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On Sombor Indices of Tricyclic Graphs

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Abstract

This paper indicates alternative ways of deriving the main results of the recent paper [M. Zhang, B. Zhao, Extremal values of the Sombor index in tricyclic graphs, MATCH Commun. Math. Comput. Chem. 89 (2023) 741-758]. The graphs possessing minimum and maximum values of the reduced Sombor index are also characterized from the class of all tricyclic connected graphs of a given order.

1 Introduction

This paper considers only finite and connected graphs. The (chemical) graph-theoretical notions and terminology that are utilized in the present paper can be found in relevant standard books like [3, 4, 16, 17].

The sets of edges and vertices of a graph G are represented by $E(G)$ and $V(G)$, respectively. Denote by d_v the degree of a vertex $v \in V(G)$. The edge between two vertices $x, y \in V(G)$ is represented by xy.

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A topological index is a numerical quantity TI that is calculated/derived from a (chemical) graph such that TI remains the same under graph isomorphism. Many topological indices being studied in chemical graph theory have several chemical applications, for example see the recent articles [13, 15].

The Sombor and reduced Sombor indices [8] are among the recently introduced topological indices. These indices are denoted as SO and SO_{red}, respectively. They are defined for a graph G as:

$$SO(G) = \sum_{xy \in E(G)} \sqrt{d_x^2 + d_y^2}\,,$$

$$SO_{red}(G) = \sum_{xy \in E(G)} \sqrt{(d_x - 1)^2 + (d_y - 1)^2}\,.$$

The Sombor and reduced Sombor indices were initially studied via a geometric approach. Soon after their discovery, various publications concerning these indices were appeared; such type of articles are still published at a considerable pace. Most of the existing mathematical results regarding Sombor indices can be found in the review articles [7, 10] and in the articles listed therein. Applications of these indices in chemistry are also well researched [6, 9, 11, 12].

A connected graph of order n and size $n + 2$ is known as a connected tricyclic graph. Quite recently, Zhang and Zhao [18] solved the problem of characterizing the graphs possessing minimum and maximum values of the Sombor index among all tricyclic connected graphs of a given order. This paper not only indicates an alternative way of solving the aforementioned problem, by utilizing the results reported in [1, 11, 14], but also gives a solution to an analogous problem regarding the reduced Sombor index.

2 Results

First, we derive the result regarding the minimum Sombor index reported in [18] by utilizing the results reported in [1, 11]. A graph in which all the vertices have the same degree is referred to as a regular graph. By a bidegreed graph G, we mean a non-regular graph in which the degree of every vertex belongs to the set $\{\delta, \Delta\}$, where δ and Δ are the minimum and maximum degrees of G. The following known result confirms that a graph with the minimum Sombor index among all connected graphs of a given order and size must be either regular or bidegreed.

Lemma 1. [1] *If $G^\star$ is a graph with the minimum Sombor index among all connected graphs of order n and size m, then $G^\star$ has $2m - n\lfloor 2m/n \rfloor$ vertices of degree $\lfloor 2m/n \rfloor + 1$ and $n + n\lfloor 2m/n \rfloor - 2m$ vertices of degree $\lfloor 2m/n \rfloor$.*

Since every connected tricyclic graph of order n has $n + 2$ edges and $\lfloor 2(n+2)/n \rfloor = 2$ whenever $n \geq 5$, the following result directly follows from Lemma 1.

Corollary. *For $n \geq 5$, if $G^\star$ is a graph with the minimum Sombor index among all connected tricyclic graphs of order n, then the minimum and maximum degrees of $G^\star$ are 2 and 3, respectively.*

In chemical graph theory, a graph of maximum degree at most 4 is referred to as a chemical graph. Denote by K_n the complete graph of order n.

Lemma 2. [11] *The graph obtained from K_4 by replacing exactly one of its edges with the path of length $n-3$ is the unique graph with the minimum Sombor index among all connected chemical tricyclic graphs of order n for every $n \geq 6$.*

Now, the next result regarding the minimum Sombor index reported in [18] follows from Corollary 2 and Lemma 2.

Corollary. [18] *The graph defined in Lemma 2 is the unique graph with the minimum Sombor index among all connected tricyclic graphs of order n for every $n \geq 6$.*

Although the second main result of [18, Theorem 3.9] regarding the maximum Sombor index can also be found in [14, Theorem 2.1], but we remark here that the proofs of this independently obtained result are entirely different, from each other, in the mentioned papers.

Next, we proceed towards characterizing the graphs possessing minimum value of the reduced Sombor index from the class of all tricyclic connected graphs of a given order. We start with the following elementary lemma.

Lemma 3. *For the real numbers a, b, c, d satisfying $a \geq b \geq c \geq d \geq 0$, it holds that*

$$\sqrt{a+c} + \sqrt{b+d} \geq \sqrt{a+b} + \sqrt{c+d}.$$

Proof. Because of the given constraints on the numbers a, b, c, d, the inequality $a(b-c) \geq d(b-c)$ holds, which is equivalent to

$$\left(\sqrt{a+c} + \sqrt{b+d}\right)^2 \geq \left(\sqrt{a+b} + \sqrt{c+d}\right)^2.$$

■

For a vertex x of a graph G, denote by $N_G(x)$ the set of those vertices of G that are adjacent with x. The member of the set $N_G(x)$ are referred to as neighbors of x. The following result (analogous to Theorem 1 of [1]) is very crucial for characterizing the graphs possessing minimum value of the reduced Sombor index from the class of all tricyclic connected graphs of a given order.

Theorem 1. *If $G^\star$ is a graph with the minimum reduced Sombor index among all connected graphs of order n and size m, then the absolute difference between the minimum and maximum degrees of $G^\star$ is at most* 1.

Proof. Let δ and Δ be the minimum and maximum degrees of $G^\star$, respectively. Contrarily, we assume that $\Delta - \delta > 1$. Take $u, v \in V(G)$ such that $d_u = \delta$ and $d_v = \Delta$. The inequality $\Delta - \delta > 1$ implies that the vertex v has at least one neighbor w such that w is not adjacent with u. Form a new graph $H^\star$ from $G^\star$ by dropping the edge wv and inserting the edge wu. Certainly, both the graphs $H^\star$ and $G^\star$ are connected and have the same number of vertices and edges. However, in the following, we have $SO_{red}(G^\star) - SO_{red}(H^\star) > 0$, a contradiction to the minimality of $SO_{red}(G^\star)$.

In the rest of the proof, we show that $SO_{red}(G^\star) - SO_{red}(H^\star) > 0$. The proof of this inequality is completed by considering two cases. Also, in what follows, when we write d_a we mean that it is the degree of the vertex $a \in V(G^\star) = V(H^\star)$ in $G^\star$ not in $H^\star$.

Case 1. $uv \notin E(G)$.
In this case, we have

$$\begin{aligned}
&SO_{red}(G^\star) - SO_{red}(H^\star)\\
&= \sum_{x \in N_{G^\star}(u)} \left(\sqrt{(d_x-1)^2 + (\delta-1)^2} - \sqrt{(d_x-1)^2 + \delta^2} \right)\\
&+ \sum_{y \in N_{G^\star}(v) \setminus \{w\}} \left(\sqrt{(d_y-1)^2 + (\Delta-1)^2} - \sqrt{(d_y-1)^2 + (\Delta-2)^2} \right)\\
&+ \sqrt{(d_w-1)^2 + (\Delta-1)^2} - \sqrt{(d_w-1)^2 + \delta^2}\,. \qquad (1)
\end{aligned}$$

Since $\Delta - \delta > 1$, that is $\Delta - 2 \geq \delta$, it holds that

$$\begin{aligned}
&\sqrt{(d_w-1)^2 + (\Delta-1)^2} - \sqrt{(d_w-1)^2 + \delta^2}\\
&\geq \sqrt{(d_w-1)^2 + (\Delta-1)^2} - \sqrt{(d_w-1)^2 + (\Delta-2)^2}.
\end{aligned}$$

Thus, Eq. (1) yields

$$\begin{aligned}
&SO_{red}(G^\star) - SO_{red}(H^\star)\\
&\geq \sum_{x \in N_{G^\star}(u)} \left(\sqrt{(d_x-1)^2 + (\delta-1)^2} - \sqrt{(d_x-1)^2 + \delta^2} \right)\\
&+ \sum_{y \in N_{G^\star}(v)} \left(\sqrt{(d_y-1)^2 + (\Delta-1)^2} - \sqrt{(d_y-1)^2 + (\Delta-2)^2} \right). \qquad (2)
\end{aligned}$$

Note that for $x \in N_{G^\star}(u)$ and $y \in N_{G^\star}(v)$ the following inequalities hold

$$\sqrt{(d_x-1)^2 + (\delta-1)^2} - \sqrt{(d_x-1)^2 + \delta^2} \geq \sqrt{2}(\delta-1) - \sqrt{(\delta-1)^2 + \delta^2} \qquad (3)$$

and

$$\sqrt{(d_y-1)^2+(\Delta-1)^2}-\sqrt{(d_y-1)^2+(\Delta-2)^2}$$
$$\geq \sqrt{2}(\Delta-1)-\sqrt{(\Delta-1)^2+(\Delta-2)^2}\,. \tag{4}$$

By utilizing (3) and (4) in (2), we get

$$SO_{red}(G^{\star})-SO_{red}(H^{\star}) \geq \delta\left(\sqrt{2}(\delta-1)-\sqrt{(\delta-1)^2+\delta^2}\,\right)$$
$$+\Delta\left(\sqrt{2}(\Delta-1)-\sqrt{(\Delta-1)^2+(\Delta-2)^2}\,\right). \tag{5}$$

We arrive at the desired conclusion, in the present case, if we prove the following inequality:

$$\delta\left(\sqrt{2}(\delta-1)-\sqrt{(\delta-1)^2+\delta^2}\,\right)$$
$$+\Delta\left(\sqrt{2}(\Delta-1)-\sqrt{(\Delta-1)^2+(\Delta-2)^2}\,\right)>0. \tag{6}$$

Note that $(3\delta-2)\delta>-1$, which is equivalent to

$$2\delta^2\Big((\delta-1)^2+\delta^2\Big)<\Big(2\delta(\delta-1)+(\delta+1)\Big)^2,$$

which yields

$$\sqrt{2}(\delta-1)-\sqrt{(\delta-1)^2+\delta^2}>-\frac{\delta+1}{\sqrt{2}\delta}. \tag{7}$$

Also, we observe that $3\Delta(\Delta-2)+1>0$, which is equivalent to

$$2\Delta^2\Big((\Delta-1)^2+(\Delta-2)^2\Big)<(\Delta-1)^2(2\Delta-1)^2,$$

which provides

$$\sqrt{2}(\Delta-1)-\sqrt{(\Delta-1)^2+(\Delta-2)^2}>\frac{\Delta-1}{\sqrt{2}\Delta}. \tag{8}$$

From (7) and (8), it follows that

$$\begin{aligned}
&\delta\left(\sqrt{2}(\delta-1)-\sqrt{(\delta-1)^2+\delta^2}\,\right)\\
&+\Delta\left(\sqrt{2}(\Delta-1)-\sqrt{(\Delta-1)^2+(\Delta-2)^2}\,\right)\\
&>\delta\left(-\frac{\delta+1}{\sqrt{2}\delta}\right)+\Delta\left(\frac{\Delta-1}{\sqrt{2}\Delta}\right)\geq 0,
\end{aligned}$$

which proves (6). Thus, (5) gives $SO_{red}(G^\star)-SO_{red}(H^\star)>0$, as desired.

Case 2. $uv \in E(G)$.
In this case, it holds that

$$\begin{aligned}
&SO_{red}(G^\star)-SO_{red}(H^\star)\\
&=\sum_{x\in N_{G^\star}(u)\backslash\{v\}}\left(\sqrt{(d_x-1)^2+(\delta-1)^2}-\sqrt{(d_x-1)^2+\delta^2}\,\right)\\
&+\sum_{y\in N_{G^\star}(v)\backslash\{w,u\}}\left(\sqrt{(d_y-1)^2+(\Delta-1)^2}-\sqrt{(d_y-1)^2+(\Delta-2)^2}\,\right)\\
&+\sqrt{(d_w-1)^2+(\Delta-1)^2}-\sqrt{(d_w-1)^2+\delta^2}\\
&+\sqrt{(\delta-1)^2+(\Delta-1)^2}-\sqrt{(\Delta-2)^2+\delta^2}\,.
\end{aligned}\tag{9}$$

Since $\Delta-2\geq\delta$, Eq. (9) gives

$$\begin{aligned}
&SO_{red}(G^\star)-SO_{red}(H^\star)\\
&\geq\sum_{x\in N_{G^\star}(u)\backslash\{v\}}\left(\sqrt{(d_x-1)^2+(\delta-1)^2}-\sqrt{(d_x-1)^2+\delta^2}\,\right)\\
&+\sum_{y\in N_{G^\star}(v)\backslash\{u\}}\left(\sqrt{(d_y-1)^2+(\Delta-1)^2}-\sqrt{(d_y-1)^2+(\Delta-2)^2}\,\right)\\
&+\sqrt{(\delta-1)^2+(\Delta-1)^2}-\sqrt{(\Delta-2)^2+\delta^2}\,.
\end{aligned}\tag{10}$$

By utilizing (3) and (4) in (10), we get

$$\begin{aligned} SO_{red}(G^\star) - SO_{red}(H^\star) \geq\, & (\delta-1)\left(\sqrt{2}(\delta-1) - \sqrt{(\delta-1)^2+\delta^2}\right) \\ & + (\Delta-1)\left(\sqrt{2}(\Delta-1) - \sqrt{(\Delta-1)^2+(\Delta-2)^2}\right) \\ & + \sqrt{(\delta-1)^2+(\Delta-1)^2} - \sqrt{(\Delta-2)^2+\delta^2}\,. \end{aligned} \tag{11}$$

By using (6) in (11), we have

$$\begin{aligned} SO_{red}(G^\star) - SO_{red}(H^\star) >\, & \sqrt{(\delta-1)^2+(\Delta-1)^2} - \sqrt{(\Delta-2)^2+\delta^2} \\ & + \sqrt{(\Delta-1)^2+(\Delta-2)^2} - \sqrt{2}(\Delta-1) \\ & + \sqrt{(\delta-1)^2+\delta^2} - \sqrt{2}(\delta-1)\,. \end{aligned} \tag{12}$$

By taking $a = b = (\Delta-1)^2$, $c = (\Delta-2)^2$, and $d = (\delta-1)^2$ in Lemma 3, we get

$$\begin{aligned} & \sqrt{(\Delta-1)^2+(\Delta-2)^2} + \sqrt{(\Delta-1)^2+(\delta-1)^2} \\ & \geq \sqrt{2}(\Delta-1) + \sqrt{(\Delta-2)^2+(\delta-1)^2}. \end{aligned} \tag{13}$$

Also, by taking $a = (\Delta-2)^2$, $b = \delta^2$, and $c = d = (\delta-1)^2$ in Lemma 3, we get

$$\begin{aligned} & \sqrt{(\Delta-2)^2+(\delta-1)^2} + \sqrt{\delta^2+(\delta-1)^2} \\ & \geq \sqrt{(\Delta-2)^2+\delta^2} + \sqrt{2}(\delta-1) \end{aligned} \tag{14}$$

By utilizing (13) first in (12) and then making use of (14) there, we arrive at the inequality $SO_{red}(G^\star) - SO_{red}(H^\star) > 0$, as desired. ■

Next, we provide a simple but notable corollary of Theorem 1. This corollary is similar to Lemma 1. For the sake of completeness, we provide its proof.

Corollary. *If $G^\star$ is a graph with the minimum value of the reduced Sombor index among all connected graphs of order n and size m, then $G^\star$ has*

$2m - n\lfloor 2m/n \rfloor$ vertices of degree $\lfloor 2m/n \rfloor + 1$ and $n + n\lfloor 2m/n \rfloor - 2m$ vertices of degree $\lfloor 2m/n \rfloor$.

Proof. If $G^\star$ is regular then the desired conclusion holds trivially. Next, assume that the minimum degree δ and maximum degree Δ of $G^\star$ are not the same. Then, Theorem 1 confirms that $\Delta - \delta = 1$. If n_i represents the number of vertices of degree i in $G^\star$, then the following equations holds

$$n_\delta + n_\Delta = n \quad \text{and} \quad \delta\, n_\delta + (\delta + 1)n_\Delta = 2m, \tag{15}$$

which give $\delta\, n = 2m - n_\Delta$, which further provides $\delta = \lfloor 2m/n \rfloor$ because $0 < \frac{n_\Delta}{n} < 1$. The value of Δ is now obtained from $\Delta - \delta = 1$. Since $\delta n = 2m - n_\Delta$, we have $n_\Delta = 2m - n\lfloor 2m/n \rfloor$. Now, the value of n_δ is deduced from the first equation of the system (15). ■

The following known result is also needed for characterizing the graphs possessing minimum value of the reduced Sombor index from the class of all tricyclic connected graphs of a given order.

Lemma 4. [11] *The graph defined in Lemma 2 is the unique graph with the minimum reduced Sombor index among all connected chemical tricyclic graphs of order n for every $n \geq 6$.*

Finally, the next result regarding the minimum reduced Sombor index of tricyclic graphs follows from Corollary 2 and Lemma 4.

Corollary. *The graph defined in Lemma 2 is the unique graph with the minimum reduced Sombor index among all connected tricyclic graphs of order n for every $n \geq 6$.*

Next, we characterize the unique graph possessing maximum value of the reduced Sombor index from the class of all tricyclic connected graphs of a given order.

For every $n \geq 5$, Das et al. [5] proved that if G^* has the maximum reduced Sombor index among all connected tricyclic graphs with order n then the maximum degree of G^* is $n - 1$; if in addition the number of pendent vertices of G^* is at most $n - 5$ then $G^* = H_{n,3}$, where a vertex of degree one is known as a pendent vertex and $H_{n,3}$ is the graph formed from the star graph S_n of order n by adding 3 edges between a fixed pendent vertex and three other pendent vertices of S_n (see [2]). However, for $n \geq 5$, there is only one connected tricyclic graph of order n and maximum degree $n-1$ having more than $n-5$ pendent vertices; this graph is depicted in Figure 1.

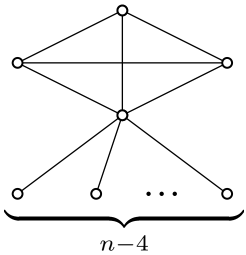

Figure 1. The unique connected tricyclic graphs of order n and maximum degree $n-1$ having more than $n-5$ pendent vertices, where $n \geq 5$.

Denote by K the graph shown in Figure 1. The reduced Sombor indices of the graphs $H_{n,3}$ and K are given below

$$3\sqrt{(n-2)^2+1}+\sqrt{(n-2)^2+9}+(n-5)(n-2)+3\sqrt{10}, \text{ and}$$

$$3\sqrt{(n-2)^2+4}+(n-4)(n-2)+6\sqrt{2},$$

respectively. Simple comparison shows that $SO_{red}(K) < SO_{red}(H_{n,3})$. Consequently, we have the next result.

Theorem 2. *The graph $H_{n,3}$ is the unique graph with the maximum reduced Sombor index among all connected tricyclic graphs of order n for every $n \geq 5$.*

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