Iranian J. Math. Chem. 13 (4) December (2022) 281 – 290

IRANIAN JOURNAL OF
Mathematical Chemistry
Journal homepage: ijmc.kashanu.ac.ir

Original Scientific Paper

Extremal Trees for Sombor Index with Given Degree Sequence

FATEME MOVAHEDI•

Department of Mathematics, Faculty of Sciences, Golestan University, Gorgan, Iran

ARTICLE INFO

Article History:

Received: 18 November 2022
Accepted: 22 November 2022
Published online: 30 December 2022
Academic Editor: Ivan Gutman

Keywords:

Sombor index
Extremal tree
Degree sequence

ABSTRACT

Let $G = (V, E)$ be a simple graph with vertex set V and edge set E. The Sombor index of the graph G is a degree-based topological index, defined as $SO(G) = \sum_{uv\in E} \sqrt{d(u)^2 + d(v)^2}$, in which $d(x)$ is the degree of the vertex $x \in V$ for $x = u, v$. In this paper, we characterize the extremal trees with given degree sequence that minimize and maximize the Sombor index.

1. INTRODUCTION

In [1], Gutman defined a new vertex degree-based topological index, named the Sombor index, and defined it for a graph G as follows

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

where $d(u)$ and $d(v)$ denote the degree of vertices u and v in G, respectively. Some chemical applications of the Sombor indices are studied in [2, 3]. Das and Gutman [4] obtained sharp bounds on the Sombor index of trees in terms of the order, independence number, and the number of pendant vertices. The minimum bounds on the Sombor index of the unicyclic graphs with fixed diameter are obtained in [5]. Chen et al. [6] determined the extremal values of the Sombor index of trees with some given parameters such as matching number, pendant vertices, diameter, segment number, and branching number. Movahedi and Akhbari [7]

•Corresponding Author (Email address: f.movahedi@gu.ac.ir)
DOI: 10.22052/IJMC.2022.248570.1676

introduced the entire Sombor index of a graph and obtained the sharp bounds for the entire Somber index.

In recent years, the extremal problem with respect to topological indices has received much attention [8]. Delorme et al. [9] proposed an algorithm for determining an extremal tree with fixed degree sequence that maximizes the general Randić index. Wang [10] characterized the extremal trees with given degree sequence for the general Randić index. Xing et al. [11] characterized the extremal trees with fixed degree sequence that maximize and minimize the atom-bond connectivity index.

In [1], the Sombor index is minimized by the path and maximized by the star among general trees of the same size. Zhou et al. [12] obtained the extremal values of the Sombor index of trees and unicyclic graphs with a given maximum degree. In [13] a sharp upper bound for the Sombor index and the reduced Sombor index among all molecular trees with fixed numbers of vertices is obtained, and those molecular trees achieving the extremal value are characterized.

In [14] the extremal graphs with respect to the Sombor index among all the trees of the same order with a given diameter are characterized. Réti et al. [15] characterized graphs with the maximum Sombor index in the classes of all connected unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs of a given order.

In this paper, we focus on the following natural extremal problem of the Sombor index.

Problem 1. Find extremal trees of Sombor indices with given degree sequence and characterize all extremal trees which attain the extremal values.

Let $T = (V, E)$ be a simple and undirected tree with vertex set $V(T) = \{v_1, \dots, v_n\}$ and the edge set $E(T) = \{e_1, \dots, e_m\}$. The set $N_T(u) = \{v \in V \mid uv \in E\}$ is called the neighborhood of vertex $u \in V$ in tree T. The number of edges incident to vertex u in T is denoted $d(u)$. A leaf is a vertex with degree 1 in tree T. The distance between vertices u and v is the minimum number of edges between u and v and is denoted by $d(u, v)$. The degree sequence of the tree is the sequence of the degrees of non-leaf vertices arranged in non-increasing order. Therefore, we consider $(d_1, d_2, \dots, d_k)$ as a degree sequence of the tree T where $d_1 \geq d_2 \geq \cdots \geq d_k \geq 2$. A tree is called a maximum (minimum) optimal tree if it maximizes (minimizes) the Sombor index among all trees with a given degree sequence.

In this paper, we investigate the extremal trees which attain the maximum and minimum Sombor index among all trees with given degree sequence.

2. Preliminaries

In this section, we prove some lemmas that are used in the next main results.

Lemma 2.1. For function $g(x,y)=\sqrt{x^2+y^2}$, if $x\leq y$ then $g(x,1)\leq g(y,1)$.

Proof. If $x\leq y$, then $x^2+1\ \leq\ y^2+1$ and consequently, $\sqrt{x^2+1}\leq\sqrt{y^2+1}$. Therefore, $g(x,1)\leq g(y,1)$. ■

Lemma 2.2. Let $f(x)=\sqrt{x^2+a^2}-\sqrt{x^2+b^2}$ with $a.b.x\geq 1$. Then $f(x)$ is an increasing function for every $a\leq b$ and a decreasing function for every $a\geq b$.

Proof. We have that $f'(x)=\frac{x}{\sqrt{x^2+a^2}}-\frac{x}{\sqrt{x^2+b^2}}$, Define the function $\hat{f}(y)=\frac{x}{\sqrt{x^2+y^2}}$, where $y\geq 1$. The derivative of this function is $\hat{f}'(y)=\frac{-xy}{(x^2+y^2)\sqrt{x^2+y^2}}<0$. Therefore, $\hat{f}(y)$ is a decreasing function for every $y\geq 1$. Hence, if $a\leq b$, $\frac{x}{\sqrt{x^2+a^2}}=\hat{f}(a)\geq\hat{f}(b)=\frac{x}{\sqrt{x^2+b^2}}$. Consequently, $f'(x)>0$ and the function $f(x)$ is an increasing function for every $x\geq 1$. Similarity, if $a\geq b$, then $f(x)$ is a decreasing function for every $x\geq 1$. ■

Lemma 2.3. Let $h(x)=\sqrt{x^2+y^2}$ with $y\geq 1$. Then $h(x)$ is an increasing function for every $x\geq 1$.

Proof. We have $h'(x)=\frac{x}{\sqrt{x^2+y^2}}$. Since $x\geq 1$, then $h'(x)>0$ and function $h(x)$ is an increasing function for every $x\geq 1$. ■

3. Extremal Trees with the Maximum Sombor Index

In this section, we characterize the extremal trees with maximum Sombor index among the trees with given degree sequence. We propose a technique to construct these trees. To do this, we first state some properties of a maximum optimal tree.

Theorem 3.1. Let T be a maximum optimal tree with a path $v_0\ v_1\ v_2\ ...\ v_k\ v_{k+1}$ in T, where v_0 and v_{k+1} are leaves. For $i\leq\frac{k+1}{2}$ and $i+1\leq j\leq\ k-i+1$,

i. if i is odd, then $d(v_i)\geq d(v_{k-i+1})\geq d\big(v_j\big)$,

ii. if i is even, then $d(v_i)\leq d(v_{k-i+1})\leq d\big(v_j\big)$.

Proof. Let T be a maximum optimal tree with the degree sequence D. We prove the result by induction on i. For $i=1$, we show that $d(v_1)\geq d(v_k)\geq\ d(v_j)$ where $2\leq j\leq k$. We suppose for contradiction that $d(v_1)<d(v_j)$ for some $2\leq j\leq k$. We consider a new tree T' obtained from T by changing edges v_0v_1 and $v_j\ v_{j+1}$ to edges v_0v_j and v_1v_{j+1} such that

no other edges are changed. Note that T and T' have the same degree sequence. Therefore, using Lemmas 2.1-2.3, and since $d(v_{j+1}) > 1$, we have

$$SO(T') - SO(T) = \sqrt{d(v_0)^2 + d(v_j)^2} + \sqrt{d(v_1)^2 + d(v_{j+1})^2} - \left(\sqrt{d(v_0)^2 + d(v_1)^2} + \sqrt{d(v_j)^2 + d(v_{j+1})^2}\right)$$
$$= \left(\sqrt{d(v_j)^2 + 1} - \sqrt{d(v_1)^2 + 1}\right) + \left(\sqrt{d(v_1)^2 + d(v_{j+1})^2} - \sqrt{d(v_j)^2 + d(v_{j+1})^2}\right)$$
$$= f(1) - f\left(d(v_{j+1})\right) > 0,$$

which is a contradiction with the maximum optimality T. Thus, $d(v_1) \geq d(v_j)$ for every $2 \leq j \leq k$. Similarity, we can get $d(v_1) \geq d(v_k)$ and $d(v_k) \geq d(v_j)$. Therefore, we have $d(v_1) \geq d(v_k) \geq d(v_j)$ where $2 \leq j \leq k$. So, we suppose that the result holds for smaller values of i.

If $i \geq 2$ is even, then $i-1$ is odd and by the induction hypothesis, $d(v_{i-1}) \geq d(v_{k-i+1}) \geq d(v_j)$ for $i+1 \leq j \leq k-i+1$. We suppose for contradiction that $d(v_i) > d(v_j)$ for some $i+1 \leq j \leq k-i+1$. We consider a new tree T'' obtained from T by changing edges $v_{i-1}v_i$ and v_jv_{j+1} to edges $v_{i-1}v_j$ and v_iv_{j+1} with the degree sequence D. Also, in tree T'', other edges are the same edges in tree T.

By the induction hypothesis, $d(v_{i-1}) \geq d(v_{j+1})$. Therefore, by applying Lemma 2.2, we have

$$SO(T'') - SO(T) = \sqrt{d(v_{i-1})^2 + d(v_j)^2} + \sqrt{d(v_i)^2 + d(v_{j+1})^2} - \left(\sqrt{d(v_{i-1})^2 + d(v_i)^2} + \sqrt{d(v_j)^2 + d(v_{j+1})^2}\right)$$
$$= \left(\sqrt{d(v_{i-1})^2 + d(v_j)^2} - \sqrt{d(v_{i-1})^2 + d(v_i)^2}\right) + \left(\sqrt{d(v_{j+1})^2 + d(v_i)^2} - \sqrt{d(v_{j+1})^2 + d(v_j)^2}\right)$$
$$= f\left(d(v_{i-1})\right) - f\left(d(v_{j+1})\right) > 0.$$

This contradiction with the maximum optimality of T. Therefore, $d(v_i) \leq d(v_j)$ for $i+1 \leq j \leq k-i+1$. Similarity, we have $d(v_i) \leq d(v_{k-i+1})$ and $d(v_{k-i+1}) \leq d(v_j)$. Consequently, for i even, $d(v_i) \leq d(v_{k-i+1}) \leq d(v_j)$ where $i+1 \leq j \leq k-i+1$. For odd $i > 2$, with the similar technique, we can get $d(v_i) \geq d(v_{k-i+1}) \geq d(v_j)$ for $i+1 \leq j \leq k-i+1$. ■

Suppose that L_i denotes the set of vertices adjacent to the closet leaf at a distance i. Thus, L_0 and L_1 denote the set of leaves and the set of vertices that are adjacent to the leaves. Let $d^m = min\{d(u) : u \in L_1\}$ and L_1^m be the set of leaves whose adjacent vertices have degree d^m in T. We suppose that $\overline{L_1^m}$ denote the set of leaves v such that $v \notin L_1^m$.

We construct a new tree T_i' from trees T and T_i rooted at v_i by identifying the root v_i with a vertex $v \in L_1^m$.

Theorem 3.2. Let T_1' and T_2' are obtained from tree T by identifying the root v_i of T_i with $u' \in L_1^m$ and $v' \in \overline{L_1^m}$, respectively. Then $SO(T_1') \geq SO(T_2')$.

Proof. We suppose that u and v are adjacent to u' and v', respectively. Using Theorem 3.1, $d(u) \leq d(v)$. Therefore, we have

$$\begin{aligned} SO(T_1') - SO(T_2') &= \sqrt{(d(v_i)+1)^2 + d(u)^2} + \sqrt{d(u)^2+1} \\ &\quad - \left(\sqrt{(d(v_i)+1)^2 + d(v)^2} + \sqrt{d(v)^2+1}\right) \\ &= \left(\sqrt{(d(v_i)+1)^2 + d(u)^2} - \sqrt{(d(v_i)+1)^2 + d(v)^2}\right) \\ &\quad + \left(\sqrt{d(v)^2+1} - \sqrt{d(u)^2+1}\right) \\ &= f(1) - f(d(v_i)+1) > 0. \end{aligned}$$

Therefore, $SO(T_1') \geq SO(T_2')$. ■

We use a similar technique in [10], for constructing tree T with a fixed degree sequence D such that T is the maximum optimal tree among the trees with degree sequence D. We propose the following algorithms to construct such trees.

Algorithm 1. (Construction of subtrees)

1. Given the degree sequence of the non-leaf vertices as $D = (d_1, d_2, \ldots, d_m)$ in descending order.
2. If $d_m \geq m-1$, then using Theorem 3.1, the vertices with degrees $d_1, d_2, \ldots, d_{m-1}$ are in L_1. Tree T produces by rooted at u with d_m children whose their degrees are $d_1, d_2, \ldots, d_{m-1}$ and $d_m - m + 1$ leaves adjacent to u.
3. If $d_m \leq m-2$, then we produce subtree T_1 by rooted at u_1 with $d_m - 1$ children with degrees $d_1, d_2, \ldots, d_{d_m - 1}$ such that $u_1 \in L_2$ and the children of u_1 are in L_1. Subtree T_2 is constructed by rooted at u_2 with $d_{m-1} - 1$ children whose degrees are $d_{d_m}, d_{d_m+1}, \ldots, d_{(d_m-1)+(d_{m-1}-1)}$. Then do the same to get subtrees $T_3, T_4, \ldots$ until T_k satisfies the condition of step (2). In this case, we have $d(v_k) = d_{m-k+1}$.

Algorithm 2. (Merge of subtrees)

1. Set $T = T_i$ and $i = k$. We produce a new tree T'_{i-1} from T and T_{i-1} rooted at v_{i-1} by identifying the root v_{i-1} with a vertex $v \in L_1^m$. Using Theorem 3.2, tree T'_{i-1} is a maximum optimal tree among trees with the same degree sequence.
2. Consider $i = k-1, k-2, \dots, 1$ and $T = T_i$. Tree T'_{i-1} from T and T_{i-1} by the same method of step (1). We construct trees $T'_{k-2}, T'_{k-3}, \dots, T'_1$.
3. $T = T'_1$ is the maximum optimal tree with given degree sequence $D = (d_1, d_2, \dots, d_m)$.

Example 3.3. In this example, we propose a maximum optimal tree with given degree sequence $D = (5,5,5,4,3,3,3,2,2)$. Using Step 3 of Algorithm 1, we have subset T_1 with 1 child whose has degree 5. For the new degree sequence $D_1 = (5,5,4,3,3,2)$, we construct tree T_2 and have a new degree sequence $D_2 = (5,4,3,3)$, Figure 1. It is easily seen that D_2 satisfies the condition of Step 2.

Using Algorithm 2, we attach subtrees T_2 to T_3 for constructing T'_2, Figure 2, and T_1 to T'_2 for constructing the maximum optimal tree $T'_1 = T$, Figure 3.

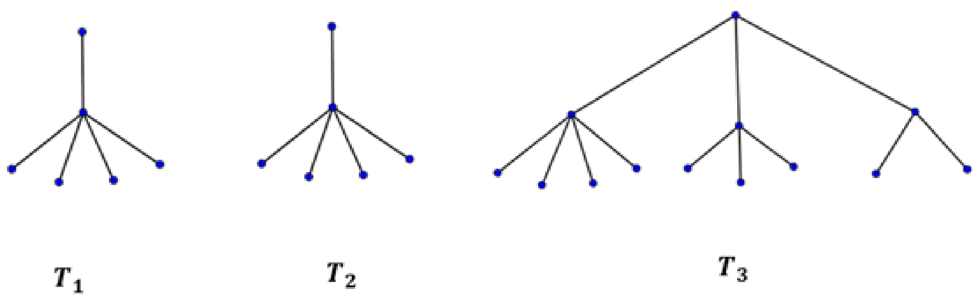


Figure 1: Construction of subtrees using Algorithm 1.

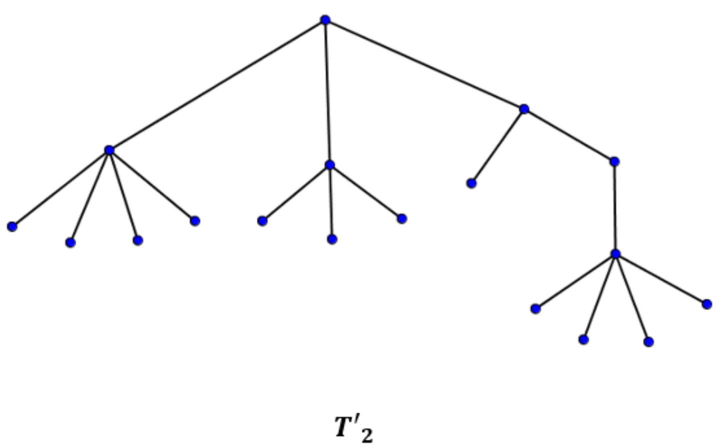
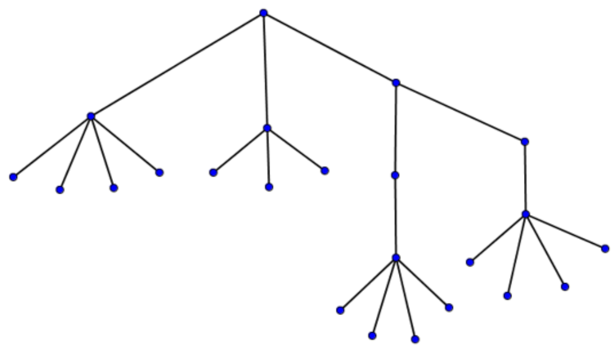


Figure 2: Merge of subtrees using Algorithm 2.

4. EXTREMAL TREES WITH THE MINIMUM SOMBOR INDEX

In this section, we characterize the extremal trees with the minimum Sombor index among the trees with given degree sequence. To do it, we state the following theorem and some properties of a minimal optimal tree.

Theorem 4.1. Let T be a minimum optimal tree with a path $v_1v_2 \dots v_k$ in T, where $k \geq 4$ and $d(v_1) < d(v_k)$. Then $d(v_2) \leq d(v_{k-1})$.



$T'_1 = T$

Figure 3: A maximum optimal tree T with degree sequence $(5, 5, 5, 4, 3, 3, 2, 2)$.

Proof. Let T be a minimum optimal tree with the degree sequence D. We suppose for contradiction that $(v_2) > d(v_{k-1})$. We consider a new tree T' obtained from T by changing edges v_1v_2 and $v_{k-1}v_k$ to edges v_1v_{k-1} and v_2v_k, respectively, such that no other edges are changed. In such a case, the degree sequence of T' is the same as T. Using Lemma 2.2 and since $d(v_1) < d(v_k)$, we have

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{d(v_1)^2 + d(v_{k-1})^2} + \sqrt{d(v_2)^2 + d(v_k)^2} \\ &\quad - \left(\sqrt{d(v_1)^2 + d(v_2)^2} + \sqrt{d(v_{k-1})^2 + d(v_k)^2}\right) \\ &= \left(\sqrt{d(v_2)^2 + d(v_k)^2} - \sqrt{d(v_{k-1})^2 + d(v_k)^2}\right) \\ &\quad - \left(\sqrt{d(v_1)^2 + d(v_2)^2} - \sqrt{d(v_1)^2 + d(v_{k-1})^2}\right) \\ &= f\big(d(v_k)\big) - f(d(v_1)) < 0, \end{aligned}$$

which is a construction with the minimum optimality T. ■

By Theorem 4.1, we can conclude the following results for an optimal tree with the minimum Sombor index. The proof technique is similar to the results in [9].

Corollary 4.2. Let T be a minimum optimal tree among the trees with given degree sequence. Then there is no path $v_1\ v_2 \dots v_k$ in the tree T, where $k \geq 3$, such that $d(v_1), d(v_k) > d(v_i)$ for $2 \leq\ i \leq k-1$.

Corollary 4.3. Let T be a minimum optimal tree among the trees with given degree sequence. Then there are no two non-adjacent edges v_1v_2 and u_1u_2 in the tree T such that $d(v_1) < d(u_1) \leq d(u_2) < d(v_2)$.

Wang [10] presented the extremal trees by the greedy algorithm. We show that trees obtained by this algorithm are optimal trees with the minimum Sombor index.

Algorithm 3. (Greedy algorithm for constructing a minimum optimal tree)

1. Given the degree sequence of the non-leaf vertices as $D = (\ d_1, d_2, \dots, d_m)$ in descending order.
2. Label the root vertex with degree d_1 as v.
3. Label the children of v as $v_1, v_2, \dots, v_{d_1}$ whose degrees are $d_2\ , d_3\ , \dots, d_{d_1+1}$, respectively.
4. Label the children of v_1 (except v) as $v_{11}, v_{12}\ , \dots, v_{1\ d_{2-1}}$whose degrees are $d_{d_1+2}, d_{d_1+3}\ , \dots, d_{d_1+d_2}$, respectively. Do the same for the vertices $v_2, v_3, \dots, v_{d_1}$, respectively.
5. Repeat (4) for all the newly labeled vertices, and always start with the neighbors of the labeled vertex with the largest degree whose neighbors are not labeled yet.

Theorem 4.4. Let T be a tree constructed by Algorithm 3 with a given degree sequence. Then T is a minimum optimal tree.

Proof. Let T be a tree constructed by Algorithm 3. It is easy to see that tree T satisfies the conditions in Theorem 4.1. We show that the Sombor index of the tree T attains the minimum among trees whose conditions in Theorem 4.1 hold. Two following conditions hold for the tree T.

(1) Using Corollary 4.2, for any path $v_1v_2 \dots v_k$, $k \geq 3$, in T, $d(v_1), d(v_k) \leq\ d(v_i)$ for $2 \leq i \leq\ k-1$, and

(2) when $d(u) \geq d(v) \geq d(z)$ and u is not adjacent to v, then using Corollary 4.3 u is not adjacent to z.

The above properties show that tree T has the minimum Sombor index. Therefore, the tree constructed by Algorithm 3 is a minimum optimal tree. ■

Example 4.5. In this example, we propose a minimum optimal tree with given degree sequence $D = (5, 5, 4, 4, 4, 3, 3, 3, 2, 2)$. Using Algorithm 3, we consider the root with degree 5 and children with degrees $5, 4, 4, 4, 3$. The first child from the left will have children of degrees $3, 3, 2, 2$ (see Figure 4).

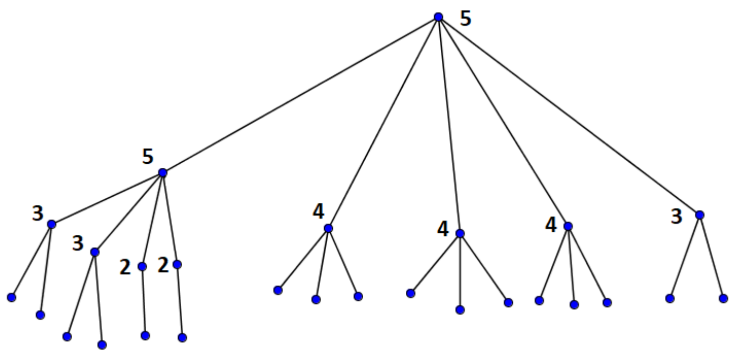


Figure 4: A minimum optimal tree T with degree sequence $(5, 5, 4, 4, 4, 3, 3, 3, 2, 2)$.

Acknowledgements. The author would like to thank Professor Ivan Gutman for suggesting the open extremal problem of the Sombor index.

References

1. I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (1) (2021) 11–16.
2. I. Redžepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc*. **86** (5) (2021) 445–457.
3. M. Mohammadi, H. Barzegar and A. R. Ashrafi, Comparisons of the Sombor index of alkane, alkyl, and annulene series with their molecular mass, *J. Chem.* **2022** (2022) 8348525.
4. K. C. Das and I. Gutman, On Sombor index of trees, *Appl. Math. Comput.* **412** (2022) 126575.
5. A. Alidadi, A. Parsian and H. Arianpoor, The minimum Sombor index for unicyclic graphs with fixed diameter, *MATCH Commun. Math. Comput. Chem.* **88** (3) (2022) 561–572.
6. H. L. Chen, W. H. Li and J. Wang, Extremal values on the Sombor index of trees, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 23–49.
7. F. Movahedi and M. H. Akhbari, Entire Sombor index of graphs, *Iranian J. Math. Chem.* (2022), DOI: 10.22052/IJMC.2022.248350.1663.
8. H. Liu, I. Gutman, L. You and Y. Huang, Sombor index: Review of extremal results and bounds, *J. Math. Chem.* **66** (2022) 771–798.

9. C. Delorme, O. Favaron and F. Rautenbach, Closed formulas for the numbers of small independent sets and matchings and an extremal problem for trees, *Discrete Appl. Math.* **130** (2003) 503–512.
10. H. Wang, Extremal trees with given degree sequence for the Randić index, *Discrete Math.* **308** (15) (2008) 3407–3411.
11. R. Xing and B. Zhou, Extremal trees with fixed degree sequence for atom-bond connectivity index, *Filomat* **26** (4) (2012) 683–688.
12. T. Zhou, Z. Lin and L. Miao, The Sombor index of trees and unicyclic graphs with given maximum degree, arXiv:2103.07947 (2021).
13. H. Deng, Z. Tang and R. Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum Chem.* **121** (2021) e26622.
14. S. Li, Z. Wang and M. Zhang, On the extremal Sombor index of trees with a given diameter, *Appl. Math. Comput.* **416** (2022) 126731.
15. T. Réti, T. Doslić and A. Ali, On the Sombor index of graphs, *Contrib. Math.* **3** (2021) 11–18.