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Research Article

On a conjecture regarding the exponential reduced Sombor index of chemical trees*

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Abstract

Let G be a graph and denote by d_u the degree of a vertex u of G. The sum of the numbers $e^{\sqrt{(d_u-1)^2+(d_v-1)^2}}$ over all edges uv of G is known as the exponential reduced Sombor index. A chemical tree is a tree with the maximum degree at most 4. In this paper, a conjecture posed by Liu et al. [*MATCH Commun. Math. Comput. Chem.* **86** (2021) 729–753] is disproved and its corrected version is proved.

Keywords: topological index; chemical graph theory; Sombor index; reduced Sombor index; exponential reduced Sombor index.

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1. Introduction

Let G be a graph. The sets of edges and vertices of G are represented by $E(G)$ and $V(G)$, respectively. For the vertex $v \in V(G)$, the degree of v is denoted by $d_G(v)$ (or simply by d_v if only one graph is under consideration). A vertex $u \in V(G)$ is said to be a pendent vertex if $d_u = 1$. The degree set of G is the set of all unequal degrees of vertices of G. The set $N_G(u)$ consists of the vertices of the graph G that are adjacent to the vertex v. The members of $N_G(u)$ are known as neighbors of u. A chemical tree is the tree of maximum degree at most 4. The (chemical-)graph-theoretical terminology and notation that are used in this study without explaining here can be found in the books [1, 2, 11].

For the graph G, the Sombor index and reduced Sombor index abbreviated as SO and SO_{red}, respectively, are defined [5] as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2} \quad \text{and} \quad SO_{red}(G) = \sum_{uv\in E(G)} \sqrt{(d_u-1)^2 + (d_v-1)^2}.$$

These degree-based graph invariants, introduced recently in [5], have attained a lot of attention from researchers in a very short time, which resulted in many publications; for example, see the review papers [4, 9], and the papers listed therein.

The following exponential version of the reduced Sombor index was considered in [10]:

$$e^{SO_{red}}(G) = \sum_{uv\in E(G)} e^{\sqrt{(d_u-1)^2+(d_v-1)^2}}.$$

Let n_i denote the number of vertices in the graph G with degree i. The cardinality of the set consisting of the edges joining the vertices of degrees i and j in the graph G is denoted by $m_{i,j}$. Denote by $\mathbb{T}_n$ the class of chemical trees of order n such that $n_2 + n_3 \le 1$ and $m_{1,3} = m_{1,2} = 0$. Deng et al. [3] proved that the members of the class $\mathbb{T}_n$ are the only trees possessing the maximum value of the reduced Sombor index for every $n \ge 11$. Keeping in mind this result of Deng et al. [3], Liu et al. [10] posed the following conjecture concerning the exponential reduced Sombor index for chemical trees.

Conjecture 1.1. [10] *Among all chemical trees of a fixed order n, the members of the class $\mathbb{T}_n$ are the only trees possessing the maximum value of the exponential reduced Sombor index for every $n \ge 11$.*

Conjecture 1.1 was also discussed in [12] and was left open. In fact, there exist counter examples to Conjecture 1.1; for instance, for the trees T_1 and T_2 depicted in Figure 1, it holds that

$$278 \approx e^{SO_{red}}(T_1) = 8e^3 + e^{3\sqrt{2}} + 2e^{\sqrt{10}} < e + 7e^3 + 2e^{3\sqrt{2}} + e^{\sqrt{10}} = e^{SO_{red}}(T_2) \approx 306.$$

The next theorem gives a corrected statement of Conjecture 1.1.

*This paper is dedicated to the memory of Professor Nenad Trinajstić (one of the pioneers of chemical graph theory).

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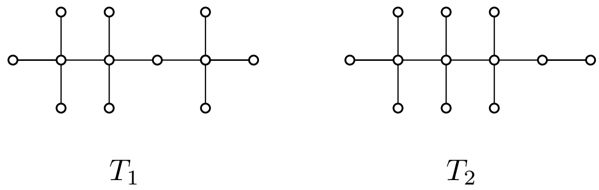

Figure 1: The trees T_1 and T_2 providing a counterexample to Conjecture 1.1.

Theorem 1.1. *For $n \geq 7$, if T is a chemical tree of order n, then*

$$e^{SO_{red}}(T) \leq \frac{1}{3}\left(2e^3 + e^{3\sqrt{2}}\right)n + \frac{1}{3}\left(2e^3 - 5e^{3\sqrt{2}}\right) + \begin{cases} \frac{1}{3}\left(3e - 5e^3 - e^{3\sqrt{2}} + 3e^{\sqrt{10}}\right) & \text{if } n \equiv 0 \pmod 3 \\ \frac{1}{3}\left(6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{\sqrt{13}}\right) & \text{if } n \equiv 1 \pmod 3 \\ 0 & \text{if } n \equiv 2 \pmod 3), \end{cases}$$

with equality if and only if
- *the degree set of T is $\{1,2,4\}$ and $n_2 = m_{2,4} = m_{1,2} = 1$, whenever $n \equiv 0 \pmod 3$;*
- *the degree set of T is $\{1,3,4\}$ and $n_3 = m_{3,4} = 1$ and $m_{1,3} = 2$, whenever $n \equiv 1 \pmod 3$;*
- *the degree set of T is $\{1,4\}$ whenever $n \equiv 2 \pmod 3$.*

2. Proof of Theorem 1.1

If T is a chemical tree of order n with $n \geq 3$, then

$$e^{SO_{red}}(T) = \sum_{1 \leq i \leq j \leq 4} m_{i,j}\, e^{\sqrt{(i-1)^2+(j-1)^2}}\,, \tag{1}$$

$$n_1 + n_2 + n_3 + n_4 = n\,, \tag{2}$$

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

$$\boxed{\sum_{\substack{1 \leq i \leq 4 \\ i \neq j}} m_{j,i} + 2m_{j,j} = j \cdot n_j \quad \text{for } j = 1,2,3,4.} \tag{4}$$

By solving the system of equations (2)–(4) for the unknowns $m_{1,4}, m_{4,4}, n_1, n_2, n_3, n_4$ and then inserting the values of $m_{4,4}$ and $m_{1,4}$ (these two values are well-known, see for example [6]) in Equation (1), one gets

$$\begin{aligned} e^{SO_{red}}(T) = {} & \frac{1}{3}\left(2e^3 + e^{3\sqrt{2}}\right)n + \frac{1}{3}\left(2e^3 - 5e^{3\sqrt{2}}\right) + \frac{1}{3}\left(3e - 4e^3 + e^{3\sqrt{2}}\right)m_{1,2} \\ & + \frac{1}{9}\left(9e^2 - 10e^3 + e^{3\sqrt{2}}\right)m_{1,3} + \frac{1}{3}\left(3e^{\sqrt{2}} - 2e^3 - e^{3\sqrt{2}}\right)m_{2,2} \\ & + \frac{1}{9}\left(9e^{\sqrt{5}} - 4e^3 - 5e^{3\sqrt{2}}\right)m_{2,3} + \frac{1}{3}\left(3e^{\sqrt{10}} - e^3 - 2e^{3\sqrt{2}}\right)m_{2,4} \\ & + \frac{1}{9}\left(9e^{2\sqrt{2}} - 2e^3 - 7e^{3\sqrt{2}}\right)m_{3,3} + \frac{1}{9}\left(9e^{\sqrt{13}} - e^3 - 8e^{3\sqrt{2}}\right)m_{3,4}. \end{aligned} \tag{5}$$

We take

$$\begin{aligned} \Gamma(T) = {} & \frac{1}{3}\left(3e - 4e^3 + e^{3\sqrt{2}}\right)m_{1,2} \\ & + \frac{1}{9}\left(9e^2 - 10e^3 + e^{3\sqrt{2}}\right)m_{1,3} + \frac{1}{3}\left(-2e^3 + 3e^{\sqrt{2}} - e^{3\sqrt{2}}\right)m_{2,2} \\ & + \frac{1}{9}\left(-4e^3 - 5e^{3\sqrt{2}} + 9e^{\sqrt{5}}\right)m_{2,3} + \frac{1}{3}\left(-e^3 - 2e^{3\sqrt{2}} + 3e^{\sqrt{10}}\right)m_{2,4} \\ & + \frac{1}{9}\left(-2e^3 + 9e^{2\sqrt{2}} - 7e^{3\sqrt{2}}\right)m_{3,3} + \frac{1}{9}\left(-e^3 - 8e^{3\sqrt{2}} + 9e^{\sqrt{13}}\right)m_{3,4}. \end{aligned} \tag{6}$$

$$\begin{aligned} \approx {} & -0.8653m_{1,2} - 7.1958m_{1,3} - 32.4742m_{2,2} - 38.2323m_{2,3} \\ & - 29.4651m_{2,4} - 41.6713m_{3,3} - 27.2888m_{3,4}. \end{aligned} \tag{7}$$

Then, Equation (5) can be written as

$$e^{SO_{red}}(T) = \frac{1}{3}\left(2e^3 + e^{3\sqrt{2}}\right)n + \frac{1}{3}\left(2e^3 - 5e^{3\sqrt{2}}\right) + \Gamma(T). \tag{8}$$

For any given integer n greater than 4, it is evident from Equation (8) that a tree T attains the greatest value of $e^{SO_{red}}$ over the class of all chemical trees of order n if and only if T possess the greatest value of Γ in the considered class. As a consequence, we consider $\Gamma(T)$ instead of $e^{SO_{red}}(T)$ in the next lemma.

Lemma 2.1. *Let T be a chemical tree of order n, where $n \geq 7$. The inequality*

$$\Gamma(T) < \frac{1}{3}\left(6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{\sqrt{13}}\right) (\approx -41.6804),$$

holds if any of the following conditions holds:

(i) $\max\{m_{3,3}, m_{2,2}, m_{2,3}\} \geq 1$,

(ii) $\max\{m_{3,4}, m_{2,4}\} \geq 2$,

(iii) $n_2 + n_3 \geq 2$.

Proof. Take an edge $uv \in E(T)$ with $d_u, d_v \in \{2, 3\}$. Since $n \geq 7$, at least one of the two vertices u, v has at least two non-pendent neighbors. Hence, if $\max\{m_{3,3}, m_{2,2}, m_{2,3}\} \geq 1$ then either $m_{3,3}+m_{2,2}+m_{2,3} \geq 2$ or $\max\{m_{3,4}, m_{2,4}\} \geq 1$ and hence the required inequality follows from (6). Also, note that the desired inequality follows from (6) whenever $\max\{m_{3,4}, m_{2,4}\} \geq 2$. In what follows, assume that $m_{3,3} = m_{2,2} = m_{2,3} = 0$, $n_2 + n_3 \geq 2$, and $\max\{m_{3,4}, m_{2,4}\} \leq 1$.

Assume that $n_3 \neq 0$. Let $w \in V(T)$ be a vertex of degree 3 and take $N_T(w) = \{w_1, w_2, w_3\}$. Since $m_{3,3} = m_{2,3} = 0$, one has $d_{w_i} \in \{1, 4\}$ for $i = 1, 2, 3$. Since $n \geq 7$, we have $d_{w_i} = 4$ for at least one $i \in \{1, 2, 3\}$. Hence, if $n_3 \geq t$ then $m_{3,4} \geq t$. Similarly, if $n_2 \geq s$ then $m_{2,4} \geq s$. Thus, if either $n_2 \geq 2$ or $n_3 \geq 2$ then we have $\max\{m_{2,4}, m_{3,4}\} \geq 2$, a contradiction. Consequently, we must have $n_2 = n_3 = 1$, which implies that $m_{2,4} \geq 1$ and $m_{3,4} \geq 1$, and hence the required inequality follows from (6).

□

Proof of Theorem 1.1. If either of the inequalities $\max\{m_{3,3}, m_{2,2}, m_{2,3}\} \geq 1$, $\max\{m_{3,4}, m_{2,4}\} \geq 2$, and $n_2 + n_3 \geq 2$, holds, then by using Lemma 2.1 and Equation (8), one has

$$\begin{aligned} e^{SO_{red}}(T) &< \frac{1}{3}\left(2e^3 + e^{3\sqrt{2}}\right)n + \frac{1}{3}\left(2e^3 - 5e^{3\sqrt{2}}\right) + \frac{1}{3}\left(6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{\sqrt{13}}\right) \\ &< \frac{1}{3}\left(2e^3 + e^{3\sqrt{2}}\right)n + \frac{1}{3}\left(2e^3 - 5e^{3\sqrt{2}}\right) + \frac{1}{3}\left(3e - 5e^3 - e^{3\sqrt{2}} + 3e^{\sqrt{10}}\right) \\ &< \frac{1}{3}\left(2e^3 + e^{3\sqrt{2}}\right)n + \frac{1}{3}\left(2e^3 - 5e^{3\sqrt{2}}\right), \end{aligned}$$

as desired.
In the rest of the proof, assume that $\max\{m_{3,3}, m_{2,2}, m_{2,3}\} = 0$, $\max\{m_{3,4}, m_{2,4}\} \leq 1$, and $n_2 + n_3 \leq 1$. Then, we note that $(n_2, n_3) \in \{(0,0), (1,0), (0,1)\}$. From Equations (2) and (3), it follows that $n_2 + 2n_3 \equiv n - 2 \pmod 3$, which gives

$$(n_2, n_3) = \begin{cases} (1,0) & \text{if } n \equiv 0 \pmod 3, \\ (0,1) & \text{if } n \equiv 1 \pmod 3, \\ (0,0) & \text{if } n \equiv 2 \pmod 3, \end{cases}$$

this together with the system of equations (4) implies that

$$(m_{1,2}, m_{1,3}, m_{2,4}, m_{3,4}) = \begin{cases} (1,0,1,0) & \text{if } n \equiv 0 \pmod 3, \\ (0,2,0,1) & \text{if } n \equiv 1 \pmod 3, \\ (0,0,0,0) & \text{if } n \equiv 2 \pmod 3). \end{cases}$$

Now, from Equation (5) the required result follows. □

3. Concluding remarks

Recently, Liu [7] reported some extremal results for the multiplicative Sombor index. For a graph G, its multiplicative Sombor index and multiplicative reduced Sombor index are defined as

$$\Pi_{SO}(G) = \prod_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \quad \text{and} \quad \Pi_{SO_{red}}(G) = \prod_{uv \in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}.$$

As expected, among all chemical trees of a fixed order $n \geq 11$, the trees attaining the maximum (reduced) Sombor index (see [3]) are same as the ones possessing the maximum multiplicative (reduced) Sombor index.

Theorem 3.1. *Among all chemical trees of a fixed order n, the members of the class $\mathbb{T}_n$ are the only trees possessing the maximum value of the multiplicative (reduced) Sombor index for every $n \geq 11$.*

Analogous to the definition of the exponential reduced Sombor index, the exponential Sombor index can be defined as

$$e^{SO}(G) = \sum_{uv \in E(G)} e^{\sqrt{(d_u)^2 + (d_v)^2}}.$$

Denote by $\mathbb{T}_n^{\star}$ the class of chemical trees of order n such that $n_2 + n_3 \leq 1$ and $m_{3,4} + m_{2,4} \leq 1$. As expected, among all chemical trees of a fixed order $n \geq 7$, the trees attaining the maximum exponential reduced Sombor index (see Theorem 1.1) are same as the ones possessing the maximum exponential Sombor index.

Theorem 3.2. *For every $n \geq 7$, the trees of the class $\mathbb{T}_n^{\star}$ uniquely attain the maximum value of the exponential Sombor index among all chemical trees of a fixed order n.*

Because the proofs of Theorems 1.1, 3.1, and 3.2 are very similar to one another, we omit the proofs of Theorems 3.1 and 3.2.

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