Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2024.254215.1814
Vol. 15, No. 4, 2024, pp. 259-268
Research Paper

Extremal Chemical Trees for a Modified Version of Sombor Index

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Keywords:
Sombor index,
Nirmala index,
Dharwad index,
F-Sombor index,
Chemical tree

AMS Subject Classification (2020):

05C35; 05C09; 05C92

Article History:

Received: 11 January 2024

Accepted: 6 March 2024

Abstract

Let G be a molecular graph, where d_u representes the degree of vertex u, and uv denotes an edge connecting vertices u and v. A few years ago, a new vertex-degree-based graph invariant (topological index) was introduced by Gutman, defined as $SO(G) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2}$, called the Sombor index. Recently, Kulli et al. compared several modified versions of Sombor index (Nirmala, Sombor, Dharwad, and F-Sombor indices), they found that these indices are highly correlated and their values for QSPR applications are nearly the same. Based on this study Kulli et al. introduced a new vertex-degree-based topological index, which is defined as $X(G) = \sum_{uv \in E} \sqrt{d_u^k + d_v^k}$, where $k \geq 1$ is a real number. In this paper, we determine the extremal chemical trees with respect to X index.

1 Introduction

In chemistry, the mathematical apparatus of graph theory is applied for modeling chemical phenomena, usually the relations between molecular structure and the physicochemical properties of the underlying chemical compounds.

Let G be a graph with vertex set V and edge set E. By $uv \in E$ we denote the edge of G, connecting the vertices u and v. The degree of the vertex u in G is denoted by d_u. A few years ago, Gutman [1] defined a new vertex-degree-based graph invariant, named "Sombor index" of a graph G, denoted by $SO(G)$, defined as:

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

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Academic Editor: Akbar Ali

The mathematical properties and the various applications of the Sombor index and its modified versions can be found in the recent articles [2–9] and cited therein.

The bond incident degree (BID) index for a graph G is defined as the total of contributions $f(d_u, d_v)$ from all edges uv of G, where f is a real-valued symmetric function. For example, if take $f(d_u, d_v) = \sqrt{d_u^2 + d_v^2}$ then we obtain the Sombor index. Albalahi et al. [10] studied the problem of finding graphs with extremum BID indices over the class of all chemical graphs of a fixed number of edges and vertices.

Kulli et al. [11] compared several modified versions of the Sombor index. They found that these indices are highly correlated and their value for QSPR applications is nearly the same. Based on this study, Kulli et al. [11] considered a new vertex-degree-based topological index

$$X(G) = \sum_{uv\in E} \sqrt{d_u^k + d_v^k},$$

where $k \geq 1$ is a real number. For $k = 1, 2, 3$ and 4, X gives Nirmala [12, 13], Sombor, Dharwad, and F-Sombor [14] indices, respectively.

In this paper, we determine the extremal chemical trees with respect to X index.

2 Main results

In [11], it was proved that $X(T) \geq X(P_n)$ for any tree T of order n. Therefore, we study the extremal chemical trees with maximum X index. For $n = 3s + 2$ with $s \geq 1$, $\mathcal{CT}_n$ is the class of chemical trees of order n such that every degree of vertices is one or four. For $n = 3s$ with $s \geq 3$, $\mathcal{CT}_n$ is the class of chemical trees of order n such that only one vertex has degree two and its neighbors have degree four, and other vertices have degree one or four. For $n = 3s + 1$ with $s \geq 4$, $\mathcal{CT}_n$ is the class of chemical trees of order n such that only one vertex has degree three and its neighbors have degree four, and other vertices have degree one or four.

If $n \leq 3$ then there is only one tree of order n. For $n = 4$, we have

$$X(P_4) = 2\sqrt{1 + 2^k} + \sqrt{2^{k+1}} < 3\sqrt{1 + 3^k} = X(S_4).$$

Thus, let T be a chemical tree of order $n \geq 5$ and v_i $(i = 1, 2, 3, 4)$ be the number of vertices of degree i in T. Also let $e_{i,j}$ $(1 \leq i \leq j \leq 4)$ be the number of edges of T connecting vertices of degree i and j. Then $e_{1,1} = 0$ and

$$\begin{aligned}
&v_1 + v_2 + v_3 + v_4 = n, \quad v_1 + 2v_2 + 3v_3 + 4v_4 = 2(n-1),\\
&e_{1,2} + e_{1,3} + e_{1,4} + e_{2,2} + e_{2,3} + e_{2,4} + e_{3,3} + e_{3,4} + e_{4,4} = n - 1,\\
&e_{1,2} + e_{1,3} + e_{1,4} = v_1, \quad e_{1,4} + e_{2,4} + e_{3,4} + 2e_{4,4} = 4v_4,\\
&e_{1,2} + 2e_{2,2} + e_{2,3} + e_{2,4} = 2v_2, \quad e_{1,3} + e_{2,3} + 2e_{3,3} + e_{3,4} = 3v_3.
\end{aligned} \tag{1}$$

Lemma 2.1. *Let T be a chemical tree of order n. If $X(T)$ is the maximum among all chemical trees of order n, then $e_{2,2} = e_{2,3} = e_{3,3} = 0$.*

Proof. First, suppose that $e_{2,2} \neq 0$. Then there are adjacent vertices u and v in T such that $d_u = d_v = 2$. Let $N_T(u) = \{v, x\}$ and $N_T(v) = \{u, y\}$. Denote $T_1 = T - vy + uy$. Then we get

$$\begin{aligned}
X(T_1) - X(T) =& \sqrt{3^k + d_x^k} + \sqrt{3^k + d_y^k} + \sqrt{3^k + 1}\\
&- \sqrt{2^k + d_x^k} - \sqrt{2^k + d_y^k} - \sqrt{2^k + 2^k} > 0,
\end{aligned}$$

using $3^k + 1 \geq 2^k + 2^k$ for all $k \geq 1$. Because the function $f(t) = (t+1)^k - t^k$ is increasing when $k \geq 1$. This is a contradiction.

Suppose now that $e_{2,3} \neq 0$. Then there are adjacent vertices u and v in T such that $d_v = 2$ and $d_u = 3$. Let $N_T(u) = \{v, x, y\}$ and $N_T(v) = \{u, z\}$. Denote $T_1 = T - vz + uz$. Then

$$\begin{aligned}X(T_1) - X(T) =& \sqrt{4^k + d_x^k} + \sqrt{4^k + d_y^k} + \sqrt{4^k + d_z^k} + \sqrt{4^k + 1} \\ &- \sqrt{3^k + d_x^k} - \sqrt{3^k + d_y^k} - \sqrt{2^k + d_z^k} - \sqrt{3^k + 2^k} > 0,\end{aligned}$$

using $4^k + 1 \geq 3^k + 2^k$ for all $k \geq 1$. This is a contradiction.

Finally, suppose that $e_{3,3} \neq 0$. Then there are adjacent vertices u and v in T such that $d_v = d_u = 3$. Let $N_T(u) = \{v, x, y\}$ and $N_T(v) = \{u, z, w\}$. Without loss of generality, we can assume that $d_x = \max\{d_x, d_y, d_z, d_w\}$. Denote $T_1 = T - uy + vy$. Then

$$\begin{aligned}X(T_1) - X(T) =& \sqrt{4^k + d_z^k} + \sqrt{4^k + d_w^k} + \sqrt{4^k + d_y^k} + \sqrt{2^k + d_x^k} + \sqrt{4^k + 2^k} \\ &- \sqrt{3^k + d_z^k} - \sqrt{3^k + d_w^k} - \sqrt{3^k + d_y^k} - \sqrt{3^k + d_x^k} - \sqrt{3^k + 3^k}.\end{aligned}$$

In order to get the inequality $X(T_1) > X(T)$, it will be enough to show that

$$\sqrt{4^k + d_y^k} + \frac{1}{3}\sqrt{2^k + d_x^k} > \sqrt{3^k + d_y^k} + \frac{1}{3}\sqrt{3^k + d_x^k}. \tag{2}$$

Because $4^k + 2^k \geq 3^k + 3^k$ for all $k \geq 1$. Then we get a contradiction and it follows that $e_{3,3} = 0$. Hence, we now will prove the inequality (2) and it is equivalent to

$$3\left(\sqrt{4^k + d_y^k} - \sqrt{3^k + d_y^k}\right) > \sqrt{3^k + d_x^k} - \sqrt{2^k + d_x^k}.$$

On the other, it is easy to see that $\sqrt{4^k + d_y^k} - \sqrt{3^k + d_y^k} \geq \sqrt{4^k + d_x^k} - \sqrt{3^k + d_x^k}$, because $d_x \geq d_y$. Therefore, we have to prove that:

$$3\left(\sqrt{4^k + d_x^k} - \sqrt{3^k + d_x^k}\right) > \sqrt{3^k + d_x^k} - \sqrt{2^k + d_x^k},$$

that is,

$$3\sqrt{4^k + d_x^k} + \sqrt{2^k + d_x^k} > 4\sqrt{3^k + d_x^k}.$$

Therefore, the proof is completed by showing that

$$\begin{aligned}\left(3\sqrt{4^k + d_x^k} + \sqrt{2^k + d_x^k}\right)^2 &> 9 \cdot 4^k + 9d_x^k + 2^k + d_x^k + 6\sqrt{(2^k + d_x^k)^2} \\ &= 9 \cdot 4^k + 7 \cdot 2^k + 16d_x^k > 16 \cdot 3^k + 16d_x^k = \left(4\sqrt{3^k + d_x^k}\right)^2,\end{aligned}$$

since $4^k + 2^k \geq 3^k + 3^k$ for all $k \geq 1$. ■

If $n = 6$ or $n = 7$ or $n = 10$ then one can easily see that $\mathcal{CT}_n = \emptyset$. For $n = 6$, $n = 7$ or $n = 10$, we denote by T_n the graph depicted in Figure 1, respectively.

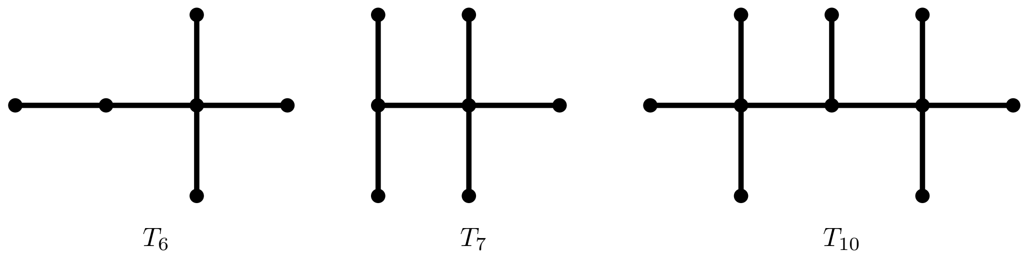

Figure 1: The graphs T_6, T_7 and T_{10} for $n = 6, 7, 10$.

Lemma 2.2. *Let T be a chemical tree of order n, where $n \in \{6, 7, 10\}$. If $X(T)$ is the maximum among all chemical trees of order n, then $T \cong T_n$.*

Proof. By Lemma 2.1, we have $e_{2,2} = e_{2,3} = e_{3,3} = 0$. If $v_4 = 0$ then we have $e_{1,2} = 2v_2$, $e_{1,3} = 3v_3$, $e_{1,2} + e_{1,3} = v_1$ and $v_1 + 2v_2 + 3v_3 = 2(n-1)$ from (1) and it follows that $v_1 = n-1$. Hence, $T \cong S_n$ and a contradiction since $\Delta(T) = n-1 \geq 5$. Therefore, we have $v_4 \geq 1$. Clearly, if $n = 6$ or $n = 7$ then $v_4 \leq 1$, and if $n = 10$ then $v_4 \leq 2$.

Let $n = 6$ or $n = 7$. Then $v_4 = 1$ and from (1), we get a system of equations: $v_1 + v_2 + v_3 = n-1$, $v_1 + 2v_2 + 3v_3 = 2n - 6$. For $n = 6$, it has only one solution that is $v_1 = 4, v_2 = 1, v_3 = 0$ and it follows that $T \cong T_6$. For $n = 7$, it has two solutions which are $(v_1, v_2, v_3) = (5, 0, 1)$ or $(4, 2, 0)$. Hence $T \in \{T_7, T_7'\}$, where T_7' is the obtained graph from P_5 by attaching two pendent vertices to the central vertex of P_5. Moreover, we have

$$X(T_7) = 2\sqrt{1+3^k} + \sqrt{3^k+4^k} + 3\sqrt{1+4^k},$$
$$X(T_7') = 2\sqrt{1+2^k} + 2\sqrt{2^k+4^k} + 2\sqrt{1+4^k}.$$

In order to get the required result, it is sufficient to prove $X(T_7) > X(T_7')$. Then

$$2\sqrt{1+3^k} + \sqrt{3^k+4^k} + \sqrt{1+4^k} > 2\sqrt{1+2^k} + 2\sqrt{2^k+4^k},$$

that is,

$$1 + 5 \cdot 3^k + 4\sqrt{(1+3^k)(3^k+4^k)} + 4\sqrt{(1+3^k)(1+4^k)} + 2\sqrt{(3^k+4^k)(1+4^k)}$$
$$> 8 \cdot 2^k + 2 \cdot 4^k + 8\sqrt{(1+2^k)(2^k+4^k)}.$$

The above inequality is true, because $(1+3^k)(1+4^k) > (1+2^k)(2^k+4^k)$, $\sqrt{(3^k+4^k)(1+4^k)} > 4^k$ and $1 + 5 \cdot 3^k \geq 8 \cdot 2^k$ for $k \geq 1$.

Let $n = 10$. Then $v_4 = 1$ or $v_4 = 2$. If $v_4 = 2$ then $v_1 + v_2 + v_3 = 8$, $v_1 + 2v_2 + 3v_3 = 10$ from (1) and it has two solutions that are $(v_1, v_2, v_3) = (7, 0, 1)$ or $(6, 2, 0)$. By Lemma 2.1, we have $e_{2,2} = e_{2,3} = e_{3,3} = 0$. Hence, all possible values of $X(T)$ are as follows:

$$2\sqrt{3^k+4^k} + 6\sqrt{1+4^k} + \sqrt{1+3^k},$$
$$\sqrt{4^k+4^k} + \sqrt{3^k+4^k} + 5\sqrt{1+4^k} + 2\sqrt{1+3^k},$$
$$\sqrt{4^k+4^k} + 2\sqrt{2^k+4^k} + 4\sqrt{1+4^k} + 2\sqrt{1+2^k},$$
$$3\sqrt{2^k+4^k} + 5\sqrt{1+4^k} + \sqrt{1+2^k}.$$

and we will show that $2\sqrt{3^k+4^k}+6\sqrt{1+4^k}+\sqrt{1+3^k}$ is maximum.

Using well-known Karamata's inequality, one can easily see that

$$3\sqrt{2^k+4^k}+5\sqrt{1+4^k}+\sqrt{1+2^k} > \sqrt{4^k+4^k}+2\sqrt{2^k+4^k}+4\sqrt{1+4^k}+2\sqrt{1+2^k},$$

since $(4^k+4^k, 2^k+4^k, 2^k+4^k, 1+4^k, 1+4^k, 1+4^k, 1+4^k, 1+2^k, 1+2^k)$ majorizes $(2^k+4^k, 2^k+4^k, 2^k+4^k, 1+4^k, 1+4^k, 1+4^k, 1+4^k, 1+4^k, 1+2^k)$ and $f(t)=\sqrt{t}$ is concave. Similarly as the above, we have

$$2\sqrt{3^k+4^k}+6\sqrt{1+4^k}+\sqrt{1+3^k} > \sqrt{4^k+4^k}+\sqrt{3^k+4^k}+5\sqrt{1+4^k}+2\sqrt{1+3^k}.$$

Now we show that:

$$2\sqrt{3^k+4^k}+6\sqrt{1+4^k}+\sqrt{1+3^k} > 3\sqrt{2^k+4^k}+5\sqrt{1+4^k}+\sqrt{1+2^k}.$$

It is enough to prove that:

$$2\sqrt{3^k+4^k}+\sqrt{1+4^k} > 3\sqrt{2^k+4^k},$$

that is,

$$4\sqrt{3^k+4^k+12^k+16^k} > 9\cdot 2^k+4\cdot 4^k-4\cdot 3^k-1.$$

Using $4\cdot 3^k \geq 6\cdot 2^k$ and $16\cdot 12^k \geq 24\cdot 8^k$, we have

$$\begin{aligned} 9\cdot 2^k+4\cdot 4^k-4\cdot 3^k-1 < 4\cdot 4^k+3\cdot 2^k &= \sqrt{16\cdot 16^k+24\cdot 8^k+9\cdot 4^k} \\ &< \sqrt{16\cdot 16^k+16\cdot 12^k+16\cdot 4^k} < 4\sqrt{3^k+4^k+12^k+16^k}. \end{aligned}$$

From the above, we conclude that $X(T)=2\sqrt{3^k+4^k}+6\sqrt{1+4^k}+\sqrt{1+3^k}$. Hence $T\cong T_{10}$.

If $v_4=1$ then $v_1+v_2+v_3=9$, $v_1+2v_2+3v_3=14$ and it has three solutions that are $(v_1,v_2,v_3)=(6,1,2)$ or $(5,3,1)$ or $(4,5,0)$. By Lemma 2.1, we have $e_{2,2}=e_{2,3}=e_{3,3}=0$. Hence, all possible values of $X(T)$ are as follows:

$$\begin{aligned} &2\sqrt{3^k+4^k}+\sqrt{1+4^k}+\sqrt{2^k+4^k}+4\sqrt{1+3^k}+\sqrt{1+2^k}, \\ &\sqrt{3^k+4^k}+3\sqrt{2^k+4^k}+2\sqrt{1+3^k}+3\sqrt{1+2^k}. \end{aligned}$$

First we show that:

$$2\sqrt{3^k+4^k}+6\sqrt{1+4^k}+\sqrt{1+3^k} > \sqrt{3^k+4^k}+3\sqrt{2^k+4^k}+2\sqrt{1+3^k}+3\sqrt{1+2^k}.$$

It is enough to prove that:

$$\sqrt{3^k+4^k}+5\sqrt{1+4^k} > 3\sqrt{2^k+4^k}+3\sqrt{1+2^k}.$$

By squaring both sides, we get:

$$A = 17\cdot 4^k+3^k+16+10\sqrt{3^k+4^k+12^k+16^k} > 18\cdot 2^k+18\sqrt{2^k+2\cdot 4^k+8^k}.$$

Since $9\cdot 4^k \geq 18\cdot 2^k$, $8\cdot 4^k+3^k = 8\sqrt{16^k}+3^k > 8\sqrt{2\cdot 8^k}+\sqrt{8^k} > 12\sqrt{8^k}$, we get

$$\begin{aligned} A &> 18\cdot 2^k+12\sqrt{8^k}+10\sqrt{0+0+12/8\cdot 8^k+16/8\cdot 8^k} > 18\cdot 2^k+27\sqrt{8^k} \\ &= 18\cdot 2^k+18\sqrt{\frac{1}{4}\cdot 8^k+2\cdot\frac{1}{2}\cdot 8^k+8^k} \geq 18\cdot 2^k+18\sqrt{2^k+2\cdot 4^k+8^k}. \end{aligned}$$

To finish the proof, we have to prove that:

$$X(T_{10}) > 2\sqrt{3^k+4^k} + \sqrt{1+4^k} + \sqrt{2^k+4^k} + 4\sqrt{1+3^k} + \sqrt{1+2^k},$$

that is,

$$5\sqrt{1+4^k} > \sqrt{2^k+4^k} + 3\sqrt{1+3^k} + \sqrt{1+2^k}. \tag{3}$$

On the other hand, one can easily see that $\sqrt{3/2(1+4^k)} > \sqrt{2^k+4^k}$, $\sqrt{3/5(1+4^k)} \geq \sqrt{1+2^k}$ and $\sqrt{3/2} + \sqrt{3/5} < 2$. Using these inequalities in (3), we get the required result. ■

Theorem 2.3. *Let T be a chemical tree of order $n > 4$, where $n \notin \{6,7,10\}$. If $X(T)$ is the maximum among all chemical trees of order n then $T \in \mathcal{CT}_n$.*

Proof. By Lemma 2.1, we have $e_{2,2} = e_{2,3} = e_{3,3} = 0$. Hence, from (1), we get

$$\begin{aligned}
&v_1 + v_2 + v_3 + v_4 = n,\\
&e_{1,2} + e_{1,3} + e_{1,4} + e_{2,4} + e_{3,4} + e_{4,4} = n-1,\\
&e_{1,2} + e_{1,3} + e_{1,4} = v_1, \quad e_{1,2} + e_{2,4} = 2v_2,\\
&e_{1,3} + e_{3,4} = 3v_3, \quad e_{1,4} + e_{2,4} + e_{3,4} + 2e_{4,4} = 4v_4.
\end{aligned}$$

From the above, we easily get the following equations:

$$\begin{aligned}
n &= \frac{3}{2}e_{1,2} + \frac{4}{3}e_{1,3} + \frac{5}{4}e_{1,4} + \frac{3}{4}e_{2,4} + \frac{7}{12}e_{3,4} + \frac{1}{2}e_{4,4},\\
e_{1,4} &= \frac{2}{3}(n+1) - \frac{2}{3}\left(2e_{1,2} + \frac{5}{3}e_{1,3} + \frac{1}{2}e_{2,4} + \frac{1}{6}e_{3,4}\right),\\
e_{4,4} &= \frac{1}{3}(n-5) + \frac{1}{3}e_{1,2} + \frac{1}{9}e_{1,3} - \frac{2}{3}e_{2,4} - \frac{8}{9}e_{3,4}.
\end{aligned} \tag{4}$$

Then, using (4), we obtain:

$$\begin{aligned}
X(T) &= \sum_{uv\in E}\sqrt{d_u^k + d_v^k} = \sum_{1\leq i\leq j\leq 4}\left[\sqrt{i^k+j^k}\right]\cdot e_{i,j}\\
&= \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3}\cdot 2^k\sqrt{2} - e_{1,2}\left(\frac{4}{3}\sqrt{1+4^k} - \frac{1}{3}\cdot 2^k\sqrt{2} - \sqrt{1+2^k}\right)\\
&\quad - e_{1,3}\left(\frac{10}{9}\sqrt{1+4^k} - \frac{2^k\sqrt{2}}{9} - \sqrt{1+3^k}\right)\\
&\quad - e_{2,4}\left(\frac{1}{3}\sqrt{1+4^k} + \frac{2^{k+1}\sqrt{2}}{3} - \sqrt{2^k+4^k}\right)\\
&\quad - e_{3,4}\left(\frac{1}{9}\sqrt{1+4^k} + \frac{8\cdot 2^k\sqrt{2}}{9} - \sqrt{3^k+4^k}\right)\\
&= \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3}\cdot 2^k\sqrt{2} - c_{12}e_{1,2} - c_{13}e_{1,3} - c_{24}e_{2,4} - c_{34}e_{3,4},
\end{aligned} \tag{5}$$

where $c_{12} = \frac{4}{3}\sqrt{1+4^k} - \frac{1}{3}\cdot 2^k\sqrt{2} - \sqrt{1+2^k}$, $c_{13} = \frac{10}{9}\sqrt{1+4^k} - \frac{2^k\sqrt{2}}{9} - \sqrt{1+3^k}$, $c_{24} = \frac{1}{3}\sqrt{1+4^k} + \frac{2^{k+1}\sqrt{2}}{3} - \sqrt{2^k+4^k}$, and $c_{34} = \frac{1}{9}\sqrt{1+4^k} + \frac{8\cdot 2^k\sqrt{2}}{9} - \sqrt{3^k+4^k}$.

First we prove that:

$$c_{12} > c_{24} > 0 \text{ and } c_{13} > c_{34} > 0. \tag{6}$$

By Karamata's inequality, we have

$$c_{12} - c_{24} = \sqrt{1+4^k} + \sqrt{2^k+4^k} - 2^k\sqrt{2} - \sqrt{1+2^k} > 0,$$

since $(4^k+4^k, 1+2^k)$ majorizes $(4^k+2^k, 4^k+1)$ and $f(t)=\sqrt{t}$ is concave. Also by Karamata's inequality, we have

$$c_{13} - c_{34} = \sqrt{1+4^k} + \sqrt{3^k+4^k} - 2^k\sqrt{2} - \sqrt{1+3^k} > 0,$$

since $(4^k+4^k, 1+3^k)$ majorizes $(4^k+3^k, 4^k+1)$. Now we show that $c_{24} > 0$ and $c_{34} > 0$. Then

$$\begin{aligned} c_{24} &= \frac{1}{3}\sqrt{1+4^k} + \frac{2^{k+1}\sqrt{2}}{3} - \sqrt{2^k+4^k} = \frac{2^k}{3}\left(\sqrt{1+\frac{1}{4^k}} + 2\sqrt{2} - 3\sqrt{1+\frac{1}{2^k}}\right) \\ &> \frac{2^k}{3}\left(1+2\sqrt{2}-3\sqrt{1+\frac{1}{2}}\right) > 0. \end{aligned}$$

$$\begin{aligned} c_{34} &= \frac{1}{9}\sqrt{1+4^k} + \frac{8\cdot 2^k\sqrt{2}}{9} - \sqrt{3^k+4^k} = \frac{2^k}{9}\left(\sqrt{1+\frac{1}{4^k}} + 8\sqrt{2} - 9\sqrt{1+\frac{3^k}{4^k}}\right) \\ &> \frac{2^k}{9}\left(1+8\sqrt{2}-9\sqrt{1+\frac{3}{4}}\right) > 0. \end{aligned}$$

We distinguish the following three cases.

(i) Let $n = 3s+2$, $s \geq 1$. Then from (5) and (6), we obtain

$$X(T) \leq \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3}\cdot 2^k\sqrt{2},$$

with equality holding if and only if

$$e_{1,2} = e_{1,3} = e_{2,2} = e_{2,3} = e_{2,4} = e_{3,3} = e_{3,4} = 0.$$

Hence we get $v_1 = e_{1,4} = 2(n+1)/3$ and $e_{4,4} = (n-5)/3$. Also we have $v_2 = v_3 = 0$. Therefore $T \in \mathcal{CT}_n$.

(ii) Let $n = 3s$, $s \geq 3$. Then $v_2 \neq 0$ or $v_3 \neq 0$. If $v_2 \geq 1$ then

$$e_{1,2} + e_{2,4} = 2v_2 \geq 2,$$

from (1). Therefore, we get

$$\begin{aligned} X(T) \leq& \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3}\cdot 2^k\sqrt{2} - c_{24}(e_{1,2}+e_{2,4}) \\ \leq& \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3}\cdot 2^k\sqrt{2} - 2c_{24} \\ =& \frac{2n}{3}\sqrt{1+4^k} + \frac{n-9}{3}\cdot 2^k\sqrt{2} + 2\sqrt{2^k+4^k}, \end{aligned} \tag{7}$$

since $c_{12} > c_{24}$ and $c_{13} > c_{34} > 0$.

If $v_2 = 0$ then we have $v_1 + v_3 + v_4 = n$ and $v_1 + 3v_3 + 4v_4 = 2(n-1)$. Thus, since $n = 3s$ we easily get $v_3 \geq 2$. Therefore, we have:

$$e_{1,3} + e_{3,4} = 3v_3 \geq 6,$$

from (1). Hence, we obtain:

$$\begin{aligned} X(T) \leq & \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3} \cdot 2^k\sqrt{2} - c_{34}(e_{1,3}+e_{3,4}) \\ \leq & \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3} \cdot 2^k\sqrt{2} - 6c_{34} \\ = & \frac{2n}{3}\sqrt{1+4^k} + \frac{n-21}{3} \cdot 2^k\sqrt{2} + 6\sqrt{3^k+4^k}, \end{aligned} \tag{8}$$

since $c_{12} > c_{24} > 0$ and $c_{13} > c_{34}$. From (7) and (8), we get the required result because $6c_{34} > 2c_{24}$ which is equivalent to $4\sqrt{2\,(16^k+8^k)}+2^k > 9 \cdot 3^k$. Moreover, by AM-GM inequality and power mean inequality, we obtain

$$4\sqrt{2\,(16^k+8^k)} + 2^k \geq 4\sqrt{4 \cdot 12^k} + 2^k > 8 \cdot (3.4)^k + 2^k > 9 \cdot \left(\frac{8 \cdot 3.4 + 2}{9}\right)^k > 9 \cdot 3^k.$$

Equality holds in (7) if and only if $v_2 = 1$, $v_3 = 0$ and $e_{2,4} = 2$. Thus $T \in \mathcal{T}_n$.

(iii) If $n = 3s+1$, $s \geq 4$ then $v_2 \neq 0$ or $v_3 \neq 0$. If $v_3 \geq 1$, then similarly as in (ii) we get:

$$\begin{aligned} X(T) \leq & \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3} \cdot 2^k\sqrt{2} - c_{34}(e_{1,3}+e_{3,4}) \\ \leq & \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3} \cdot 2^k\sqrt{2} - 3c_{34} \\ = & \frac{2n+1}{3}\sqrt{1+4^k} + \frac{n-13}{3} \cdot 2^k\sqrt{2} + 3\sqrt{3^k+4^k}. \end{aligned} \tag{9}$$

Let now $v_3 = 0$. If $v_2 = 1$, then the system of equations $v_1 + v_4 = n-1$ and $v_1 + 4v_4 = 2(n-2)$ has no integer solution. Thus $v_2 \geq 2$ and similarly as in (ii), we also get:

$$\begin{aligned} X(T) \leq & \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3} \cdot 2^k\sqrt{2} - c_{24}(e_{1,2}+e_{2,4}) \\ \leq & \frac{2}{3}(n+1)\sqrt{1+4^k} + \frac{n-5}{3} \cdot 2^k\sqrt{2} - 4c_{24} \\ = & \frac{2}{3}(n-1)\sqrt{1+4^k} + \frac{n-13}{3} \cdot 2^k\sqrt{2} + 4\sqrt{2^k+4^k}, \end{aligned}$$

from $4c_{24} < 3c_{34}$. Because $4c_{24} < 3c_{34}$ is equivalent to $\sqrt{1+4^k}+3\sqrt{4^k+3^k} > 4\sqrt{4^k+2^k}$. Now we prove this inequality. Then

$$\begin{aligned} \sqrt{1+4^k} + 3\sqrt{4^k+3^k} & \geq 4\sqrt[8]{(1+4^k)(4^k+3^k)^3} \\ & = 4\sqrt[8]{27^k + 3 \cdot 36^k + 3 \cdot 48^k + 64^k + 108^k + 3 \cdot 144^k + 3 \cdot 192^k + 256^k} \\ & > 4\sqrt[8]{16^k + 3 \cdot 32^k + 32^k + (2 \cdot 48^k + 64^k + 108^k + 2 \cdot 144^k) + 128^k + 3 \cdot 128^k + 256^k} \\ & > 4\sqrt[8]{16^k + 4 \cdot 32^k + 6 \cdot ((2 \cdot 48 + 64 + 108 + 2 \cdot 144)/5)^k + 4 \cdot 128^k + 256^k} \\ & > 4\sqrt[8]{16^k + 4 \cdot 32^k + 6 \cdot 64^k + 4 \cdot 128^k + 256^k} = 4\sqrt{4^k+2^k}, \end{aligned}$$

by AM-GM inequality and power mean inequality. Hence, equality holds in (9) if and only if $v_2 = 0$, $v_3 = 1$ and $e_{3,4} = 3$. Thus $T \in \mathcal{CT}_n$.

On the other hand, in each case we easily conclude that the equality holds if and only if $T \in \mathcal{CT}_n$. ∎

Remark. In the introduction, we have mentioned that the investigation of chemical graphs with extreme BID indices has been studied in [10]. In this paper, we have characterized extremal chemical trees with respect to X index and highlight that Theorem 2.3 can also be addressed using Theorem 2 in [10].

Conflicts of interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

Acknowledgment. This manuscript is dedicated to the memory of Prof. Ali Reza Ashrafi, whom B. Horoldagva had the privilege of meeting in person at The International Congress of Mathematicians (ICM2014) in Seoul. The authors are grateful to anonymous referees for their helpful suggestions.

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