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Research Article

On the Conjugated Chemical Trees of a Given Order and Their Extremum Bond Incident Degree Indices

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Abstract: A *conjugated tree* is defined as a tree that possesses a perfect matching. A *chemical tree* is a tree in which the degree of every vertex is at most 4. Let T be a conjugated chemical tree with edge set E. For any vertex u in T, let $d(u)$ denote its degree. This study investigates a family of graph invariants defined as $B_\ell(T) = \sum_{uv\in E} \ell(d(u), d(v))$, where ℓ is a symmetric, real-valued function of the degrees of adjacent vertices of T. The principal objective is to determine those trees, among all conjugated chemical trees with a fixed order, that minimize or maximize B_ℓ, subject to specific assumptions on the function ℓ.

Keywords: graph invariant, topological index, bond incident degree index, chemical tree, perfect matching

MSC: 05C05, 05C07, 05C09

1. Introduction

This study is devoted exclusively to a particular class of graphs, namely, trees of maximum degree at most 4. The graph-theoretical terminology employed in this work, where not explicitly defined, follows standard usage as presented in common books on graph theory such as [1–3]. Likewise, terminology specific to chemical graph theory is adopted in accordance with the conventions outlined in [4, 5].

Within the domain of chemical graph theory, a central focus is the study of graph-based numerical descriptors known as *topological indices* [4, 5]. These are real-valued quantities assigned to graphs that remain unchanged under graph isomorphism; that is, they are independent of any specific labeling or graphical representation. Their importance stems from their ability to encode structural information about molecular graphs into single numerical values that correlate with chemical or physical properties. These indices have proven to be helpful tools in the prediction of a wide range of physicochemical characteristics of chemical compounds [6].

This work focuses on a notable subclass of topological indices, formally defined by the following expression [7, 8]. Given a graph G with edge set $E(G)$, we define:

$$\mathscr{B}_\ell(G) = \sum_{uv \in E(G)} \ell(d(u),\, d(v)), \tag{1}$$

where $d(u)$ denotes the degree of vertex u in G. When needed, we will write $d_G(u)$ to indicate the graph explicitly. Here, the function ℓ is assumed to be symmetric and real-valued. Indices of the form (1) are commonly known as Bond Incident Degree (BID) indices [9–11], a term introduced in [12] to provide a unified nomenclature for this important class of topological indices. The study of BID indices remains a vibrant area of research, with ongoing contributions found in a wide range of contemporary literature, including [13–17].

A *conjugated tree* is defined as a tree that admits a perfect matching. A *chemical tree* is a tree in which every vertex has degree at most 4. The primary aim of the present paper is to address the extremal problem of identifying those trees among all conjugated chemical trees with a fixed order that minimize or maximize the BID index B_ℓ, under explicit assumptions on the function ℓ.

2. Results

Before presenting the main findings of this paper, it is essential to introduce a set of foundational terms and concepts. This preliminary review is intended to establish a common understanding of the terminology and theoretical framework underlying the subsequent discussions.

Let G be a graph with vertex set denoted by $V(G)$. A graph is referred to as an *n-order graph* if it contains exactly n vertices. For any vertex $w \in V(G)$, the *neighborhood* of w, denoted $N_G(w)$, is defined as the set of all vertices in G that are adjacent to w; that is, all vertices connected to w by an edge. Each element $w' \in N_G(w)$ is called a *neighbor* of w. A vertex of degree one is called a *pendent vertex*.

A non-trivial path $P: w_1 w_2 \ldots w_p$ in a graph G is said to be pendent (internal, respectively) if $\max\{d_G(w_1),\, d_G(w_p)\} \geq 3$, $\min\{d_G(w_1),\, d_G(w_p)\} = 1$ ($\min\{d_G(w_1),\, d_G(w_p)\} \geq 3$, respectively) and $d_G(w_i) = 2$ whenever $2 \leq i \leq p-1$.

Lemma 1 Let ℓ be a real-valued and symmetric function of two variables, both of which are at least 1. The conditions listed below are assumed to be true.

(i) The function ϕ defined as $\phi(x) = \ell(x,\, \eta_1) - \ell(x,\, \eta_2)$, with $x \geq 1$, is increasing in x for given integers η_1 and η_2 satisfying $\eta_1 \geq \eta_2 + 1 \geq 2$.

If $\ell(x,\, y) = \sqrt{xy}$, then $\phi'(x) = \dfrac{1}{2\sqrt{x}}(\sqrt{\eta_1} - \sqrt{\eta_2}) > 0$ for $\eta_1 \geq \eta_2 + 1 \geq 2$ and $x \geq 1$.

(ii) The following inequality holds:

$$\begin{aligned} &\max\{\ell(3,\, 4) - \ell(2,\, 4) + \ell(2,\, 3),\, \ell(3,\, 3)\} \\ &+ 2\ell(2,\, 3) - 4\ell(2,\, 4) + \ell(1,\, 3) - \ell(1,\, 4) + \ell(3,\, 4) < 0. \end{aligned} \tag{2}$$

(iii) For every $c \in \{2,\, 3,\, 4\}$, it holds that

$$2\ell(c,\, 3) - \ell(c,\, 2) - \ell(c,\, 4) + 2\ell(2,\, 3) - 3\ell(2,\, 4) + \ell(1,\, 3) - \ell(1,\, 4) + \ell(4,\, 3) < 0. \tag{3}$$

If G is a tree that maximizes $\mathscr{B}_\ell$ among all chemical n-order trees with perfect matching, then G does not contain more than one vertex of degree 3.

Proof. Let M denote the unique perfect matching of G. We contrarily suppose that G contains more than one vertex of degree 3. Let $v,\ w \in V(G)$ such that $d_G(v) = 3 = d_G(w)$. Let $N_G(v) = \{v_1,\ v_2,\ v_3\}$ and $N_G(w) = \{w_1,\ w_2,\ w_3\}$. Without loss of generality, we assume that v_3 and w_3 lie on the unique path connecting v and w, and that v_1v does not belong to M. Then, $d_G(v_1) \geq 2$ and M is also the unique perfect matching of the tree G' formed from G by deleting v_1v and inserting v_1w. Additionally, we note that at most one of w_1 and w_2 is pendent.

Case 1: $vw \notin E(G)$.

Here, we have two possibilities: either $v_3 \neq w_3$ or $v_3 = w_3$.

Case 1.1: $v_3 \neq w_3$.

By using condition (i) and inequality (2), we have

$$\begin{aligned}
\mathscr{B}_\ell(G) - \mathscr{B}_\ell(G') = &\sum_{i=2}^{3}[\ell(d_G(v_i),\ 3) - \ell(d_G(v_i),\ 2)] + \sum_{i=1}^{3}[\ell(d_G(w_i),\ 3) - \ell(d_G(w_i),\ 4)] \\
&+ \ell(d_G(v_1),\ 3) - \ell(d_G(v_1),\ 4) \\
&\leq 2[\ell(4,\ 3) - \ell(4,\ 2)] + 3[\ell(2,\ 3) - \ell(2,\ 4)] + \ell(1,\ 3) - \ell(1,\ 4) < 0,
\end{aligned}$$

a contradiction.

Case 1.2: $v_3 = w_3$.

In this case, by using condition (i) and inequality (3), we have

$$\begin{aligned}
\mathscr{B}_\ell(G) - \mathscr{B}_\ell(G') = &\sum_{i=1}^{2}[\ell(d_G(w_i),\ 3) - \ell(d_G(w_i),\ 4))] + \ell(d_G(v_1),\ 3) - \ell(d_G(v_1),\ 4) \\
&+ \ell(d_G(v_2),\ 3) - \ell(d_G(v_2),\ 2) \\
&+ 2\ell(d_G(v_3),\ 3) - \ell(d_G(v_3),\ 2) - \ell(d_G(v_3),\ 4) \\
&\leq 2[\ell(2,\ 3) - \ell(2,\ 4)] + \ell(1,\ 3) - \ell(1,\ 4) + \ell(4,\ 3) - \ell(4,\ 2) \\
&+ 2\ell(d_G(v_3),\ 3) - \ell(d_G(v_3),\ 2) - \ell(d_G(v_3),\ 4) < 0,
\end{aligned}$$

a contradiction.

Case 2: $vw \in E(G)$.

In this case, $v_3 = w$ and $w_3 = v$. By using condition (i) and inequality (2), we have

$$\begin{aligned}
\mathscr{B}_\ell(G) - \mathscr{B}_\ell(G') = &\sum_{i=1}^{2}[\ell(d_G(w_i),\ 3) - \ell(d_G(w_i),\ 4))] + \ell(d_G(v_1),\ 3) - \ell(d_G(v_1),\ 4) \\
&+ \ell(d_G(v_2),\ 3) - \ell(d_G(v_2),\ 2) + \ell(3,\ 3) - \ell(2,\ 4) \\
&\leq 2[\ell(2,\ 3) - \ell(2,\ 4)] + \ell(1,\ 3) - \ell(1,\ 4) + \ell(4,\ 3) + \ell(3,\ 3) - 2\ell(2,\ 4) < 0,
\end{aligned}$$

a contradiction. $\square$

The following lemma's proof is not provided because its reasoning closely mirrors the one given in Lemma 1's proof.

Lemma 2 Let ℓ be a real-valued and symmetric function of two variables, both of which are at least 1. The conditions listed below are assumed to be true.

(i) The function ϕ defined as $\phi(x) = \ell(x,\ \eta_1) - \ell(x,\ \eta_2)$, with $x \geq 1$, is decreasing in x for given integers η_1 and η_2 satisfying $\eta_1 \geq \eta_2 + 1 \geq 2$.

(ii) The following inequality holds:

$$\max\{\ell(3,\ 4) - \ell(2,\ 4) + \ell(2,\ 3),\ \ell(3,\ 3)\}$$

$$+ 2\ell(2,\ 3) - 4\ell(2,\ 4) + \ell(1,\ 3) - \ell(1,\ 4) + \ell(3,\ 4) > 0. \tag{4}$$

(iii) For every $c \in \{2,\ 3,\ 4\}$, it holds that

$$2\ell(c,\ 3) - \ell(c,\ 2) - \ell(c,\ 4) + 2\ell(2,\ 3) - 3\ell(2,\ 4) + \ell(1,\ 3) - \ell(1,\ 4) + \ell(4,\ 3) > 0. \tag{5}$$

If G is a tree that minimizes $\mathscr{B}_\ell$ among all chemical n-order trees with perfect matching, then G does not contain more than one vertex of degree 3.

Lemma 3 Let ℓ be the function from Lemma 1 that satisfies the conditions given therein. Also, assume that, for every $c \in \{2,\ 3\}$, the following inequalities hold:

$$c[\ell(c,\ 2) - \ell(c+1,\ 2)] - \ell(c+1,\ 1) + \ell(2,\ 2) < 0, \tag{6}$$

and

$$(c-1)[\ell(c,\ 2) - \ell(c+1,\ 2)] + \ell(2,\ 2) - \ell(2,\ c+1) + \ell(c,\ 4) - \ell(c+1,\ 1) + \ell(1,\ 2) - \ell(1,\ 4) < 0. \tag{7}$$

Additionally, assume that

$$2\ell(1,\ 2) - 3\ell(1,\ 4) + \ell(c,\ 2) + \ell(c,\ 4) - \ell(c-1,\ 4) + \ell(c,\ 2) - \ell(c,\ 4) < 0, \tag{8}$$

for $c \in \{2,\ 3,\ 4\}$, and

$$2\ell(1,\ 2) + 3\ell(2,\ 4) - \ell(2,\ 3) - 2\ell(1,\ 4) - \ell(3,\ 1) - \ell(3,\ 4) < 0. \tag{9}$$

If G is a tree that maximizes $\mathscr{B}_\ell$ among all chemical n-order trees with perfect matching M, then every edge in M is incident with a pendent vertex of G.

Proof. We suppose contrarily that there exists at least one edge $vw \in M$ of G whose both end vertices are non-pendent. Without loss of generality, let $d_G(v) \leq d_G(w)$. Since $vw \in M$, each neighbor of v as well as of w is non-pendent.

Case 1: $d_G(w) \leq 3$.

By Lemma 1, $d_G(v)=2$. Let $N_G(v)=\{v',\ w\}$. Let G' denote the tree form from G by deleting $v'v$ and inserting $v'w$. We note that M is also the perfect matching of G'. However, by condition (i) of Lemma 1 and (6), we have

$$\begin{aligned}\mathscr{B}_\ell(G)-\mathscr{B}_\ell(G') = &\sum_{w'\in N_G(w)\setminus\{v\}}[\ell(d_G(w),\ d_G(w'))-\ell(d_G(w)+1,\ d_G(w'))]+\ell(d_G(w),\ 2)-\ell(d_G(w)+1,\ 1)\\ &+\ell(d_G(v'),\ 2)-\ell(d_G(v'),\ d_G(w)+1)\\ &\le (d_G(w)-1)[\ell(d_G(w),\ 2)-\ell(d_G(w)+1,\ 2)]+\ell(d_G(w),\ 2)-\ell(d_G(w)+1,\ 1)\\ &+\ell(2,\ 2)-\ell(2,\ d_G(w)+1)<0,\end{aligned}$$

a contradiction.

Case 2: $d_G(w)=4$.

We recall that each neighbor of v as well as of w is non-pendent because $vw\in M$. Let $w_1,\ w_2\in N_G(w)\setminus\{v\}$. Among all the paths that start at w and contain w_1, let P be a longest one. Then, the other end vertex of P must be pendent; we name such a vertex as $z_1\in V(G)$. Let y_1 be the unique neighbor of z_1. Since P is a longest path starting at w and containing w_1, and since every vertex of G has at most one pendent neighbor, we have $d_G(y_1)=2$. Let $N_G(y_1)=\{y_1',\ z_1\}$.

Case 2.1: $d_G(v)\le 3$.

Let G'' be the tree obtained from G by removing the edge(s) of the set $\{v''v : v''\in N_G(v)\setminus\{w\}\}$ and inserting the edge(s) of the set $\{v''y_1 : v''\in N_G(v)\setminus\{w\}\}$. We note that M is also the perfect matching of G''. However, by condition (i) of Lemma 1 and (7), we have

$$\begin{aligned}\mathscr{B}_\ell(G)-\mathscr{B}_\ell(G'') = &\sum_{v''\in N_G(v)\setminus\{w\}}[\ell(d_G(v),\ d_G(v''))-\ell(d_G(v)+1,\ d_G(v''))]+\ell(d_G(y_1'),\ 2)-\ell(d_G(y_1'),\ d_G(v)+1)\\ &+\ell(d_G(v),\ 4)-\ell(d_G(v)+1,\ 1)+\ell(1,\ 2)-\ell(1,\ 4)\\ &\le (d_G(v)-1)[\ell(d_G(v),\ 2)-\ell(d_G(v)+1,\ 2)]+\ell(2,\ 2)-\ell(2,\ d_G(v)+1)\\ &+\ell(d_G(v),\ 4)-\ell(d_G(v)+1,\ 1)+\ell(1,\ 2)-\ell(1,\ 4)<0,\end{aligned}$$

a contradiction.

Case 2.2: $d_G(v)=4$.

Let $N_G(w)=\{v,\ w_1,\ w_2,\ w_3\}$ and $N_G(v)=\{w,\ v_1,\ v_2,\ v_3\}$. For every $i\in\{1,\ 2,\ 3\}$, let $T(w_i)$ be the component of $G-w$ that contains w_i. Similarly, for every $i\in\{1,\ 2,\ 3\}$, let $T(v_i)$ be the component of $G-v$ that contains v_i. By Lemma 1, at most one of $T(v_1)$, $T(v_2)$, $T(v_3)$, $T(w_1)$, $T(w_2)$ and $T(w_3)$ contains a vertex of degree 3 in G. Without loss of generality, let $d_G(u)\ne 3$ for every

$$u\in\left(\bigcup_{i=1}^{2}V(T(w_i))\right)\cup\left(\bigcup_{i=1}^{3}V(T(v_i))\right).$$

For every $i \in \{1,\ 2,\ 3\}$, let $P^{(i)}: w_i^{(0)} w_i^{(1)} w_i^{(2)} \dots w_i^{(\alpha_i)}$ be a longest path starting at w and containing w_i, where $\alpha_i \geq 2$, $w_i^{(0)} = w$ and $w_i^{(1)} = w_i$. Certainly, $d_G\left(w_i^{(\alpha_i)}\right) = 1$ for $i = 1,\ 2,\ 3$. Since every vertex of G has at most one pendent neighbor, we have $d_G\left(w_i^{(\alpha_i - 1)}\right) = 2$ for $i = 1,\ 2,\ 3$. Similarly, for every $i \in \{1,\ 2,\ 3\}$, let $Q^{(i)}: v_i^{(0)} v_i^{(1)} v_i^{(2)} \dots v_i^{(\beta_i)}$ be a longest path starting at v and containing v_i, where $\beta_i \geq 2$, $v_i^{(0)} = v$ and $v_i^{(1)} = v_i$.

Case 2.2.1: At least one of the paths $P^{(1)}$, $P^{(2)}$, $P^{(3)}$, $Q^{(1)}$, $Q^{(2)}$ and $Q^{(3)}$ has a length of at least 3.

Without loss of generality, we assume that the path $P^{(1)}$ has a length of at least 3, and if $P^{(2)}$ also has a length of at least 3 then we assume that

$$d_G\left(w_1^{(\alpha_1 - 2)}\right) \leq d_G\left(w_2^{(\alpha_2 - 2)}\right). \tag{10}$$

Let G''' denote the tree formed from G by removing the edges $v_1 v$, $w_1^{(\alpha_1-2)} w_1^{(\alpha_1-1)}$, $w_1^{(\alpha_1-1)} w_1^{(\alpha_1)}$, ww_3 and inserting $v_1 w_2^{(\alpha_2-1)}$, $w_2^{(\alpha_2-1)} w_3$, $vw_1^{(\alpha_1-1)}$, $ww_1^{(\alpha_1)}$. We note that if the length of $P^{(1)}$ is 3, then $d_G\left(w_1^{(\alpha_1-2)}\right) \geq 3$ because in this case the edges $w_1^{(\alpha_1-3)} w_1^{(\alpha_1-2)}$ and $w_1^{(\alpha_1-2)} w_1^{(\alpha_1-1)}$ would not belong to the perfect matching M of G. Hence, the following set of edges of G''' forms a perfect matching of G''':

$$\left(M \setminus \left\{vw,\ w_1^{(\alpha_1)} w_1^{(\alpha_1-1)}\right\}\right) \cup \left\{vw_1^{(\alpha_1-1)},\ ww_1^{(\alpha_1)}\right\}.$$

However, by condition (i) of Lemma 1, inequalities (8) and (10), we have

$$\begin{aligned}
\mathscr{B}_\ell(G) - \mathscr{B}_\ell(G''') &= 2\ell(1,\ 2) - 3\ell(1,\ 4) + \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right),\ 2\right) \\
&\quad + \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right),\ d_G\left(w_1^{(\alpha_1-3)}\right)\right) - \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right) - 1,\ d_G\left(w_1^{(\alpha_1-3)}\right)\right) \\
&\quad + \ell\left(d_G\left(w_2^{(\alpha_2-2)}\right),\ 2\right) - \ell\left(d_G\left(w_2^{(\alpha_2-2)}\right),\ 4\right) \\
&\leq 2\ell(1,\ 2) - 3\ell(1,\ 4) + \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right),\ 2\right) \\
&\quad + \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right),\ 4\right) - \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right) - 1,\ 4\right) \\
&\quad + \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right),\ 2\right) - \ell\left(d_G\left(w_1^{(\alpha_1-2)}\right),\ 4\right) < 0,
\end{aligned}$$

a contradiction.

Case 2.2.2: None of the paths $P^{(1)}$, $P^{(2)}$, $P^{(3)}$, $Q^{(1)}$, $Q^{(2)}$ and $Q^{(3)}$ has a length of at least 3.

In this case, each of the paths $P^{(1)}$, $P^{(2)}$, $P^{(3)}$, $Q^{(1)}$, $Q^{(2)}$ and $Q^{(3)}$ has lenth 2, and hence G is isomorphic to the tree T_2 of order 14 depicted in Figure 1.

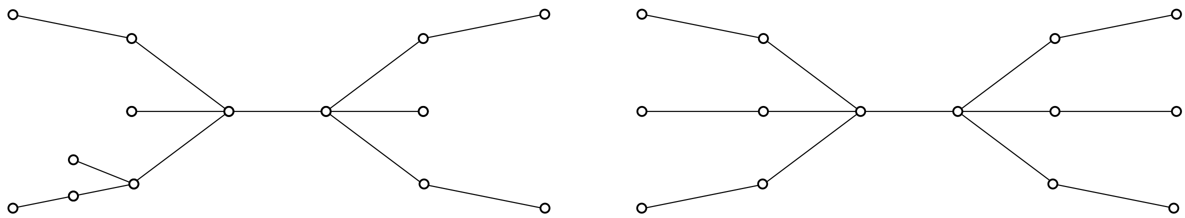

Figure 1. The trees T_1 and T_2 considered in Case 2.2.2 of Lemma 3

We observe that the tree T_1 depicted in Figure 1 also has order 14 and perfect matching. But, by (9), it holds that

$$\mathcal{B}_\ell(T_2) - \mathcal{B}_\ell(T_1) = 2\ell(1,\ 2) + 3\ell(2,\ 4) - \ell(2,\ 3) - 2\ell(1,\ 4) - \ell(3,\ 1) - \ell(3,\ 4) < 0,$$

and hence, $\mathcal{B}_\ell(G) = \mathcal{B}_\ell(T_2) < \mathcal{B}_\ell(T_1)$, which is a contradiction to the definition of G. $\square$

The following lemma's proof is not provided because its reasoning closely mirrors the one given in Lemma 3's proof.

Lemma 4 Let ℓ be the function from Lemma 2 that satisfies the conditions given therein. Also, assume that, for every $c \in \{2,\ 3\}$, the following inequalities hold:

$$c[\ell(c,\ 2) - \ell(c+1,\ 2)] - \ell(c+1,\ 1) + \ell(2,\ 2) > 0, \tag{11}$$

and

$$(c-1)[\ell(c,\ 2) - \ell(c+1,\ 2)] + \ell(2,\ 2) - \ell(2,\ c+1) + \ell(c,\ 4) - \ell(c+1,\ 1) + \ell(1,\ 2) - \ell(1,\ 4) > 0. \tag{12}$$

Additionally, assume that

$$2\ell(1,\ 2) - 3\ell(1,\ 4) + \ell(c,\ 2) + \ell(c,\ 4) - \ell(c-1,\ 4) + \ell(c,\ 2) - \ell(c,\ 4) > 0, \tag{13}$$

for $c \in \{2,\ 3,\ 4\}$, and

$$2\ell(1,\ 2) + 3\ell(2,\ 4) - \ell(2,\ 3) - 2\ell(1,\ 4) - \ell(3,\ 1) - \ell(3,\ 4) > 0. \tag{14}$$

If G is a tree that minimizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching M, then every edge in M is incident with a pendent vertex of G.

Lemma 5 Let ℓ be the function from Lemma 1 that satisfies the conditions given therein. Also, assume that inequalities (6), (7), (8) and (9) hold. If G is a tree that maximizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching, then G does not contain any edge with both end vertices of degrees 2, where $n \geq 6$.

Proof. Contrarily, let vw be an edge of G whose both end vertices have degrees 2. Let M be the unique perfect matching of G. Let $N_G(v) = \{v', w\}$ and $N_G(w) = \{w', v\}$. By Lemma 3, $vw \notin M$. Thus, $v'v, w'w \in M$, and hence (by Lemma 3) $d_G(v') = 1 = d_G(w')$, which contradicts the assumption $n \geq 6$. $\square$

The next lemma's proof is not provided because its reasoning closely mirrors the one given in the proof of Lemma 5.

Lemma 6 Let ℓ be the function from Lemma 2 that satisfies the conditions given therein. Also, assume that inequalities (11), (12), (13) and (14) hold. If G is a tree that minimizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching, then G does not contain any edge with both end vertices of degrees 2, where $n \geq 6$.

Lemma 7 Let ℓ be the function from Lemma 1 that satisfies the conditions given therein. Also, assume that inequalities (6), (7), (8) and (9) hold. If G is a tree that maximizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching, then G does not contain any vertex of degree 2 with both non-pendent neighbors. (That is, G neither contains any internal path of length larger than 1 nor has any pendent path of length larger than 2).

Proof. Contrarily, let $v \in V(G)$ be a vertex of degree 2 such that its both neighbors, say v' and v'', are non-pendent. By Lemma 3, neither $v'v$ nor $v''v$ is a member of the perfect matching of G. Hence, v is not incident with any edge of the perfect matching of G, which is a contradiction. $\square$

The following lemma's proof is not provided because its reasoning closely mirrors the one given in Lemma 8's proof.

Lemma 8 Let ℓ be the function from Lemma 2 that satisfies the conditions given therein. Also, assume that inequalities (11), (12), (13) and (14) hold. If G is a tree that minimizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching, then G does not contain any vertex of degree 2 with both non-pendent neighbors.

We note that the path graph is the unique n-order tree with perfect matching for each $n \in \{2, 4\}$. Also, for $n = 6$, there are only two n-order trees with perfect matching, namely, the path graph and the graph T_6^* obtained from the 5-order path graph P_5 by attaching a pendent vertex to the central vertex of P_5. Hence, in what follows, we assume that $n \geq 8$.

Lemma 9 Let ℓ be the function from Lemma 1 that satisfies the conditions given therein. Also, assume that inequalities (6), (7), (8) and (9) hold. Let G be a tree that maximizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching such that it contains a vertex v of degree 3, where $n \geq 8$. If $N_G(v) = \{v_1, v_2, v_3\}$ such that $d_G(v_1) \leq d_G(v_2) \leq d_G(v_3)$ then $(d_G(v_1), d_G(v_2), d_G(v_3)) \in \{(1, 2, 4), (1, 4, 4)\}$.

Proof. By Lemma 1, $d_G(v_i) \neq 3$ for every $i \in \{1, 2, 3\}$. Also, by Lemma 3, we have $d_G(v_1) = 1 < d_G(v_2)$. Thus, we have $(d_G(v_2), d_G(v_3)) \in \{(2, 2), (2, 4), (4, 4)\}$. If $(d_G(v_2), d_G(v_3)) = (2, 2)$, then Lemma 3 confirms that the neighbors of v_2 and v_3 distinct from v are pendent, and hence $n = 6$, which contradicts $n \geq 8$. $\square$

The following lemma's proof is not provided because its reasoning closely mirrors the one given in Lemma 9's proof.

Lemma 10 Let ℓ be the function from Lemma 2 that satisfies the conditions given therein. Also, assume that inequalities (11), (12), (13) and (14) hold. Let G be a tree that minimizes $\mathcal{B}_\ell$ among all chemical n-order trees with perfect matching such that it contains a vertex v of degree 3, where $n \geq 8$. If $N_G(v) = \{v_1, v_2, v_3\}$ such that $d_G(v_1) \leq d_G(v_2) \leq d_G(v_3)$ then $(d_G(v_1), d_G(v_2), d_G(v_3)) \in \{(1, 2, 4), (1, 4, 4)\}$.

For a given graph G, let $\mathscr{n}_r(G) = |\{v \in V(G) : d_G(v) = r\}|$ and

$$\mathscr{m}_{s,\,t}(G) = |\{vw \in E(G) : d_G(v) = s \text{ and } d_G(w) = t\}|.$$

Theorem 1 Let ℓ be the function from Lemma 1 that satisfies the conditions given therein. Also, assume that inequalities (6), (7), (8) and (9) hold. If T is a chemical n-order tree with perfect matching such that $n \geq 8$, then

$$
\mathscr{B}_\ell(T) \leq \begin{cases} [\ell(1,\, 2)+\ell(2,\, 4)]\left(\dfrac{n+4}{4}\right)+\ell(1,\, 4)\left(\dfrac{n-4}{4}\right)+\ell(4,\, 4)\left(\dfrac{n-8}{4}\right) & \text{if } n \equiv 0 \pmod 4, \\ \ell(1,\, 2)\left(\dfrac{n+2}{4}\right)+\ell(2,\, 4)\left(\dfrac{n-2}{4}\right)+\ell(1,\, 4)\left(\dfrac{n-6}{4}\right)+\ell(4,\, 4)\left(\dfrac{n-10}{4}\right) & \\ +\ell(1,\, 3)+\ell(2,\, 3)+\ell(3,\, 4) & \text{otherwise.} \end{cases}
$$

When $n \equiv 0 \pmod 4$, the bound is achieved if and only if

$$
m_{1,\, 2}(T) = m_{2,\, 4}(T) = \frac{n+4}{4} = m_{1,\, 4}(T)+2 = m_{4,\, 4}(T)+3,
$$

and $m_{r,\, s}(T) = 0$ for remaining values of r and s. Also, when $n \equiv 2 \pmod 4$, the bound is achieved if and only if

$$
m_{1,\, 2}(T) = \frac{n+2}{4} = m_{2,\, 4}(T)+1 = m_{1,\, 4}(T)+2 = m_{4,\, 4}(T)+3,
$$

$$
m_{1,\, 3}(T) = 1 = m_{2,\, 3}(T) = m_{3,\, 4}(T),
$$

and $m_{r,\, s}(T) = 0$ for the remaining values of r and s. Two trees (one for each case) that attain the bound are depicted in Figure 2.

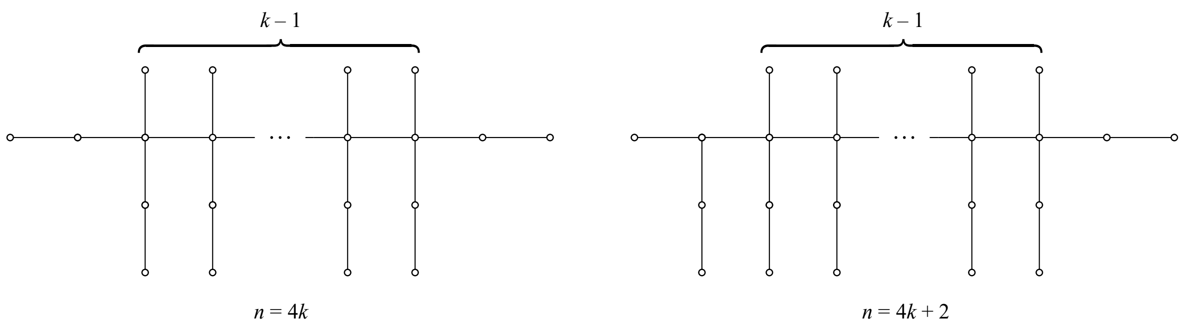

Figure 2. Two trees attaining the bound given in Theorem 1, where $k \geq 2$

Proof. Let G be a tree that maximizes $\mathscr{B}_\ell$ among all chemical n-order trees with perfect matching, where $n \geq 8$. Throughout this proof, we assume that $n_r(G) := n_r$ and $m_{s,\, t}(G) := m_{s,\, t}$. The following equations hold:

$$
\sum_{r=1}^{4} n_r = n \tag{15}
$$

$$\sum_{r=1}^{4} rn_r = 2(n-1) \tag{16}$$

$$\sum_{t=2}^{4} m_{1,\, t} = n_1 \tag{17}$$

$$\sum_{t=1}^{4} m_{2,\, t} + m_{2,\, 2} = 2n_2 \tag{18}$$

$$\sum_{t=1}^{4} m_{3,\, t} + m_{3,\, 3} = 3n_3 \tag{19}$$

$$\sum_{t=1}^{4} m_{4,\, t} + m_{4,\, 4} = 4n_4. \tag{20}$$

Lemma 5 gives

$$m_{2,\, 2} = 0. \tag{21}$$

By Lemma 1, it holds that

$$n_3 \leq 1. \tag{22}$$

Also, by Lemma 3, we have

$$n = 2n_1. \tag{23}$$

Case 1: $n \equiv 0 \pmod 4$.

Let $n = 4k$ for some integer k greater than 1. If $n_3 = 1$, then by (23), we have $n_1 + n_3 = 2k+1$, a contradiction to the fact that every graph contains an even number of vertices of odd degrees. Thus, (22) yields

$$n_3 = 0, \tag{24}$$

and hence from Lemma 7 and (21) it follows that $m_{2,\, 4} = m_{1,\, 2} = n_2$. Now, using (23) and (24) in (15) and (16), we obtain $n_2 = k+1$ and $n_4 = k-1$. Therefore,

$$m_{1,\, 2} = m_{2,\, 4} = k+1. \tag{25}$$

Consequently, from (17)-(20), we have

$$m_{1,\,4} = k-1 \quad \text{and} \quad m_{4,\,4} = k-2. \tag{26}$$

Therefore,

$$\mathscr{B}_\ell(G) = [\ell(1,\,2)+\ell(2,\,4)]\,(k+1)+\ell(1,\,4)\,(k-1)+\ell(4,\,4)\,(k-2),$$

or

$$\mathscr{B}_\ell(G) = [\ell(1,\,2)+\ell(2,\,4)]\left(\frac{n+4}{4}\right)+\ell(1,\,4)\left(\frac{n-4}{4}\right)+\ell(4,\,4)\left(\frac{n-8}{4}\right).$$

Case 2: $n \equiv 2 \pmod 4$.

Let $n = 4k+2$ for some integer k greater than 1. If $n_3 = 0$, then by (23), we have $n_1 + n_3 = 2k+1$, a contradiction to the fact that every graph contains an even number of vertices of odd degrees. Thus, (22) yields

$$n_3 = 1. \tag{27}$$

Now, using (23) and (27) in (15) and (16), we obtain $n_2 = k+1$ and $n_4 = k-1$.

Let $v \in V(G)$ be the unique vertex of degree 3. Let $N_G(v) = \{v_1,\, v_2,\, v_3\}$ such that $d_G(v_1) \le d_G(v_2) \le d_G(v_3)$. Then, by Lemma 9, either $(d_G(v_1),\, d_G(v_2),\, d_G(v_3)) = (1,\,2,\,4)$ or $(d_G(v_1),\, d_G(v_2),\, d_G(v_3)) = (1,\,4,\,4)$.

Case 2.1: $(d_G(v_1),\, d_G(v_2),\, d_G(v_3)) = (1,\,2,\,4)$.

In this case, we have

$$m_{1,\,3} = m_{2,\,3} = m_{3,\,4} = 1,$$

and hence, from Lemma 7 it follows that

$$m_{1,\,2} = n_2 = k+1. \tag{28}$$

Consequently, from (17)-(21), we have

$$m_{2,\,4} = k, \quad m_{1,\,4} = k-1 \quad \text{and} \quad m_{4,\,4} = k-2. \tag{29}$$

Therefore,

$$\mathscr{B}_\ell(G) = \ell(1,\,2)\,(k+1)+\ell(2,\,4)\,k+\ell(1,\,4)\,(k-1)+\ell(4,\,4)\,(k-2)+\ell(1,\,3)+\ell(2,\,3)+\ell(3,\,4) := \Theta_1. \tag{30}$$

Case 2.2: $(d_G(v_1),\, d_G(v_2),\, d_G(v_3)) = (1,\, 4,\, 4)$.
In this case, we have $k \geq 3$ and

$$m_{1,\,3} = 1,\; m_{2,\,3} = 0,\; m_{3,\,4} = 2,$$

and hence from Lemma 7 and (21) it follows that

$$m_{2,\,4} = m_{1,\,2} = n_2 = k+1. \tag{31}$$

Consequently, from (17)-(20), we have

$$m_{1,\,4} = k-1 \quad \text{and} \quad m_{4,\,4} = k-3. \tag{32}$$

Therefore,

$$\mathscr{B}_\ell(G) = [\ell(1,\,2)+\ell(2,\,4)](k+1)+\ell(1,\,4)\,(k-1)+\ell(4,\,4)\,(k-3)+\ell(1,\,3)+2\ell(3,\,4) := \Theta_2. \tag{33}$$

From (30) and (33), we have $\Theta_1 - \Theta_2 = \ell(4,\,4) - \ell(2,\,4) - [\ell(4,\,3) - \ell(2,\,3)] > 0$, by condition (i) of Lemma 1. Therefore, when $n \equiv 2 \pmod 4$, we must have

$$\mathscr{B}_\ell(G) = \Theta_1 = \ell(1,\,2)\left(\frac{n+2}{4}\right) + \ell(2,\,4)\left(\frac{n-2}{4}\right)$$

$$+\,\ell(1,\,4)\left(\frac{n-6}{4}\right) + \ell(4,\,4)\left(\frac{n-10}{4}\right) + \ell(1,\,3) + \ell(2,\,3) + \ell(3,\,4).$$

$\square$

Table 1. Some indices covered by Theorem 1

$\ell(d(v),\, d(u))$	Equation (1) yields	Symbol
$\sqrt{d(v)d(u)}$	reciprocal Randić index [18]	$\mathscr{RR}$
$(d(v)+d(u)-2)^2$	reformulated first Zagreb index [19, 20]	$\mathscr{EM}_1$
$(d(v)+d(u))\sqrt{(d(v))^2+(d(u))^2}$	elliptic Sombor index [21]	$\mathscr{ESO}$
$d(v)d(u)\sqrt{(d(v))^2+(d(u))^2}$	Zagreb-Sombor index [22, 23]	$\mathscr{ZSO}$
$(d(v)+d(u))\sqrt{d(v)d(u)}$	arithmetic-geometric product index	$\mathscr{AGP}$
$(d(v)+d(u))\sqrt{(d(v))^3+(d(u))^3}$	elliptic cubic Sombor index	$\mathscr{ECS}$
$d(v)d(u)\sqrt{(d(v))^3+(d(u))^3}$	Zagreb cubic Sombor index	$\mathscr{ZCS}$

Remark 1 Given that each function corresponding to the indices listed in Table 1 meets all the criteria specified for ℓ in Theorem 1, the conclusions drawn in that theorem can be readily invoked for these indices without the need for additional justification.

Remark 2 There exists a strong negative linear relationship between the elliptic Sombor index and entropy for the set of octane isomers; particularly, the correlation coefficient between these two quantities is -0.958 (see [21]), which indicates that the association is not only inverse in direction but also very close to a perfect linear dependence. This implies that variations in molecular structure captured by the elliptic Sombor index are strongly reflected in the entropy values of the isomers. Specifically, as the elliptic Sombor index increases, the entropy tends to decrease in a highly predictable manner. On the other hand, by Theorem 1 and Remark 1, among all octane isomers possessing a perfect matching, 3-ethyl-3-methylpentane uniquely attains the maximum value of the elliptic Sombor index. In view of the strong negative correlation observed between the elliptic Sombor index and entropy, one may reasonably expect 3-ethyl-3-methylpentane to exhibit the minimum entropy within the considered class of isomers, which is true according to the experimental values available at the following link: https://web.archive.org/web/20180830013934if_/http://moleculardescriptors.eu/dataset/dataset.htm.

The following theorem's proof is not provided because its reasoning closely mirrors the one given in Theorem 1's proof.

Theorem 2 Let ℓ be the function from Lemma 2 that satisfies the conditions given therein. Also, assume that inequalities (11), (12), (13) and (14) hold. If T is a chemical n-order tree with perfect matching such that $n \geq 8$, then the inequality regarding $\mathscr{B}_\ell(T)$ given in Theorem 1 is reversed, and the equality characterization in this inequality remains the same.

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Data availability

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Conflict of interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

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