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Research Article

Further Results on Bond Incident Degree Indices of Molecular Trees With Perfect Matchings

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Abstract

In chemical graph theory, a tree with maximum degree at most four is called a molecular tree. Let T be such a tree, with edge set $E(T)$, and let $d(u)$ denote the degree of a vertex u in T. A bond incident degree (BID) index of T is defined by $\mathcal{BID}_\phi(T) = \sum_{xy\in E(T)} \phi\big(d(x), d(y)\big)$, where ϕ is a real-valued symmetric function. The primary objective of this paper is to establish unified extremal results for BID indices of molecular trees of fixed order that admit perfect matchings, under certain conditions on ϕ. One of the main results applies, among others, to the atom-bond connectivity (ABC) index, the refined diminished Sombor index, and the atom-bond sum-connectivity (ABS) index. Another main result covers, among others, the reciprocal hyper-Zagreb index, the reciprocal reformulated first Zagreb index, the reciprocal mean square index, and the reciprocal mean cube index. The conclusions concerning the ABC and ABS indices are already known, whereas those for the other aforementioned indices are new.

Keywords: degree-based topological indices; bond incident degree indices; tree; perfect matching.

2020 Mathematics Subject Classification: 05C05, 05C07, 05C09.

1. Introduction

All the graphs considered in this paper are simple, finite, and connected. Unless otherwise stated, the graph-theoretic terminology used in this paper follows the standard conventions adopted in widely used graph theory books, such as [10, 13, 19].

Topological indices are numerical graph invariants that encode structural information of graphs and have long been used in chemical graph theory [32, 34]. Their role in quantitative structure-activity relationships and quantitative structure-property relationships is well documented in the literature; see, for example, the book [16]. Topological indices can be classified into several categories. One of such categories consists of indices defined in terms of the vertex degrees of a graph; these are commonly referred to as degree-based topological indices [20, 30]. Among the most extensively studied indices of this type are the Zagreb indices [11, 21] and the Randić index [12, 27]. Most of the degree-based topological indices can be defined through contributions assigned to the edges according to the degrees of their end-vertices [22]; such indices are called bond incident degree indices [33], or BID indices for short. For a graph G with edge set $E(G)$, the general form of BID indices is given by

$$\mathcal{BID}_\phi(G) = \sum_{xy\in E(G)} \phi\left(d(x), d(y)\right), \tag{1}$$

where ϕ is a real-valued symmetric function, while $d(x)$ and $d(y)$ are the degrees of vertices x and y in G, respectively; when context requires, we write $d_G(x)$ to explicitly indicate the underlying graph G. This framework allows one to treat extremal problems concerning BID indices in a unified manner; for example, see the survey paper [5]. Recent developments on BID indices can be found, for example, in [29, 31].

In chemical graph theory, trees with maximum degree at most four are usually called molecular trees. In the present paper, as a continuation of the study reported in [1], we investigate BID indices for molecular trees of fixed order that admit perfect matchings. Our aim is to derive unified extremal results for BID indices under certain conditions on the function ϕ. One of the main results covers, among others, the reciprocal hyper-Zagreb, reciprocal reformulated first Zagreb, reciprocal mean square, and reciprocal mean cube indices, whereas another applies, among others, to the atom-bond connectivity (ABC), refined diminished Sombor, and atom-bond sum-connectivity (ABS) indices. The choices of the function ϕ in Equation (1) corresponding to these particular BID indices are listed in Tables 3.1 and 3.2. The conclusions concerning the ABC and ABS indices are not new, whereas those for the other aforementioned indices are new.

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The remainder of the paper is organized as follows. In Section 2, we recall the necessary terminology and notation and establish several lemmas used in the subsequent section. In Section 3, we present the main results and identify several specific BID indices to which the main results apply.

2. Preliminaries and Lemmas

Let G be a graph with edge set $E(G)$ and vertex set $V(G)$. We say G is an n-vertex graph if $|V(G)| = n$. If w and w' are adjacent vertices in G, we say w' is a neighbor of w. We denote by $N_G(w)$ the set of all neighbors of w in G. A pendent vertex is a vertex that has only one neighbor. A non-trivial path $v_1v_2 \dots v_s$ in a graph G is called a pendent path if $\max(d_G(v_1), d_G(v_s)) \geq 3$, $\min(d_G(v_1), d_G(v_s)) = 1$, and $d_G(v_i) = 2$ when $2 \leq i \leq s-1$. If $u, v, x, y \in V(G)$ such that $uv \in E(G)$ and $xy \notin E(G)$, then we denote by $G - uv + xy$ the graph obtained from G by removing the edge uv and adding the edge xy.

Lemma 2.1. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies the following conditions.*

(i). *For all $\alpha_0, \alpha_1, \alpha_2, \alpha_3 \in \{2, 3, 4\}$ with $\max(\alpha_0, \alpha_1, \alpha_2) \leq \alpha_3$, it holds that*

$$\sum_{i=0}^{2} \big[\phi(\alpha_i, 3) - \phi(\alpha_i, 4)\big] + \phi(\alpha_3, 3) - \phi(\alpha_3, 2) + \phi(3, 3) - \phi(2, 4) > 0. \tag{2}$$

(ii). *For every $s \in \{2, 3\}$ and $\beta_1, \beta_2, \dots, \beta_s \in \{2, 3, 4\}$ with $(\beta_1, \beta_2, \dots, \beta_s) \neq (4, 4, \dots, 4)$, it holds that*

$$\sum_{i=1}^{s-1} \big[\phi(s, \beta_i) - \phi(s+1, \beta_i)\big] + \phi(2, \beta_s) - \phi(s+1, \beta_s) + \phi(2, s) - \phi(1, s+1) > 0. \tag{3}$$

(iii). *For all $s \in \{2, 3\}$, $\gamma_1 \in \{1, 2, 3, 4\}$ and $\gamma_2, \gamma_3, \gamma_4 \in \{2, 3, 4\}$, it holds that*

$$\begin{aligned}\sum_{i=1}^{3} \big[\phi(4, \gamma_i) - \phi(3, \gamma_i)\big] + \phi(2, \gamma_4) - \phi(3, \gamma_4) + \phi(2, s) - \phi(1, s+1) + (s-1)\big[\phi(s, 4) - \phi(s+1, 4)\big] - \phi(3, s+1) \\ + \phi(1, 2) - \phi(1, 3) + \phi(2, 4) > 0.\end{aligned} \tag{4}$$

(iv). *For all $\eta_2, \eta_3, \eta_4 \in \{2, 3, 4\}$, it holds that*

$$\sum_{i=2}^{3} \big[\phi(3, \eta_i) - \phi(4, \eta_i)\big] + \phi(2, \eta_4) - \phi(4, \eta_4) + \phi(3, 4) + \phi(1, 2) - 2\phi(1, 4) > 0. \tag{5}$$

Also, assume that ϕ satisfies the following inequality:

$$\phi(4, 4) + \phi(1, 2) - \phi(1, 4) - \phi(2, 4) > 0. \tag{6}$$

If G is a graph minimizing $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings, then every edge of the unique perfect matching of G is incident with a pendent vertex of G.

Proof. Let M be the unique perfect matching of G. Suppose, to the contrary, that there exists an edge $vw \in M$ such that neither v nor w is pendent. We may assume that $2 \leq d_G(v) \leq d_G(w) \leq 4$. We first note that every pendent edge of G must belong to M. Consequently, no vertex can have two pendent neighbors. Set $U = \big(N_G(v) \cup N_G(w)\big) \setminus \{v, w\}$. Since $vw \in M$, every vertex in U has degree at least 2.

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

Case 1.1. $d_G(v) = d_G(w) = 3$.
We choose a vertex $u_0 \in U$ having maximum degree among the vertices of U. Without loss of generality, assume that $u_0 \in N_G(v)$. Let $N_G(v) = \{u_0, v_1, w\}$ and $N_G(w) = \{w_1, w_2, v\}$. Define $G' = G - vv_1 + wv_1$. Since $vv_1 \notin M$, the matching M remains a perfect matching of G'. By the choice of u_0, it holds that $\max\big(d_G(w_1), d_G(w_2), d_G(v_1)\big) \leq d_G(u_0)$. Hence, by (2), we have

$$\begin{aligned}\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G') = &\sum_{i=1}^{2} \big[\phi(3, d_G(w_i)) - \phi(4, d_G(w_i))\big] + \phi(3, d_G(v_1)) - \phi(4, d_G(v_1)) + \phi(3, d_G(u_0)) - \phi(2, d_G(u_0)) \\ &+ \phi(3, 3) - \phi(2, 4) > 0,\end{aligned}$$

a contradiction to the definition of G.

Case 1.2. $d_G(v) = 2$.
Let $s = d_G(w)$. Then, $s \in \{2, 3\}$. Take $N_G(v) = \{x, w\}$ and $N_G(w) = \{v, w_1, \ldots, w_{s-1}\}$. We note that all the vertices $x, w_1, \ldots, w_{s-1}$ have degrees in $\{2, 3, 4\}$.

Case 1.2.1. At least one of the vertices $x, w_1, \ldots, w_{s-1}$ has degree less than 4 in G.
Let $G' = G - vx + wx$. Since $vx \notin M$, the matching M is also the perfect matching of G'. Therefore, by (3), we have

$$\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G') = \sum_{i=1}^{s-1} \big[\phi(s, d_G(w_i)) - \phi(s+1, d_G(w_i))\big] + \phi(2, s) - \phi(1, s+1) + \phi(2, d_G(x)) - \phi(s+1, d_G(x)) > 0.$$

a contradiction.

Case 1.2.2. Each of the vertices $x, w_1, \ldots, w_{s-1}$ has degree 4 in G.
We choose a non-pendent vertex $x_0 \in N_G(x) \setminus \{v\}$ and, among all paths starting at x and containing x_0, we choose one, say P, of a maximum length. We denote the terminal vertex of P, different from x, by z. Then, $d_G(z) = 1$. Let y be the neighbor of z. The maximality of P and the fact that no vertex of G has more than one pendent neighbor imply that $d_G(y) = 2$. Let y' be the neighbor of y different from z. Define $G'' = G - vx + wy$. Since the edge vx does not belong to M, the set M remains the perfect matching of G''. Let $N_G(x) \setminus \{v\} = \{x_0, x_1, x_2\}$.

Case 1.2.2.1. The vertices x and y' coincide.
By using (4) with $\gamma_3 = 3$ and $\gamma_4 = 4$, we obtain

$$\begin{aligned}\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G'') = {} & \sum_{i=1}^{2} \big[\phi(4, d_G(x_i)) - \phi(3, d_G(x_i))\big] + 2\phi(2, 4) - \phi(3, 3) - \phi(3, s+1) \\ & + \phi(1, 2) - \phi(1, 3) + \phi(2, s) - \phi(1, s+1) + (s-1)\big[\phi(s, 4) - \phi(s+1, 4)\big] > 0,\end{aligned}$$

a contradiction.

Case 1.2.2.2. The vertices x and y' do not coincide.
Since x can have at most one pendent neighbor and $d_G(y') \in \{2, 3, 4\}$, by using (4), we have

$$\begin{aligned}\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G'') = {} & \sum_{i=0}^{2} \big[\phi(4, d_G(x_i)) - \phi(3, d_G(x_i))\big] + \phi(2, d_G(y')) - \phi(3, d_G(y')) + \phi(1, 2) - \phi(1, 3) \\ & + \phi(2, 4) - \phi(3, s+1) + \phi(2, s) - \phi(1, s+1) + (s-1)\big[\phi(s, 4) - \phi(s+1, 4)\big] > 0,\end{aligned}$$

a contradiction.

Case 2. $d_G(w) = 4$.
We choose a vertex $w_0 \in N_G(w) \setminus \{v\}$ and, among all paths starting at w and containing w_0, choose one of a maximum length. Let z be the terminal vertex of this path, different from w. Then, $d_G(z) = 1$. Let y be the neighbor of z and let y' be the other neighbor of y. Let $s = d_G(v)$. Take $N_G(v) \setminus \{w\} = \{v_2, \ldots, v_s\}$. Then, we have $d_G(v_i) \in \{2, 3, 4\}$ for every i with $2 \le i \le s$.

Case 2.1. $s \in \{2, 3\}$.
Let G' be obtained from G by deleting every edge $vv_i,\ 2 \le i \le s$, and adding every edge $yv_i,\ 2 \le i \le s$. Certainly, M is also the perfect matching of G'. Here, we have

$$\begin{aligned}\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G') = {} & \sum_{i=2}^{s} \big[\phi(s, d_G(v_i)) - \phi(s+1, d_G(v_i))\big] + \phi(s, 4) - \phi(1, 4) + \phi(1, 2) - \phi(1, s+1) \\ & + \phi(2, d_G(y')) - \phi(s+1, d_G(y')).\end{aligned} \tag{7}$$

In the rest of Case 2.1, we show that the right-hand side of (7) is positive, which is a contradiction.

If $s = 3$, then the right-hand side of (7) is positive by (5).

If $s = 2 = d_G(v_2) = d_G(y')$, then by taking $s = \beta_1 = \beta_2 = 2$ in (3), $(s, \gamma_1, \gamma_2, \gamma_3, \gamma_4) = (3, 2, 2, 4, 2)$ in (4) and adding the two resulting inequalities to (6), we obtain

$$4\phi(2, 2) - 4\phi(2, 3) + 2\phi(2, 4) - 2\phi(1, 4) + 2\phi(1, 2) - 2\phi(1, 3) > 0,$$

and hence, the right-hand side of (7) is positive.

If $s = 2 = d_G(y')$ and $d_G(v_2) = 3$, then taking $(s, \gamma_1, \gamma_2, \gamma_3, \gamma_4) = (3, 3, 4, 4, 2)$ in (4) gives

$$\phi(2,4) - \phi(3,3) - \phi(1,4) + \phi(1,2) - \phi(1,3) + \phi(2,2) > 0,$$

and hence, the right-hand side of (7) is positive.

If $s = 2 = d_G(y')$ and $d_G(v_2) = 4$, then (4) with $(s, \gamma_1, \gamma_2, \gamma_3, \gamma_4) = (3, 2, 4, 4, 2)$, gives

$$2\phi(2,4) - \phi(3,4) - \phi(1,4) + \phi(1,2) - \phi(1,3) + \phi(2,2) - \phi(2,3) > 0,$$

which implies that the right-hand side of (7) is positive.

If $s = 2$ and $d_G(y') = 3$ ($d_G(y') = 4$, respectively), then by using (4) with $(s, \gamma_1, \gamma_2, \gamma_3) = (3, 3, 4, 4)$ ($(s, \gamma_1, \gamma_2, \gamma_3) = (3, 2, 4, 4)$, respectively), we note that the right-hand side of (7) is positive.

Case 2.2. $s = 4$.
In this case, we construct a new graph G'' by deleting every edge $vv_i,\ 2 \le i \le 4$, and adding every edge $zv_i,\ 2 \le i \le 4$. Then, M remains the perfect matching of G''. Therefore, by (6), we have

$$\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G'') = \phi(4,4) + \phi(1,2) - \phi(1,4) - \phi(2,4) > 0,$$

a contradiction. □

The proof of the following lemma is completely analogous to that of Lemma 2.1, and hence, it is stated without proof.

Lemma 2.2. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies the following conditions.*

(i). *For all $\alpha_0, \alpha_1, \alpha_2, \alpha_3 \in \{2, 3, 4\}$ with $\max(\alpha_0, \alpha_1, \alpha_2) \le \alpha_3$, it holds that*

$$\sum_{i=0}^{2} \big[\phi(\alpha_i, 3) - \phi(\alpha_i, 4)\big] + \phi(\alpha_3, 3) - \phi(\alpha_3, 2) + \phi(3,3) - \phi(2,4) < 0. \tag{8}$$

(ii). *For every $s \in \{2, 3\}$ and $\beta_1, \beta_2, \dots, \beta_s \in \{2, 3, 4\}$ with $(\beta_1, \beta_2, \dots, \beta_s) \neq (4, 4, \dots, 4)$, it holds that*

$$\sum_{i=1}^{s-1} \big[\phi(s, \beta_i) - \phi(s+1, \beta_i)\big] + \phi(2, \beta_s) - \phi(s+1, \beta_s) + \phi(2, s) - \phi(1, s+1) < 0. \tag{9}$$

(iii). *For all $s \in \{2, 3\}$, $\gamma_1 \in \{1, 2, 3, 4\}$ and $\gamma_2, \gamma_3, \gamma_4 \in \{2, 3, 4\}$, it holds that*

$$\begin{aligned}\sum_{i=1}^{3} \big[\phi(4, \gamma_i) - \phi(3, \gamma_i)\big] + \phi(2, \gamma_4) - \phi(3, \gamma_4) + \phi(2, s) - \phi(1, s+1) + (s-1)\big[\phi(s, 4) - \phi(s+1, 4)\big] - \phi(3, s+1) \\ + \phi(1,2) - \phi(1,3) + \phi(2,4) < 0.\end{aligned} \tag{10}$$

(iv). *For all $\eta_2, \eta_3, \eta_4 \in \{2, 3, 4\}$, it holds that*

$$\sum_{i=2}^{3} \big[\phi(3, \eta_i) - \phi(4, \eta_i)\big] + \phi(2, \eta_4) - \phi(4, \eta_4) + \phi(3,4) + \phi(1,2) - 2\phi(1,4) < 0. \tag{11}$$

Also, assume that ϕ satisfies the following inequality:

$$\phi(4,4) + \phi(1,2) - \phi(1,4) - \phi(2,4) < 0. \tag{12}$$

If G is a graph maximizing $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings, then every edge of the unique perfect matching of G is incident with a pendent vertex of G.

Lemma 2.3. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (2), (3), (4), (5) and (6). Also, assume that ϕ satisfies the following inequality for all $\xi_1, \xi_2, \xi_3, \xi_4 \in \{3, 4\}$:*

$$\sum_{i=2}^{4}[\phi(\xi_i, 4) - \phi(\xi_i, 3)] + \phi(\xi_1, 2) - \phi(\xi_1, 3) + \phi(1,4) + \phi(1,2) - 2\phi(1,3) > 0. \tag{13}$$

Let G be an n-vertex molecular tree admitting perfect matching. If G contains a vertex u of degree 4 having no neighbor of degree 2, then G does not minimize $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings.

Proof. We suppose, to the contrary, that G minimizes $\mathcal{BID}_\phi$ among all n-vertex molecular trees with perfect matchings. Let M be the unique perfect matching of G. Let $N_G(u) = \{u_1, u_2, u_3, u_4\}$. Without loss of generality, we assume that $u_1u \in M$. Then, by Lemma 2.1, $d_G(u_1) = 1$, and so $d_G(u_i) \geq 3$ for every $i \in \{2, 3, 4\}$. Among all the paths that start at u and contain u_2, let P be a longest one. Then, the other end vertex of P must be pendent, say $v_1 \in V(G)$. Let v be the only vertex adjacent to v_1. We observe that $d_G(v) = 2$. Let v_2 be the other neighbor of v. Then, $d_G(v_2) \geq 3$ by Lemma 2.1. Denote by G' the graph constructed from G by dropping the edge u_4u and adding u_4v. We observe that M is also the perfect matching of G' because $u_4u \notin M$. Whether $v_2 = u_2$ or $v_2 \neq u_2$, in each case, by applying (13), we obtain

$$\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G') = \sum_{i=2}^{4}[\phi(d_G(u_i), 4) - \phi(d_G(u_i), 3)] + \phi(d_G(v_2), 2) - \phi(d_G(v_2), 3) + \phi(1, 4) + \phi(1, 2) - 2\phi(1, 3) > 0,$$

a contradiction. □

The next lemma's proof is fully analogous to that of Lemma 2.3, and hence, it is stated without proof.

Lemma 2.4. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (8), (9), (10), (11) and (12). Also, assume that ϕ satisfies the following inequality for all $\xi_1, \xi_2, \xi_3, \xi_4 \in \{3, 4\}$:*

$$\sum_{i=2}^{4}[\phi(\xi_i, 4) - \phi(\xi_i, 3)] + \phi(\xi_1, 2) - \phi(\xi_1, 3) + \phi(1, 4) + \phi(1, 2) - 2\phi(1, 3) < 0. \tag{14}$$

Let G be an n-vertex molecular tree admitting perfect matching. If G contains a vertex of degree 4 having no neighbor of degree 2, then G does not maximize $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings.

Lemma 2.5. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (2), (3), (4), (5), (6) and (13). Let G be an n-vertex molecular tree admitting perfect matching, where $n \geq 10$. If G contains a vertex u of degree 4 such that u does not have exactly two neighbors of degree 2, then G does not minimize $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings, where $n \geq 10$.*

Proof. We suppose, to the contrary, that G minimizes $\mathcal{BID}_\phi$ among all n-vertex molecular trees with perfect matchings, where $n \geq 10$. From Lemmas 2.1 and 2.3, we conclude that u has exactly one pendent neighbor and at least one neighbor of degree 2. Let M be the perfect matching of G. Let $N_G(u) = \{u_1, u_2, u_3, u_4\}$, where $d_G(u_1) = 1$ and $d_G(u_2) = 2$. Let $N_G(u_2) = \{u, v\}$. Then, from Lemma 2.1, we conclude that the vertex v is pendent. If $d_G(u_3) = d_G(u_4) = 2$, then by Lemma 2.1, we have $n = 8$, which contradicts $n \geq 10$. Thus, $d_G(u_3) \geq 3$ and $d_G(u_4) \geq 3$. Denote by G' the graph constructed by dropping the edge u_3u from G and adding the edge u_3u_2. We note that M is also the unique perfect matching of G'. Now, using (13) with $\xi_1 = 4$ and $\xi_4 = 3$, we obtain

$$\mathcal{BID}_\phi(G) - \mathcal{BID}_\phi(G') = \sum_{i=3}^{4}[\phi(d_G(u_i), 4) - \phi(d_G(u_i), 3)] + \phi(2, 4) - \phi(3, 3) + \phi(1, 2) + \phi(1, 4) - 2\phi(1, 3) > 0,$$

a contradiction. □

The following lemma's proof is completely analogous to the one given for Lemma 2.5, and hence, it is stated without proof.

Lemma 2.6. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (8), (9), (10), (11), (12) and (14). Let G be an n-vertex molecular tree admitting a perfect matching, where $n \geq 10$. If G contains a vertex u of degree 4 such that u does not have exactly two neighbors of degree 2, then G does not maximize $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings, where $n \geq 10$.*

3. Main Results

Let n be an even integer larger than 5. Denote by $T_n^\dagger$ the n-vertex tree obtained from the $\frac{n}{2}$-vertex path graph $P_{n/2}$ by attaching a pendent vertex to each vertex of $P_{n/2}$; see Figure 3.1. For an even integer larger than 11 (larger than 7, respectively), let T_n^* ($T_n^\diamond$, respectively) be the n-vertex tree obtained from the tree $T_{n-4}^\dagger$ ($T_{n-2}^\dagger$, respectively) by attaching a pendent path of length 2 to the non-pendent neighbor of each vertex (exactly one vertex, respectively) of degree 2; see Figure 3.2.

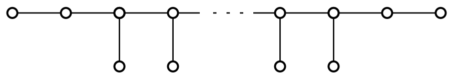

Figure 3.1: The tree $T_n^{\dagger}$.

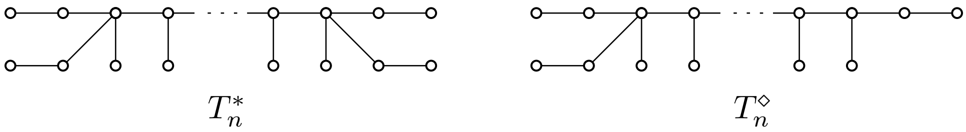

Figure 3.2: The trees T_n^* and $T_n^{\diamond}$.

Theorem 3.1. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (2), (3), (4), (5), (6) and (13). Let H be a molecular n-vertex tree with perfect matching such that $n \in \{6, 8, 10, 12\}$. Then, the following statements hold.*

(i). *If $n = 6$, then $\mathcal{BID}_\phi(H) \geq 2\phi(1,2) + \phi(1,3) + 2\phi(2,3)$, where the equality holds if and only if $H \cong T_6^{\dagger}$.*

(ii). *If $n \in \{8, 10\}$, $H \ncong T_n^{\dagger}$ and $H \ncong T_n^{\diamond}$, then*

$$\mathcal{BID}_\phi(H) > \min\left\{\mathcal{BID}_\phi(T_n^{\dagger}), \mathcal{BID}_\phi(T_n^{\diamond})\right\},$$

where

$$\begin{aligned}
\mathcal{BID}_\phi(T_n^{\dagger}) &= \frac{n-4}{2}\,\phi(1,3) + \frac{n-6}{2}\,\phi(3,3) + 2[\phi(1,2) + \phi(2,3)],\\
\mathcal{BID}_\phi(T_8^{\diamond}) &= 3\phi(1,2) + \phi(1,4) + 3\phi(2,4),\\
\mathcal{BID}_\phi(T_{10}^{\diamond}) &= \phi(1,3) + \phi(1,4) + \phi(2,3) + \phi(3,4) + 3\phi(1,2) + 2\phi(2,4).
\end{aligned}$$

(iii). *If $n = 12$, $H \ncong T_{12}^{\dagger}$, $H \ncong T_{12}^*$ and $H \ncong T_{12}^{\diamond}$ then*

$$\mathcal{BID}_\phi(H) > \min\left\{\mathcal{BID}_\phi(T_{12}^{\dagger}), \mathcal{BID}_\phi(T_{12}^{\diamond}), \mathcal{BID}_\phi(T_{12}^*)\right\},$$

where

$$\begin{aligned}
\mathcal{BID}_\phi(T_{12}^{\dagger}) &= 4\phi(1,3) + 3\phi(3,3) + 2\big[\phi(1,2) + \phi(2,3)\big],\\
\mathcal{BID}_\phi(T_{12}^{\diamond}) &= 2\phi(1,3) + \phi(3,3) + \phi(1,4) + \phi(2,3) + \phi(3,4) + 3\phi(1,2) + 2\phi(2,4),\\
\mathcal{BID}_\phi(T_{12}^*) &= 4\phi(1,2) + 2\phi(1,4) + 4\phi(2,4) + \phi(4,4).
\end{aligned}$$

Proof. Let G be a tree minimizing $\mathcal{BID}_\phi$ among all n-vertex molecular trees admitting perfect matchings, and let M be its perfect matching. Then,

$$\mathcal{BID}_\phi(H) \geq \mathcal{BID}_\phi(G). \tag{15}$$

By Lemma 2.1, every edge of M is incident with a pendent vertex. Since every pendent edge necessarily belongs to M, it follows that every non-pendent vertex of G has exactly one pendent neighbor. Since G has perfect matching, no vertex of G can have two pendent neighbors. Let G^- be the tree obtained from G by deleting all its pendent vertices. Then,

$$|V(G^-)| = \frac{n}{2}$$

and $d_G(v) = d_{G^-}(v) + 1$ for every $v \in V(G^-)$. Hence, the maximum degree of G^- is at most 3. Consequently, the following hold:

- If $n = 6$, then G^- is isomorphic to the 3-vertex path graph P_3.
- If $n = 8$, then G^- is isomorphic to either the 4-vertex path graph P_4 or the 4-vertex star graph S_4.
- If $n = 10$, then G^- is isomorphic to either the 5-vertex path graph P_5 or $P_5^{\diamond}$, where $P_5^{\diamond}$ is the graph obtained from $T_{10}^{\diamond}$ by removing its pendent vertices.

Therefore, for $n \in \{6, 8, 10\}$, the desired conclusion follows from (15).

In what follows, we assume that $n = 12$. Then, Lemma 2.5 implies that every vertex of degree 3 in G^- has exactly two pendent neighbors; however, there are only three non-isomorphic 6-vertex trees of maximum degree at most 3 with this property, namely the 6-vertex path graph P_6, $P_6^\diamond$ and $S_{3,3}$, where $P_6^\diamond$ and $S_{3,3}$ are the graphs obtained, respectively, from $T_{12}^\diamond$ and T_{12}^* by removing their pendent vertices. Thus, the required conclusion follows from (15). □

We state the next result without proof because its proof is similar to that of Theorem 3.1.

Theorem 3.2. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (8), (9), (10), (11), (12) and (14). Let H be a molecular n-vertex tree with perfect matching such that $n \in \{6, 8, 10, 12\}$. Then, the following statements hold.*

(i). *If $n = 6$, then $\mathcal{BID}_\phi(H) \leq 2\phi(1,2) + \phi(1,3) + 2\phi(2,3)$, where the equality holds if and only if $H \cong T_6^\dagger$.*

(ii). *If $n \in \{8, 10\}$, $H \ncong T_n^\dagger$ and $H \ncong T_n^\diamond$, then*

$$\mathcal{BID}_\phi(H) < \max\left\{\mathcal{BID}_\phi(T_n^\dagger), \mathcal{BID}_\phi(T_n^\diamond)\right\},$$

where the values of $\mathcal{BID}_\phi(T_n^\dagger)$ and $\mathcal{BID}_\phi(T_n^\diamond)$ for $n \in \{8, 10\}$ are given in Theorem 3.1(ii).

(iii). *If $n = 12$, $H \ncong T_{12}^\dagger$, $H \ncong T_{12}^*$ and $H \ncong T_{12}^\diamond$ then*

$$\mathcal{BID}_\phi(H) < \max\left\{\mathcal{BID}_\phi(T_{12}^\dagger), \mathcal{BID}_\phi(T_{12}^\diamond), \mathcal{BID}_\phi(T_{12}^*)\right\},$$

where the values of $\mathcal{BID}_\phi(T_{12}^\dagger)$, $\mathcal{BID}_\phi(T_{12}^\diamond)$ and $\mathcal{BID}_\phi(T_{12}^*)$ are given in Theorem 3.1(iii).

Theorem 3.3. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (2), (3), (4), (5), (6) and (13). Let H be a molecular n-vertex tree with perfect matching such that $n \geq 14$. Let $\Theta = 2[\phi(1,3) + \phi(3,3) - \phi(2,4)] + \phi(2,3) - \phi(3,4) - \phi(1,2) - \phi(1,4)$.*

(i). *If $\Theta < 0$, then*

$$\mathcal{BID}_\phi(H) \geq \frac{n-4}{2}\,\phi(1,3) + \frac{n-6}{2}\,\phi(3,3) + 2[\phi(1,2) + \phi(2,3)], \tag{16}$$

where the equality in (16) is achieved if and only if H is isomorphic to $T_n^\dagger$; see Figure 3.1.

(ii). *If $\Theta > 0$, then*

$$\mathcal{BID}_\phi(H) \geq \frac{n-12}{2}\,\phi(1,3) + \frac{n-14}{2}\,\phi(3,3) + 2[\phi(1,4) + \phi(3,4)] + 4[\phi(1,2) + \phi(2,4)], \tag{17}$$

where the equality in (17) is achieved if and only if H is isomorphic to T_n^*; see Figure 3.2.

(iii). *If $\Theta = 0$, then both (16) and (17) hold; that is, the bounds in (i) and (ii) coincide. The equality in this case is achieved if and only if H is isomorphic to $T_n^\diamond$ or $T_n^\dagger$ or T_n^* (see Figures 3.1 and 3.2).*

Proof. Let G be a tree minimizing $\mathcal{BID}_\phi$ among all molecular n-vertex trees with perfect matchings, where $n \geq 14$. Then,

$$\mathcal{BID}_\phi(H) \geq \mathcal{BID}_\phi(G). \tag{18}$$

Case 1. Maximum degree of G is 4.
Let u be a vertex of G such that $d_G(u) = 4$. Keeping in mind Lemmas 2.1 and 2.5 and the assumption $n \geq 14$, we may assume that $N_G(u) = \{u_1, u_2, u_3, u_4\}$ such that $d_G(u_1) = 1$ and $d_G(u_2) = d_G(u_3) = 2$, $d_G(u_4) = 3$, and each of the vertices u_2 and u_3 has a pendent neighbor. Among all the paths that start at u_1 and contain u_4, let P be a longest one. Then, the other end vertex of P must be pendent, say $v_1 \in V(G)$. Let v be the vertex adjacent to v_1. Then, $d_G(v) = 2$. Let $N_G(v) = \{v_1, v_2\}$. Then, by Lemma 2.1, $d_G(v_2) \geq 3$. By keeping in mind Lemma 2.1, we note that if y is any vertex of P such that $y \notin \{u_1, v_1, v\}$, then y has exactly one pendent neighbor in G and $d_G(y) \geq 3$. Thus, by Lemmas 2.1 and 2.5, we conclude that every vertex of P other than u_1, u, v_1, v_2, and v, has degree 3 in G and only one of its neighbors is pendent in G. Consequently, the graph G is isomorphic to either T_n^* or $T_n^\diamond$ depicted in Figure 3.2. Here, we have

$$\mathcal{BID}_\phi(T_n^*) = \frac{n-12}{2}\,\phi(1,3) + \frac{n-14}{2}\,\phi(3,3) + 2[\phi(1,4) + \phi(3,4)] + 4[\phi(1,2) + \phi(2,4)]$$

and

$$\mathcal{BID}_\phi(T_n^\diamond) = \frac{n-8}{2}\,\phi(1,3) + \frac{n-10}{2}\,\phi(3,3) + \phi(1,4) + \phi(2,3) + \phi(3,4) + 3\phi(1,2) + 2\phi(2,4).$$

Hence,

$$\mathcal{BID}_\phi(T_n^\diamond) - \mathcal{BID}_\phi(T_n^*) = 2[\phi(1,3) + \phi(3,3) - \phi(2,4)] + \phi(2,3) - \phi(3,4) - \phi(1,2) - \phi(1,4) = \Theta. \tag{19}$$

Case 2. Maximum degree of G is 3.
Let $P' : w_1 w_2 \dots w_k$ be a longest path in G. Then, $d_G(w_1) = 1 = d_G(w_k)$. Since G has perfect matching, by the definition of P', we have $d_G(w_2) = 2 = d_G(w_{k-1})$. Also, by Lemma 2.1, w_i has exactly one pendent neighbor in G for every $i \in \{3, 4, \dots, k-2\}$ with $k \geq 9$ as $n \geq 14$. Therefore, G is isomorphic to $T_n^\dagger$ depicted in Figure 3.1. But,

$$\mathcal{BID}_\phi(T_n^\dagger) = \frac{n-4}{2}\,\phi(1,3) + \frac{n-6}{2}\,\phi(3,3) + 2[\phi(1,2) + \phi(2,3)].$$

Now, combining the conclusions in Cases 1 and 2, we deduce that G is isomorphic to T_n^* or $T_n^\dagger$ or $T_n^\diamond$. We note that

$$\begin{aligned}\mathcal{BID}_\phi(T_n^\dagger) - \mathcal{BID}_\phi(T_n^*) &= 2[\mathcal{BID}_\phi(T_n^\dagger) - \mathcal{BID}_\phi(T_n^\diamond)]\\ &= 4[\phi(1,3) + \phi(3,3) - \phi(2,4)] + 2[\phi(2,3) - \phi(3,4) - \phi(1,2) - \phi(1,4)]\\ &= 2\Theta. \end{aligned} \tag{20}$$

Consequently, the desired conclusions follow from (18), (19) and (20). □

Remark 3.1. *We note that the inequalities* (2)*,* (3)*,* (4)*,* (5)*,* (6) *and* (13) *hold for each of the functions given in Table 3.1. Thus, Theorem 3.1 covers all the indices listed in Table 3.1. Also, we observe that* Θ *given in Theorem 3.3 is negative for the first five functions, positive for the sixth and seventh functions, and zero for the last function of the aforementioned table. Therefore, the first five indices of Table 3.1 are covered by Theorem 3.3(i), the sixth and seventh by Theorem 3.3(ii), and the final index by Theorem 3.3(iii).*

Table 3.1: Some indices covered by Theorems 3.1 and 3.3.

$\phi\,(d(x), d(y))$	Equation (1) yields
$\dfrac{1}{(d(x)+d(y))^2}$	Reciprocal HZ (hyper-Zagreb) index; see [15, 28] for the HZ index
$\dfrac{1}{(d(x)+d(y)-2)^2}$	Reciprocal RFZ (reformulated first Zagreb) index; see [23, 24] for the RFZ index
$\dfrac{1}{d(x)^2+d(y)^2}$	RMS (reciprocal mean square) index [2, 3]
$\dfrac{1}{d(x)^3+d(y)^3}$	Reciprocal mean cube index
$\dfrac{1}{d(x)\,d(y)} + \dfrac{1}{d(x)^2+d(y)^2}$	Sum of the MSZ (modified second Zagreb) index [8, 26] and RMS index
$\dfrac{1}{(d(x)+d(y)+1)^2}$	Reciprocal half-increased hyper-Zagreb index
$\dfrac{1}{\left(d(x)+\frac{1}{2}\right)^2 + \left(d(y)+\frac{1}{2}\right)^2}$	Half-increased RMS index
$\dfrac{7}{d(x)+d(y)} + \dfrac{6}{d(x)\,d(y)}$	A linear combination of the harmonic index [9, 18] and MSZ index

The next theorem's proof is completely analogous to that of Theorem 3.3, and therefore, it is stated without proof.

Theorem 3.4. *Let $\mathcal{BID}_\phi$ be a BID index such that the function ϕ satisfies (8), (9), (10), (11), (12) and (14). Let H be a molecular n-vertex tree with perfect matching such that $n \geq 14$. Let Θ be the same as defined in Theorem 3.3.*

(i). *If $\Theta > 0$, then*

$$\mathcal{BID}_\phi(H) \leq \frac{n-4}{2}\,\phi(1,3) + \frac{n-6}{2}\,\phi(3,3) + 2[\phi(1,2)+\phi(2,3)], \tag{21}$$

where the equality in (21) is achieved if and only if H is isomorphic to $T_n^{\dagger}$; see Figure 3.1.

(ii). *If $\Theta < 0$, then*

$$\mathcal{BID}_\phi(H) \leq \frac{n-12}{2}\,\phi(1,3) + \frac{n-14}{2}\,\phi(3,3) + 2[\phi(1,4)+\phi(3,4)] + 4[\phi(1,2)+\phi(2,4)], \tag{22}$$

where the equality in (22) is achieved if and only if H is isomorphic to T_n^{*}; see Figure 3.2.

(iii). *If $\Theta = 0$, then both (21) and (22) hold; that is, the bounds in (i) and (ii) coincide. The equality in this case is achieved if and only if H is isomorphic to $T_n^{\diamond}$ or $T_n^{\dagger}$ or T_n^{*} (see Figures 3.1 and 3.2).*

Table 3.2: Some indices covered by Theorems 3.2 and 3.4.

$\phi\,(d(x), d(y))$	Equation (1) yields
$\sqrt{\dfrac{d(x)+d(y)-2}{d(x)d(y)}}$	Atom-bond connectivity index [4, 17]
$\dfrac{\sqrt{d(x)^2+d(y)^2+2(d(x)d(y)-1)}}{d(x)+d(y)}$	Refined DSO (diminished Sombor) index; see [14, 25] for the DSO index
$\sqrt{\dfrac{d(x)+d(y)-2}{d(x)+d(y)}}$	Atom-bond sum-connectivity index [6, 37]

Remark 3.2. *We observe that the inequalities (8), (9), (10), (11), (12) and (14) hold for each of the functions given in Table 3.2. Thus, Theorem 3.2 covers all the indices listed in Table 3.2. Also, we note that Θ given in Theorem 3.3 is positive (negative, respectively) for the first two functions (last function, respectively) of the aforementioned table. Therefore, the first two indices of Table 3.2 are covered by Theorem 3.4(i) and the third index by Theorem 3.4(ii). The conclusions concerning the atom-bond connectivity (ABC) index and the atom-bond sum-connectivity (ABS) index are not new; the corresponding result for the ABS index can be found in [35], while that for the ABC index follows from Theorem 1 of [36]. Moreover, we remark that, for the following function, $\Theta = 0$ and each of the inequalities (8), (9), (10), (11), (12) and (14) holds, and hence, Theorem 3.4(iii) covers the BID index corresponding to this function:*

$$\phi(d(x), d(y)) = 2 - \frac{1}{d(x)+d(y)} - \frac{6}{7\,d(x)\,d(y)}.$$

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