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ON THE SOMBOR INDEX OF CHEMICAL TREES

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Summary. We give sharp bounds on the Sombor index of chemical trees and characterize the cases of the equalities. We stated conjectures regarding second maximal chemical trees of order n with respect to Sombor index, when $n \equiv 0 \pmod 3$ and $n \equiv 1 \pmod 3$.

1 INTRODUCTION

Molecular descriptors are mathematical values used in evaluation and prediction of properties of chemical compounds. They are used to describe the structure and shape of molecules of even more not yet synthesized compounds and so play significant role in mathematical chemistry and pharmacology [11, 13]. Topological indices are type of molecular descriptors calculated on the graphs associated to molecules of chemical compounds. In the literature of mathematical chemistry several dozens of topological indices have been introduced and studied [4-8,12].

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex $v \in V(G)$, the degree of v is denoted by $d_G(v)$, or simply $d(v)$ whenever the graph is clear from the context. The Sombor index is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}. \tag{1}$$

This index, abbreviated as SO index, has been proposed recently by Gutman in [8]. The contribution of the edge $uv \in E(G)$ to SO(G) is

$$s_G(uv) = \sqrt{d^2(u) + d^2(v)} \tag{2}$$

and we will use the next form of equation (1)

$$SO(G) = \sum_{e \in E(G)} s_G(e). \tag{3}$$

A tree is connected graph with no cycles. The problem of finding extreme values of topological indices over chemical trees, that is trees with vertex degrees less or equal 4, has attracted

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considerable attention in the mathematical-chemistry literature [1-3,9,12-14]. In this paper we consider the problem of extreme values of SO index among chemical trees with n-vertices. We stated conjectures regarding second maximal chemical trees with respect to Sombor index, when $n \equiv 0 \pmod 3$ and $n \equiv 1 \pmod 3$.

2 DEFINITIONS AND PRELIMINARIES

Let T be a chemical tree of order n. Throughout the paper, the number of vertices with degree i is denoted by n_i, for every $i = \overline{1,4}$, and for every $1 \leq i \leq j \leq n-1$, m_{ij} denotes the number of edges of T between a vertex with degree i and a vertex with degree j. Now, in this notation, formula (1) takes the form

$$SO(T) = \sum_{1 \leq i \leq j \leq n-1} m_{ij} \sqrt{i^2 + j^2}. \tag{4}$$

which will be used, for the most part.

It has be shown by Gutman [8] that the path graph and the star graph are the graphs with extremal values of SO index among all n-vertex trees. Since the path is chemical tree, the minimum of the SO index in the set of chemical trees with a constant number of vertices is achieved for path graphs, while the maximum is achieved for star graphs only for $n \leq 5$. Our goal here is to characterize the chemical trees of order $n \geq 6$ that maximize SO index.

3 ON THE BOUNDS OF TNE NUMBERS n_i AND m_{ij}

In this section we are going to present and prove two statements that will be crucial in proving the final theorem that gives the upper bound of SO index and complete characterization of the chemical trees on which SO index attains the maximum value.

Lemma 1. *Let T be a n-vertex, $n \geq 6$, chemical tree with maximum value of SO-index. Then, in T holds the following:*

$$m_{22} = 0, m_{23} = 0, m_{33} = 0, \; m_{12} \leq 1.$$

Proof. Let us prove the first claim $m_{22} = 0$. In the contrary, suppose that there is an edge $e = uv \in E(T)$ whose endpoints u and v have degrees 2. Let uu_1 and vv_1 be the remaining edges incident with vertices u and v, respectively, and let $T' = T - vv_1 + uv_1$. Note that, since T is acyclic, u_1 and v_1 are distinct vertices. Therefore, due to (3),

$$\begin{aligned} SO(T') - SO(T) = & (s_{T'}(uu_1) + s_{T'}(uv) + s_{T'}(uv_1)) - \\ & - (s_T(uu_1) + s_T(uv) + s_T(vv_1)) \end{aligned}$$

To obtain the contradiction with the assumption that T is maximal, we need to prove that this difference is positive. Since $d_T(u) = d_T(v) = 2$, $d_{T'}(u) = 3$ and $d_{T'}(v) = 1$, it holds: $s_T(uu_1) < s_{T'}(uu_1)$, $s_T(uv) = \sqrt{8} < \sqrt{10} = s_{T'}(uv)$ and $s_T(vv_1) < s_{T'}(vv_1)$, that is $SO(T') > SO(T)$.

The next claim, $m_{23} = 0$, will be proved in the same manner, by the similar graph transformation. Suppose to the contrary that in T there is an edge $e_0 = uv \in E(T)$ such that $d(u) = 3$ and $d(v) = 2$. Let $e_1 = vw$ be the remaining edge incident with vertex v and let e_2, e_3 be the remaining edges incident with vertex u. Now, for the graph $T' = T - vw + uw$ holds

$$SO(T') - SO(T) = \sum_{i=0}^{3} s_{T'}(e_i) - \sum_{i=0}^{3} s_T(e_i),$$

and $s_{T'}(e_0) = \sqrt{17} < \sqrt{13} = s_T(e_0)$. Since, vertex degree of the only one of two endpoints of edge e_i is increased and the other one is unchanged, we obtain that $s_{T'}(e_i) > s_T(e_i)$, for each $i = \overline{1,3}$. Hence, $SO(T') > SO(T)$.

The claim, $m_{33} = 0$, is going to be proved similarly. Let us suppose that $e_0 = uv \in E(T)$ is an edge whose the both endpoints have degrees 3. Further, let $e_1 = vw_1$ and $e_2 = vw_2$ be the remaining edges incident with vertex v and e_3 and e_4 be the remaining edges incident with vertex u. Without losing the generality, suppose that $d(w_1) \le d(w_2)$ and let us construct a new chemical tree T' from T, by relocating its edge e_1 as follows: $T' = T - vw_1 + uw_1$. Then,

$$SO(T') - SO(T) = \sum_{i=0}^{4} s_{T'}(e_i) - \sum_{i=0}^{4} s_T(e_i)$$

In view of the definition of graph T', $d_T(u) = d_T(v) = 3$, $d_{T'}(u) = 4$ and $d_{T'}(v) = 2$, so $s_{T'}(e_i) > s_T(e_i)$ for $i \in \{0,3,4\}$. It remains to be seen how the sum of contributions of the edges e_1 and e_2 has been changed.

$$s_T(e_1) + s_T(e_2) = \sqrt{9 + d_{w_1}^2} + \sqrt{9 + d_{w_2}^2}$$
$$s_{T'}(e_1) + s_{T'}(e_2) = \sqrt{16 + d_{w_1}^2} + \sqrt{4 + d_{w_2}^2}$$

Using the assumption that $d(w_1) \le d(w_2)$ and $d(w_1), d(w_2) \in \{1, \ldots, 4\}$, by checking of ten cases, we obtain that $s_T(e_1) + s_T(e_2) < s_{T'}(e_1) + s_{T'}(e_2)$. It follows that $SO(T') > SO(T)$.

At the end, we want to argue that $m_{12} \le 1$. Assume for contradiction that, in some maximal tree T of order $n \ge 6$, there are two edges $e = uv$ and $g = ab$ whose endpoints have vertex degrees 2 and 1, that is $d(u) = d(a) = 2$ and $d(v) = d(b) = 1$. Because of assumption $n \ge 6$, u and a are distinct vertices. Let us denote by w and c the remaining vertices adjacent with the vertices u and a, respectively, and let $T' = T - uv + av$. Due to previously proved claims, w and c are vertices, not necessarily distinct, with degree 4 and so

$$s_T(uw) = s_T(ac) = \sqrt{20}, s_T(uv) = s_T(ab) = \sqrt{5},$$
$$s_{T'}(uw) = \sqrt{17}, s_{T'}(ac) = 5, s_{T'}(ab) = \sqrt{10}, s_{T'}(av) = \sqrt{10}$$

Hence, graph T' is a new chemical tree whose SO-index is greater than $SO(T)$, because of

$$SO(T') - SO(T) = (\sqrt{17} + 5 + 2\sqrt{10}) - 2(\sqrt{20} + \sqrt{5}) \approx 2.031 > 0$$

$\square$

Lemma 2. *Let T be a chemical tree with maximum value of SO-index. Then, in T holds the following:* $n_2 \le 1$, $n_3 \le 1$, $n_2 = 1 \Rightarrow n_3 = 0$ *and* $n_3 = 1 \Rightarrow n_2 = 0$.

Proof.
Proof of the claim $n_2 \le 1$: Assume that u and a are two vertices of chemical tree T with degree 2, a let us denote by v_1, v_2 and b_1, b_2 their first neighbors, respectively. Due to Lemma 1,

degrees of the each of the four vertices v_i, b_i, $i = 1,2$ belongs to $\{1,4\}$. Since T is connected graph, the both first neighbors of u can not be pendant vertices, that is at least on of its first neighors has degree 4. The same holds for the vertex a. Without losing the generality suppose that $d(v_1) = d(b_1) = 4$. Vertices v_1 and b_1 are not necessarily distinct. Now we construct a graph T' by removing edge uv_2 from graph T and inserting a new edge among a and v_2, that is $T' = T - uv_2 + av_2$. The following holds

$$\begin{aligned}
s_T(uv_1) = &\quad s_T(ab_1) = \sqrt{20}, \\
s_T(uv_2) = &\quad \sqrt{4+d(v_2)^2}, \qquad s_T(ab_2) = \sqrt{4+d(b_2)^2} \\
s_{T'}(uv_1) = &\quad \sqrt{17}, \qquad s_{T'}(ab_1) = 5, \\
s_{T'}(ab_2) = &\quad \sqrt{9+d(b_2)^2}, \qquad s_{T'}(av_2) = \sqrt{9+d(v_2)^2}.
\end{aligned}$$

Hence,

$$\begin{aligned}
SO(T') - SO(T) = &\quad (5 + \sqrt{17} + \sqrt{9+d(b_2)^2} + \sqrt{9+d(v_2)^2} \\
&-(2\sqrt{20} + \sqrt{4+d(v_2)^2} + \sqrt{4+d(b_2)^2} \\
&> 5 + \sqrt{17} - 2\sqrt{20} \\
&\approx 0.1788337156 > 0
\end{aligned}$$

This is opposite with the assumption that T is a chemical tree with maximum value of Sombor index.

Proof of the claim $n_3 \leq 1$**:** Assume for contradiction that there are two vertices $u, a \in V(T)$ with degree 3, and let v_i and b_i, $i = \overline{1,3}$ be their first neighbors, respectively. Due to Lemma 1, u and a are not adjacent vertices and degrees $d(v_i)$, $d(b_i)$, for each $i = \overline{1,3}$, belongs to $\{1,4\}$. As in the proof of the previous claim, assume that $d(v_1) = d(b_1) = 4$ Now, we distinguished the next three cases:

Case 1: $d(v_2) = d(v_3) = d(b_2) = d(b_3) = 4$.

In this case, we transform graph T to a new on T' as follows: $T' = T - uv_2 + av_2$. The next is worth

$$\begin{aligned}
s_T(uv_i) = &\quad s_T(ab_i) = \quad 5,\ i = \overline{1,3} \\
s_{T'}(uv_1) = &\quad s_{T'}(uv_3) = \quad 2\sqrt{5}, \\
s_{T'}(av_2) = &\quad s_{T'}(ab_i) = \quad 4\sqrt{2},\ i = \overline{1,3}.
\end{aligned}$$

that is

$$SO(T') - SO(T) = (4\sqrt{5} + 16\sqrt{2}) - 30 \approx 1.571688908 > 0.$$

So, T is not a chemical tree with maximum value of Sombor index. **Case 2:** The both of vertices v_2, v_3 have degrees 1, or the both of vertices b_2, b_3 have degrees 1. Without losing generality, let us assume that $d(v_2) = d(v_3) = 1$. Let $T' = T - uv_2 + av_2$. Then,

$$\begin{aligned}
s_T(uv_1) = &\quad s_T(ab_1) = 5, \\
s_T(uv_2) = &\quad s_T(uv_3) = \sqrt{10}, \\
s_T(ab_i) < &\quad s_{T'}(ab_i), \quad i = \overline{1,2}, \\
s_{T'}(uv_1) = &\quad 2\sqrt{5}, \quad s_{T'}(uv_3) = \quad \sqrt{5}, \\
s_{T'}(ab_1) = &\quad 4\sqrt{2}, \quad s_{T'}(av_2) = \quad \sqrt{17}.
\end{aligned}$$

It follows that

$$SO(T') - SO(T) > (3\sqrt{5} + 4\sqrt{2} + \sqrt{17}) - (10 + 2\sqrt{10}) \approx 0.1636 > 0,$$

and again T is not maximal.

Case 3: Previous two cases have not been satisfied. In this case, without losing generality, we may assume that $d(v_2) = 4$ and $d(v_3) = 1$. Since in this, third case, the both of vertices b_2, b_3 are not pendant, let as suppose that $d(b_2) = 4$. Denote by T' chemical tree obtained from T on the same way as in the previous, that is $T' = T - uv_2 + av_2$. We obtain

$$\begin{array}{lll}
s_T(uv_1) = & s_T(uv_2) = 5, & s_T(uv_3) = \sqrt{10} \\
s_T(ab_1) = & s_T(ab_2) = 5, & s_T(ab_3) = \sqrt{9 + d(b_3)^2} \\
s_{T'}(uv_1) = & 2\sqrt{5}, & s_{T'}(uv_3) = \sqrt{5}, \\
s_{T'}(av_2) = & s_{T'}(ab_i) = 4\sqrt{2}, & i = 1,2. \\
s_{T'}(ab_3) = & \sqrt{16 + d(b_3)^2} &
\end{array}$$

and conclude that

$$SO(T') - SO(T) > (12\sqrt{2} + 3\sqrt{5}) - (20 + \sqrt{10}) \approx 0.51649 > 0,$$

that is T is not maximal.

Proof of the claim $n_2 = 1 \Rightarrow n_3 = 0$: Assume for the contradiction that u and a are the vertices of T such that $d(u) = 2$ and $d(a) = 3$. In the same manner as in the previous, u and a are not the first neighbors and there are vertices u_1 and b_1 with degrees 4, adjecent with the verticees u and b, respectively. Since $d(u) = 2$, denote by v_2 remaining vertex adjacent with u and by by b_2, b_3 remaining vertices adjacent with a. We do the same graph transformation $T' = T - uv_2 + av_2$ as in the previous two cases, and obtain the following values

$$\begin{array}{lll}
s_T(uv_1) = & 2\sqrt{5}, & s_T(uv_2) = \sqrt{4 + v_2^2} \\
s_T(ab_1) = & 5, & s_T(ab_i) = \sqrt{9 + d(b_i)^2}, i = 2,3 \\
s_{T'}(uv_1) = & \sqrt{17}, & s_{T'}(ab_1) = 4\sqrt{2}, \\
s_{T'}(av_2) = & \sqrt{16 + v_2^2} & s_{T'}(ab_i) = \sqrt{16 + d(b_i)^2}, i = 2,3
\end{array}$$

Hence,

$$SO(T') - SO(T) > (\sqrt{17} + 4\sqrt{2}) - (5 + 2\sqrt{5}) \approx 0.3078239 > 0,$$

and the claim is proven.

Proof of the claim $n_3 = 1 \Rightarrow n_2 = 0$: This claim is direct consequence of the first and the previous one. □

4 CHEMICAL TREES WITH EXTREME VALUES OF SOMBOR INDEX

For $n = 3k$, $k \geq 2$, let $\mathscr{T}_n$ be the family of chemical trees with n vertices such that: $k-1$ vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and its single vertex with degree 2 is adjacent to the vertices of degree 4, in the case $k \geq 3$. In the case $k = 2$, that is $n = 6$, there is only one graph in $\mathscr{T}_6$ and its single vertex with degree 2 is adjacent with one pendant vertex and one vertex with degree 4.

For $n = 3k+1$, $k \geq 2$, denote by $\mathscr{T}_n$ the family of chemical trees with n vertices such that: $k-1$ vertices have degree 4, one vertex has degree 3, all other vertices are pendant and, in the case $k \geq 4$, its single vertex with degree 3 is adjacent with vertices of degree 4. In the case $k = 2$, that is $n = 7$, there is only one graph in $\mathscr{T}_7$ and its single vertex with degree 3 is adjacent with two pendant vertices and one vertex with degree 4. In the case $k = 3$, that is $n = 10$, there is only one graph in $\mathscr{T}_{10}$ and its single vertex with degree 3 is adjacent with one pendant vertex and two vertices with degree 4.

For $n = 3k+2 \geq 5$, $\mathscr{T}_n$ is the family of chemical trees with n vertices such that: k vertices have degree 4 and remaining are pendant.

Our the main result is presented through the next three theorems, in which the following easy observation will be important:

Let T be a chemical tree with n. Then,

$$n_1 + n_2 + n_3 + n_4 = n \tag{5}$$

and from handshaking lemma

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1). \tag{6}$$

From (5) and (6) we conclude that

$$n_2 + 2n_3 + 3n_4 = n - 2. \tag{7}$$

Theorem 1. *Let T be chemical tree of order $n \geq 6$, such that $n \equiv 0 \pmod 3$. Then*

$$SO(T) \leq 2\frac{n}{3}(\sqrt{17}+2\sqrt{2}) + \\ + \begin{cases} 4\sqrt{5} - 12\sqrt{2}, & n \geq 9 \\ 3\sqrt{5} - \sqrt{17} - 8\sqrt{2} & n = 6 \end{cases}$$

The equality is attained if and only if $T \in \mathscr{T}_n$.

Proof. Let us suppose that $n = 3k$, for some $k \geq 2$. In this case, equality (7) implies that $n_4 \leq k-1$.

First, let's see what's going on when n_4 takes values less then $k-1$. Substituting $n_4 \leq k-2$ into (7) gives $n_2 + 2n_3 \geq 4$. This is impossible because of first two claims from Lemma 2.

Otherwise, when $n_4 = k-1$, (7) gives $n_2 + 2n_3 = 1$, that is $n_2 = 1$ and $n_3 = 0$. This implies that, for $k \geq 3$, there are two possibilities, that is two potential types of maximal graphs:

Type 1: Chemical tree in which $k-1$ vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and the both first neighbors of its single vertex with degree 2 have degree 4

Type 2: Chemical tree in which $k-1$ vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and only one of the first neighbors of its single vertex with degree 2 has degree 4 but the other one is pendant.

Denote by G_1 graph of the first type and by G_2 the graph of the second type. We will prove that $SO(G_1) > SO(G_2)$.

In the both of G_1 anf G_2 holds $n_1 = n - n_4 - 1 = 2k$. Further, in G_1 holds:

$$\begin{aligned} SO(G_1) = {} & m_{24}\sqrt{20} + m_{14}\sqrt{17} + m_{44}\sqrt{32} \\ = {} & 2k(\sqrt{17}+2\sqrt{2}) + 4\sqrt{5} - 12\sqrt{2} \qquad (8) \\ \approx {} & 2k(\sqrt{17}+2\sqrt{2}) - 8.0262908, \qquad (9) \end{aligned}$$

since in this type of graphs $m_{24} = 2$, $m_{14} = n_1 = 2k$, $m_{44} = k-3$ and $m_{ij} = 0$ for all other values of i and j.

On the other side, in G_2 holds:

$$\begin{aligned} SO(G_2) = & \quad m_{12}\sqrt{5}+m_{24}\sqrt{20}+m_{14}\sqrt{17}+m_{14}\sqrt{32} \\ = & \quad 2k(\sqrt{17}+2\sqrt{2})+3\sqrt{5}-\sqrt{17}-8\sqrt{2} \qquad (10) \\ \approx & \quad 2k(\sqrt{17}+2\sqrt{2})-8.728610192, \qquad (11) \end{aligned}$$

since in this type of graphs $m_{12}=1$, $m_{24}=1$, $m_{14}=n_1-1=2k-1$, $m_{44}=k-2$. From (9) and (11) follows that $SO(G_1)>SO(G_2)$.

In the case when $k=2$, that is $n=6$, there is no graph type 1. Moreover there is only one graph G_2 type 2 and from (10) we obtain that its SO index is equal $4(\sqrt{17}+2\sqrt{2})+3\sqrt{5}-\sqrt{17}-8\sqrt{2}$. □

Theorem 2. *Let T be chemical tree of order $n\geq 7$, such that $n\equiv 1\,(\mathrm{mod}\,3)$. Then*

$$\begin{aligned} SO(T) \leq & \quad 2\lfloor\frac{n}{3}\rfloor(\sqrt{17}+2\sqrt{2})+ \\ & + \begin{cases} 15+\sqrt{17}-16\sqrt{2}, & n\geq 13 \\ 10+\sqrt{10}-12\sqrt{2}, & n=10 \\ 5+2\sqrt{10}-\sqrt{17}-8\sqrt{2}, & n=7 \end{cases} \end{aligned}$$

The equality is attained if and only if $T\in\mathscr{T}_n$.

Proof. Let $n=3k+1$, for some $k\geq 2$. As in the previous, equality (7) implies that $n_4\leq k-1$. If n_4 takes values less then $k-1$, substituting into (7) gives $n_2+2n_3\geq 5$, which is impossible by Lemma 2.

Let $n_4=k-1$. From (7) follows that $n_2+2n_3=2$, that is $n_2=0$ and $n_3=1$. Now, for $k\geq 4$, we distinguish three cases, that is tree potential types of maximal trees, regarding the degrees of the first neighbors of its single vertrex with degree 3:

Type 1: Chemical tree in which $k-1$ vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and each of the first neighbors of its single vertex with degree 3 have degree 4 .

Type 2: Chemical tree in which $k-1$ vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and two of the first neighbors of its single vertex with degree 3 have degree 4 and third one is pendant.

Type 3: Chemical tree in which $k-1$ vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and only one the first neighbors of its single vertex with degree 3 has degree 4 and the two are pendants.

In the case $k=3$, that is $n=10$, there is no graph type 3 and for $k=2$, what is equivalent with $n=7$, there is only graph type 1.

Denote by G_1 the graph of the first type, by G_2 the graph of the second type and by G_3 the graph of the third type. We are going to prove that

$$SO(G_1)>SO(G_2)>SO(G_3) \qquad (12)$$

The number n_1 of pendant vertices in each of this graphs is the same $n_1 = n - n_4 - 1 = 2k+1$. In G_1 holds

$$\begin{aligned} SO(G_1) = & \quad m_{34}\sqrt{25} + m_{14}\sqrt{17} + m_{44}\sqrt{32} \\ = & \quad 2k(\sqrt{17}+2\sqrt{2}) + 15 + \sqrt{17} - 16\sqrt{2} \qquad (13) \\ \approx & \quad 2k(\sqrt{17}+2\sqrt{2}) - 3.504311372, \qquad (14) \end{aligned}$$

since in the graphs of type 1 is valid: $m_{34} = 3$, $m_{14} = n_1 = 2k+1$, $m_{44} = k-4$ and $m_{ij} = 0$ for all other values of i and j.

In G_2 numbers m_{ij} take the values: $m_{13} = 1, m_{34} = 2, m_{14} = 2k, m_{44} = k-3$, so it follows

$$\begin{aligned} SO(G_2) = & \quad m_{13}\sqrt{10} + m_{34}\sqrt{25} + m_{14}\sqrt{17} + m_{44}\sqrt{32} \\ = & \quad 2k(\sqrt{17}+2\sqrt{2}) + 10 + \sqrt{10} - 12\sqrt{2} \qquad (15) \\ \approx & \quad 2k(\sqrt{17}+2\sqrt{2}) - 3.808285088 \qquad (16) \end{aligned}$$

Finally, in G_3 nonzero numbers m_{ij} take the values: $m_{13} = 2, m_{34} = 1, m_{14} = 2k-1, m_{44} = k-2$, so

$$\begin{aligned} SO(G_3) = & \quad m_{13}\sqrt{10} + m_{34}\sqrt{25} + m_{14}\sqrt{17} + m_{44}\sqrt{32} \\ = & \quad 2k(\sqrt{17}+2\sqrt{2}) + 5 + 2\sqrt{10} - \sqrt{17} - 8\sqrt{2} \qquad (17) \\ \approx & \quad 2k(\sqrt{17}+2\sqrt{2}) - 4.112258804. \qquad (18) \end{aligned}$$

Thefore, we get to be valid $SO(G_1) > SO(G_2) > SO(G_3)$.

The assertion of the theorem follows. □

Theorem 3. *Let T be chemical tree of order n, such that $n \equiv 2 \pmod 3$. Then*

$$SO(T) \leq 2\frac{n-2}{3}(\sqrt{17}+2\sqrt{2}) + 2\sqrt{17} - 4\sqrt{2}.$$

The equality is attained if and only if $T \in \mathcal{T}_n$.

Proof. Let $n = 3k+2$, for some $k \geq 1$. In this case, equality (7) implies that $n_4 \leq k$. When $n_4 < k$, from (7) follows $n_2 + 2n_3 \geq 3$. Based on the first two claims of Lemma 2, this is valid only for $n_2 = n_3 = 1$, but this is impossible due to the last claims of the same Lemma.

Let us assume that $n_4 = k$. Equality (7) gives $n_2 + 2n_3 = 0$, that is $n_2 = n_3 = 0$. It follows that is in this graph numbers m_{ij} take the next values: $m_{14} = n_1 = 2k+2$, $m_{44} = k-1$, and $m_{ij} = 0$ for all other values of i and j. Hence,

$$\begin{aligned} SO(G_1) = & \quad m_{14}\sqrt{17} + m_{44}\sqrt{32} \\ = & \quad 2k(\sqrt{17}+2\sqrt{2}) + 2\sqrt{17} - 4\sqrt{2} \qquad (19) \\ = & \quad 2\tfrac{n-2}{3}(\sqrt{17}+2\sqrt{2}) + 2\sqrt{17} - 4\sqrt{2}. \qquad (20) \end{aligned}$$

The proof is completed. □

5 CONCLUDING REMARKS AND FURTHER WORK

Sombor index is a recently introduced vertex-degree-based topological index. This paper is one of the several studies ([3], [12]) produced immediately after [7] became available. In this paper we consider its bounds of over the chemical trees and characterize the appropriate extreme cases.

Based on the proofs of Theorem 1 and Theorem 2 we have the following conjectures

Conjecture 1. *Let T be a chemical tree of order $n \geq 9$, such that $n \equiv 0\ (mod\, 3)$, with the second maximum of SO index. Then,*

$$SO(T) \leq 2\frac{n}{3}\left(\sqrt{17}+2\sqrt{2}\right)+3\sqrt{5}-\sqrt{17}-8\sqrt{2}.$$

The equality is attained if and only if T is chemical tree in which $\frac{n}{3}-1$ vertices have degree 4, one vertex has degree 2, remaining vertices are pendant and only one of the first neighbors of its single vertex with degree 2 has degree 4 but the other one is pendant.

Conjecture 2. *Let T be a chemical tree of order $n \geq 10$, such that $n \equiv 1\ (mod\, 3)$, with the second maximum of SO index. Then,*

$$SO(T) \leq 2\frac{n-1}{3}\left(\sqrt{17}+2\sqrt{2}\right)+10+\sqrt{10}-12\sqrt{2}.$$

The equality is attained if and only if T is chemical tree in which $\frac{n-1}{3}-1$ vertices have degree 4, one vertex has degree 3, remaining vertices are pendant and two of the first neighbors of its single vertex with degree 3 has degree 4 but the third one is pendant.

REFERENCES

[1] B. Borovićanin, K.C. Das, B. Furtula, I. Gutman, "Zagreb indices: Bounds and extremal graphs", *MATCH Commun. Math. Comput. Chem.*, **78**, 67-153 (2017).

[2] R. Cruz, J. Monsalve, J. Rada, "Extremal values of vertex-degree-based topological indices of chemical trees", *App. Math and Comp.* , **380**(C), 125281 (2020).

[3] R. Cruz, I. Gutman, J. Rada, "Sombor index of chemical graphs", *Appl. Math. Comput.* **399**, 126018 (2021).

[4] K.C. Das, "Maximizing the sum of the squares of the degrees of a graph", *Discrete Math.*, **285**, 57-66 (2004).

[5] K.C. Das, K. Xu, I. Gutman, "On Zagreb and Harary indices", *MATCH Commun. Math. Comput. Chem*, **70**, 301-314 (2013).

[6] B. Furtula, A. Graovac, D. Vukičević, "Atom-bond connectivity index of trees", *Discret. Appl. Math.* **157**, 2828-2835 (2009)

[7] I. Gutman, O. Miljković, G. Caporossi, P. Hansen, "Alkanes with small and large Randić connectivity indices", *Chem. Phys. Lett.* **306**, 366-372 (1999).

[8] I. Gutman, "Geometric Aproach to Degree-Based Topologocal Indices: Sombor Idices", *MATCH Commun. Math. Comput. Chem*, **86**, 11-16 (2021).

[9] I. Gutman, K.C. Das, "The first Zagreb index 30 years after", *MATCH Commun. Math. Comput. Chem*, **50**, 83-92 (2004).

[10] Ž. Kovijanić Vukićević, G. Popivoda, "Chemical Trees with Extreme Values of Zagreb Indices and Coindices", *Iranial Journa of Math. Chem.*, **5**, 19-29 (2014).

[11] V. R. Kulli, Graph indices, in:M. Pal, S. Samanta, A. Pal (Eds.), *Handbook of Research of Advanced Applications of Graph Theory in Modern Society,* Global, Hershey, 66-91.

[12] I. Redzepovic, "Chemical applicability of Sombor indices", *J. Serb. Chem. Soc.*, https://doi.org/10.2298/JSC201215006R

[13] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics,* Wiley-VCH, Weinheim, (2009).

[14] K. Xu, Y. Alizadeh, K.C.Das, "On two eccentricity-based topological indices of graphs", *Discrete Appl. Math.*, **233**, 240–251 (2017).

[15] K. Xu, K.C. Das, H. Liu, ”Some extremal results on the connective eccentricity index of graphs”, *J. Math. Anal. Appl.*, **433**, 803-817 (2016).
[16] B. Zhou, N. Trinajstić, ”On a novel connectivity index”, *J. Math. Chem*. **46** 1252-1270 (2009).

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