_t - 2) = f(n(T_4), \gamma_t(T_4))$ . If  $T_4 \in \mathfrak{T}$ , it is clear that  $T \in \mathfrak{T}$ , so  $T_4 \notin \mathfrak{T}$ , which is a contradiction because  $n(T_4) < n$ . If we have the situation given in Case 3.2.2.2, we can do exactly the same to get the same contradiction.

## 4. Conclusion

Currently, the study of the behavior of topological indices has attracted the attention of researchers. In addition, many studies have been done on the relationship between topological indices and some well-known parameters in the graph. In this work we have improved the known lower bounds for the Sombor index of trees. A lower bound for the Sombor index of any tree, which depends only on the order of the tree, was given in [10] in 2022, and, the same year, another lower bound for the Sombor index of any tree, which depends on the order and the domination number of the tree, was given in [24]. In this paper, we present a lower bound of the Sombor index of trees, which improves the mentioned bounds in many cases, and depends on the order and the total dominant number of the tree. We have also characterized all the trees attaining the new bound.

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