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On Bond Incident Molecular Descriptors of Molecular Trees with Perfect Matching

Abeer M. Albalahi[1], Zhibin Du[2], Akhlaq A. Bhatti[3], Amjad E. Hamza[1], Akbar Ali[1,*]

[1]*Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia*
[2]*School of Artificial Intelligence, South China Normal University, Foshan, Guangdong, China*
[3]*Department of Sciences and Humanities, National University of Computer and Emerging Sciences, B-block, Faisal Town, Lahore, Pakistan*

a.albalahi@uoh.edu.sa, zhibindu@126.com, akhlaq.ahmad@nu.edu.pk, boaljod2@hotmail.com, akbarali.maths@gmail.com

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Abstract

A molecular tree is defined as a tree in which no vertex has degree exceeding 4. Consider such a tree T with edge set E. For each vertex u in T, let $d(u)$ represent its degree. In this paper, we study a class of molecular descriptors defined by $\mathscr{B}_f(T) = \sum_{uv\in E} f(d(u), d(v))$, where f is a symmetric real-valued function that depends on the degrees of adjacent vertices in T. The primary aim of this work is to identify those graphs, in the class of all molecular trees of a given order and admitting a perfect matching, that attain extremum (i.e., minimum or maximum) values of the index $\mathscr{B}_f$, under certain assumptions imposed on the function f. As an application of one of the main results, graphs that maximize the Sombor index and Euler–Sombor index (along with their reduced versions) as well as the

*Corresponding author.

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reciprocal sum-connectivity index, cubic Sombor index and Platt–Sombor index are characterized over the aforementioned class of molecular trees.

1 Introduction

This study is exclusively concerned with a special class of graphs; namely, trees. Unless otherwise specified, the graph-theoretical terminology used herein follows standard conventions as found in common books on graph theory such as [8, 9, 14]. Terminology specific to chemical graph theory is adopted in accordance with standard references including [24, 26].

Within the field of chemical graph theory, particular attention is given to a class of molecular descriptors known as topological indices [24, 26]. These are real-valued functions defined on graphs that are invariant under graph isomorphism; in other words, they depend solely on the abstract structure of the graph and not on any specific vertex labeling or drawing. Topological indices serve as compact mathematical encodings of molecular structures, and have been widely used to correlate structural features of chemical compounds with a variety of physicochemical properties [11].

This paper focuses on a subclass of topological indices defined through vertex degrees. Given a graph G with edge set $E(G)$, we consider indices of the following form [18]:

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

where $d(u)$ denotes the degree of the vertex u in G, and f is a real-valued symmetric function defined on degrees of adjacent vertices. When context requires, the degree will be denoted by $d_G(u)$ to emphasize the underlying graph. Expressions of the form (1) are commonly referred to as bond incident degree (BID) indices [6,23,27], a terminology first proposed in [25]. The study of BID indices remains an active area of research, with numerous recent contributions such as [12, 13, 21, 30].

A molecular tree is a tree in which no vertex has degree greater than 4. The main objective of the present work is to investigate extremal properties

of BID indices within the class of molecular trees of fixed order that admit perfect matchings. Specifically, the primary goal of the present paper is to characterize those trees that minimize or maximize $\mathscr{B}_f$, under certain conditions imposed on the function f. These conditions concerning f are satisfied by several well-known indices; for instance, see Remark 1. This paper extends the recent study [1]. Since none of the main results of [1] is applicable to any of the indices listed in Table 1, this limitation serves as a motivation for the present study. In the applications of the main results, the constraints on the function f are verified using the symbolic computation software Mathematica.

2 Results

Before presenting the results of this paper, we first recall some foundational definitions and concepts.

Let G be a graph with vertex set $V(G)$. We say that G is an n-order graph if $|V(G)| = n$. For any vertex $w \in V(G)$, denote by $N_G(w)$ the set of all those vertices in G that are adjacent to w. Each vertex $w' \in N_G(w)$ is called a neighbor of w. A vertex of degree one is referred to as a pendent vertex. The complement of G, denoted by $\overline{G}$, is the graph with vertex set $V(\overline{G}) = V(G)$ and edge set $E(\overline{G}) = \{uv : \ u \neq v \text{ and } uv \notin E(G)\}$. Let $A \subseteq E(G)$ and $B \subseteq E(\overline{G})$. We define $G - A + B$ to be the graph obtained from G by deleting all edges in A and adding all edges in B. If A or B is a singleton, we write its unique element instead of the corresponding set. For example, if $A = \{uv\}$ and $B = \{xy\}$, then we write $G - uv + xy$ instead of $G - A + B$.

Now, we state and prove our first lemma.

Lemma 1. *Let $\mathscr{B}_f$ be a BID index such that f satisfies the conditions given below.*

(i). The inequality $f(x+1, \eta_1) - f(x+1, \eta_2) < f(x, \eta_1) - f(x, \eta_2)$ holds for all $x, \eta_1, \eta_2 \in \{1, 2, 3, 4\}$ provided that $x \leq 3$ and $\eta_2 < \eta_1$.

(ii). It holds that

$$\max\{f(4,3)-f(4,4)+f(2,3)-f(2,2), f(3,3)-f(2,4)\} \\ +3[f(4,3)-f(4,4)]+f(1,3)-f(1,2)<0. \tag{2}$$

If a graph G maximizes $\mathscr{B}_f$ among all molecular n-order trees with perfect matching, then G possesses at most one vertex of degree 3.

Proof. Let M be the unique perfect matching of G. Suppose, for the sake of contradiction, that G contains at least two vertices of degree 3. Let $u, v \in V(G)$ such that $d_G(u) = d_G(v) = 3$. Take $N_G(u) = \{u_1, u_2, u_3\}$ and $N_G(v) = \{v_1, v_2, v_3\}$. Without loss of generality, suppose that u_3 and v_3 lie on the path connecting the vertices u and v, and that $vv_1 \notin M$, and that $d_G(u_1) \geq d_G(u_2)$. Then, we have $\min\{d_G(u_1), d_G(u_3)\} \geq 2$ and $\min\{d_G(v_1), d_G(v_3)\} \geq 2$. Let $G' := G - vv_1 + v_1u$. Then, M remains the perfect matching of G'.

Case 1. $uv \notin E(G)$.
From condition (i), it follows that

$$\sum_{i=2}^{3}[f(d_G(v_i),3)-f(d_G(v_i),2)] \leq f(1,3)-f(1,2)+f(2,3)-f(2,2),$$

and hence, by using condition (i) and inequality (2), (whether v_3 and u_3 coincide or not, in either of the cases) we have

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

a contradiction.

Case 2. $uv \in E(G)$.
Here, $(u_3, v_3) = (v, u)$. Due to condition (i) and inequality (2), we obtain

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

a contradiction. ■

The proof of the following lemma is analogous to that of Lemma 1 and is therefore omitted.

Lemma 2. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given below.*

(i). The inequality $f(x+1,\eta_1) - f(x+1,\eta_2) > f(x,\eta_1) - f(x,\eta_2)$ holds for all $x, \eta_1, \eta_2 \in \{1,2,3,4\}$ provided that $x \leq 3$ and $\eta_2 < \eta_1$.

(ii). For every $c \in \{1,2,3,4\}$,

$$\begin{aligned}\min\{&f(4,3) - f(4,4) + f(2,3) - f(2,2), f(3,3) - f(2,4)\} \\ &+3[f(4,3) - f(4,4)] + f(1,3) - f(1,2) > 0.\end{aligned}$$

If a graph G minimizes $\mathscr{B}_f$ among all molecular n-order trees with perfect matching, then G possesses at most one vertex of degree 3.

Lemma 3. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given in Lemma 1. Also, for each $c \in \{2,3\}$, assume that*

$$(c-1)[f(c,4) - f(c+1,4)] + f(c,2) - f(c+1,1) - f(c+1,4) + f(4,2) < 0 \quad (5)$$

and

$$c[f(c,4)-f(c+1,4)]-f(c+1,1)+f(4,2)+f(1,2)-f(1,4)<0. \quad (6)$$

If a graph G maximizes $\mathscr{B}_f$ among all molecular n-order trees with perfect matching M, then every $ts \in M$ satisfies $\min\{d_G(t), d_G(s)\} = 1$.

Proof. For the sake of contradiction, assume that there exists $uv \in M$ such that $\min\{d_G(u), d_G(v)\} \geq 2$. We may, without loss of generality, suppose that $d_G(u) \geq d_G(v)$.

Case 1. $d_G(u) \in \{2, 3\}$.
Lemma 1 assures $d_G(v) = 2$. Let $N_G(v) = \{u, v_1\}$, $N_G(u) \setminus \{v\} := \{u_1\}$ when $d_G(u) = 2$, and $N_G(u) \setminus \{v\} := \{u_1, u_2\}$ when $d_G(u) = 3$. Since no edge adjacent to uv belongs to M, we have $\min\{d_G(u_i), d_G(v_1)\} \geq 2$ for any $u_i \in N_G(u) \setminus \{v\}$. Let $G' := G - v_1v + v_1u$. Then, M remains the perfect matching of the graph G'. Now, because of condition (i) of Lemma 1 and (5), we obtain

$$\begin{aligned}\mathscr{B}_f(G) - \mathscr{B}_f(G') = &\sum_{i=1}^{d_G(u)-1} [f(d_G(u), d_G(u_i)) - f(d_G(u)+1, d_G(u_i))] \\ &+ f(d_G(u), 2) - f(d_G(u)+1, 1) \\ &+ f(d_G(v_1), 2) - f(d_G(v_1), d_G(u)+1) \qquad (7) \\ \leq\ & (d_G(u)-1)[f(d_G(u), 4) - f(d_G(u)+1, 4)] \\ &+ f(d_G(u), 2) - f(d_G(u)+1, 1) \\ &+ f(4, 2) - f(4, d_G(u)+1) < 0,\end{aligned}$$

a contradiction.

Case 2. $d_G(u) = 4$.
Let $u' \in N_G(u) \setminus \{v\}$. Consider all paths that originate at u and contain u', and let P be a longest such path. Then, the endvertex of P different from u must be a pendent vertex, which we denote by z. Let $N_G(z) = \{y\}$. By the definition of P and because of the fact that each vertex of G has no more than one pendent neighbor, it follows that $d_G(y) = 2$. Let $N_G(y) = \{y', z\}$.

Case 2.1. $d_G(v) \in \{2, 3\}$.
Let $G'' := G - \{v_i v : v_i \in N_G(v) \setminus \{u\}\} + \{v_i y : v_i \in N_G(v) \setminus \{u\}\}$. Then, M remains the perfect matching of G''. Because of condition (i) of Lemma 1 and (6), it follows that

$$\begin{aligned}\mathscr{B}_f(G) - \mathscr{B}_f(G'') = &\sum_{i=1}^{d_G(v)-1} [f(d_G(v), d_G(v_i)) - f(d_G(v)+1, d_G(v_i))] \\ &+ f(d_G(y'), 2) - f(d_G(y'), d_G(v)+1) \\ &+ f(d_G(v), 4) - f(d_G(v)+1, 1) \\ &+ f(1,2) - f(1,4) \qquad (8) \\ \leq\ &(d_G(v)-1)[f(d_G(v), 4) - f(d_G(v)+1, 4)] \\ &+ f(4,2) - f(4, d_G(v)+1) \\ &+ f(d_G(v), 4) - f(d_G(v)+1, 1) + f(1,2) - f(1,4) < 0,\end{aligned}$$

which is a contradiction.

Case 2.2. $d_G(v) = 4$.
Let $G''' := G - \{v_i v : v_i \in N_G(v) \setminus \{u\}\} + \{v_i z : v_i \in N_G(v) \setminus \{u\}\}$. Then, M remains the perfect matching of G'''. Due to condition (i) of Lemma 1, we obtain

$$\mathscr{B}_f(G) - \mathscr{B}_f(G''') = f(4,4) - f(1,4) - [f(4,2) - f(1,2)] < 0, \qquad (9)$$

a contradiction. ■

The proof of the following result proceeds along the same lines as that of Lemma 3 and is thus omitted.

Lemma 4. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given in Lemma 2. Also, for each $c \in \{2, 3\}$, assume that*

$$(c-1)[f(c,4) - f(c+1,4)] + f(c,2) - f(c+1,1) - f(c+1,4) + f(4,2) > 0 \quad (10)$$

and

$$c[f(c,4) - f(c+1,4)] - f(c+1,1) + f(4,2) + f(1,2) - f(1,4) > 0. \quad (11)$$

If a graph G minimizes $\mathscr{B}_f$ among all molecular n-order trees with perfect matching M, then every $ts \in M$ satisfies $\min\{d_G(t), d_G(s)\} = 1$.

Lemma 5. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given in Lemma 1. Also, assume that* (5) *and* (6) *hold. If G is a tree that maximizes $\mathscr{B}_f$ among all molecular n-order trees with perfect matching, then G does not contain any vertex of degree* 2 *with both non-pendent neighbors, where $n \geq 8$.*

Proof. Suppose, for contradiction, that there exists a vertex $v \in V(G)$ with $d_G(v) = 2$ such that both its neighbors, denoted by v' and v'', are non-pendent. By Lemma 3, the edges vv' and vv'' are not contained in the perfect matching of G. It follows that v is not covered by the perfect matching, contradicting the fact that G has perfect matching. ■

The proof of the following lemma is considerably similar to that of Lemma 5 and is therefore omitted.

Lemma 6. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given in Lemma 2. Also, assume that inequalities* (10) *and* (11) *hold. If G is a tree that minimizes $\mathscr{B}_f$ among all molecular n-order trees with perfect matching, then G does not contain any vertex of degree* 2 *with both non-pendent neighbors, where $n \geq 8$.*

For a graph G, let n_i represent the number of those vertices of G that have degree i, and let $m_{i,j}$ represent the number of those edges of G whose one endvertex has degree i and the other endvertex has degree j.

We note that there is only one molecular 4-order tree with perfect matching, namely the path graph P_4. Also, we observe that there are only two non-isomorphic molecular 6-order trees with perfect matching, namely the path graph P_6 and the graph obtained from the 4-order star graph S_4 by subdividing its two edges. Thus, in the following, we consider trees of order at least 8.

Theorem 1. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given in Lemma 1. Also, assume that inequalities* (5) *and* (6) *hold. If T is a molecular n-order tree with perfect matching, where $n \geq 8$, then*

$$\mathscr{B}_f(T) \leq \begin{cases} [f(1,2)+f(2,4)]\left(\frac{n+4}{4}\right) & \\ +f(1,4)\left(\frac{n-4}{4}\right)+f(4,4)\left(\frac{n-8}{4}\right) & \text{if } n \equiv 0 \ (mod\ 4), \\ 3f(1,2)+2f(2,4)+f(1,4) & \\ +f(1,3)+f(2,3)+f(3,4) & \text{if } n = 10, \\ [f(1,2)+f(2,4)]\left(\frac{n+2}{4}\right)+f(1,4)\left(\frac{n-6}{4}\right) & \\ +f(4,4)\left(\frac{n-14}{4}\right)+f(1,3)+2f(3,4) & \text{otherwise.} \end{cases}$$

For $n \equiv 0 \ (mod\ 4)$, the equality holds if and only if

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

and $m_{i,j} = 0$ for the rest of the values of i and j; for example, see Figure 1. For $n = 10$, the equality holds if and only if T is isomorphic to the 10*-vertex tree shown in Figure 1. For $n \equiv 2 \ (mod\ 4)$ with $n \geq 14$, the equality holds if and only if*

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

and $m_{i,j} = 0$ for the rest of the values of i and j; for example, see Figure 1.

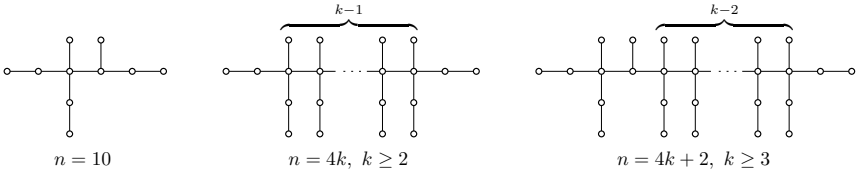

Figure 1. Examples of extremal trees characterized in Theorem 1.

Proof. Among all molecular n-order trees with perfect matching, let G be

a graph maximizing $\mathscr{B}_f$, provided that $n \geq 8$. Then,

$$\sum_{i=1}^{4} n_i = n \tag{12}$$

$$\sum_{i=1}^{4} i n_i = 2(n-1) \tag{13}$$

$$\sum_{i=2}^{4} m_{1,i} = n_1 \tag{14}$$

$$\sum_{i=1}^{4} m_{i,j} + m_{j,j} = j n_j, \quad j = 2, 3, 4. \tag{15}$$

If $m_{2,2} \neq 0$, then by Lemma 3, any edge $xy \in E(G)$ connecting vertices of degrees 2 must not belong to the perfect matching of G, and hence each of x and y must have a pendent neighbor, which contradicts $n \geq 8$. Thus,

$$m_{2,2} = 0. \tag{16}$$

From Lemma 1, it follows that

$$n_3 \leq 1. \tag{17}$$

Also, Lemma 3 guaranties

$$n = 2n_1. \tag{18}$$

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

In the present case, we have $n = 4k$ for some integer $k \geq 2$. If $n_3 = 1$, then (18) yields $n_1 + n_3 = 2k + 1$, which is a contradiction to the well-known fact that vertices of odd degree occur in an even number in a graph. Hence, (17) implies that

$$n_3 = 0, \tag{19}$$

and therefore by Lemma 5 and (16), we obtain $m_{2,4} = m_{1,2} = n_2$. From (12), (13), (18) and (19), it follws that $(n_2, n_4) = (k+1, k-1)$. Thus, $m_{1,2} = k + 1 = m_{2,4}$. Consequently, using (14) and (15), we have that

$m_{1,4} = k-1$ and $m_{4,4} = k-2$. Hence,

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

Case 2. $n \equiv 2 \pmod 4$.
In the present case, we have $n = 4k+2$ for some integer $k \geq 2$. The choice $n_3 = 0$, due to (18), yields a contradiction to the fact that vertices of odd degree occur in an even number in a graph. Hence, (17) gives

$$n_3 = 1. \tag{20}$$

From (12), (13), (18) and (20), it follows that $(n_2, n_4) = (k+1, k-1)$.

Let $v \in V(G)$ be the vertex with degree 3. Take $N_G(v) = \{v_1, v_2, v_3\}$ such that $d_G(v_1) \leq d_G(v_2) \leq d_G(v_3)$. Then, by (20), $d_G(v_i) \neq 3$ for every $i \in \{1,2,3\}$. Also, from Lemma 3, it follows that $d_G(v_1) = 1 < d_G(v_2)$. Hence, $(d_G(v_2), d_G(v_3)) \in \{(2,2),(2,4),(4,4)\}$. If $(d_G(v_2), d_G(v_3)) = (2, 2)$, then by Lemma 3 we have $n = 6$, a contradiction because $n \geq 8$. Thus, $(d_G(v_2), d_G(v_3)) \in \{(2,4),(4,4)\}$.

Case 2.1. $(d_G(v_2), d_G(v_3)) = (2,4)$.
Here, $m_{1,3} = m_{2,3} = m_{3,4} = 1$, and therefore, by Lemma 5 and (16), we obtain $m_{2,4} + 1 = m_{1,2} = k+1 = n_2$. Consequently, using (14) and (15), we obtain $m_{1,4} = k-1$ and $m_{4,4} = k-2$. Therefore,

$$\begin{aligned}\mathscr{B}_f(G) &= f(2,4)\,k + f(1,2)\,(k+1) + f(4,4)\,(k-2) + f(1,4)\,(k-1) \\ &\quad + f(1,3) + f(3,4) + f(2,3) \\ &:= \Theta_1. \end{aligned} \tag{21}$$

Case 2.2. $(d_G(v_2), d_G(v_3)) = (4,4)$.
Here, it holds that $k \geq 3$ and $m_{2,3} = 0,\ m_{1,3} = 1,\ m_{3,4} = 2$, and thus, by using Lemma 5 and (16), we obtain $m_{2,4} = k+1 = m_{1,2} = n_2$. Hence,

using (14) and (15), we obtain $m_{1,4} = k-1$ and $m_{4,4} = k-3$. Thus,

$$\begin{aligned}\mathscr{B}_f(G) &= f(1,4)\,(k-1) + [f(1,2) + f(2,4)](k+1) + f(4,4)\,(k-3) \\ &\quad + 2f(3,4) + f(1,3) \\ &:= \Theta_2. \end{aligned} \tag{22}$$

From (21) and (22), it follows that

$$\Theta_1 - \Theta_2 = f(4,4) - f(2,4) - [f(4,3) - f(2,3)] < 0,$$

by condition (i) of Lemma 1. Consequently, for $n \equiv 2 \pmod 4$ with $n \geq 14$, we have

$$\begin{aligned}\mathscr{B}_f(G) &= \Theta_2 \\ &= [f(1,2) + f(2,4)] \left(\frac{n+2}{4}\right) + f(1,4) \left(\frac{n-6}{4}\right) + f(4,4) \left(\frac{n-14}{4}\right) \\ &\quad + f(1,3) + 2f(3,4).\end{aligned}$$

Also, for $n = 10$, we have $\mathscr{B}_f(G) = \Theta_1$. ■

Remark 1. Since each of the functions associated with the indices listed in Table 1 satisfies all the conditions imposed on f in Theorem 1, the conclusion of this theorem is directly applicable to all these indices.

The proof of the following theorem is omitted, as it follows almost the same reasoning as the proof of Theorem 1.

Theorem 2. *Let $\mathscr{B}_f$ be a BID index such that f meets the conditions given in Lemma 2. Also, assume that inequalities* (10) *and* (11) *hold. If T is a molecular n-order tree with perfect matching with $n \geq 8$, then the upper bound for $\mathscr{B}_f(T)$ given in Theorem 1 becomes a lower bound of $\mathscr{B}_f(T)$, while the characterization of equality remains unchanged.*

3 Concluding remarks

We note that Equation (1) yields the augmented Sombor (ASO) index [10] or the reciprocal augmented Sombor (RASO) index [10] for the choice

Table 1. Selected indices encompassed by Theorem 1. Here, we used the notations $d'(v) := d(v) - 1$ and $d'(u) := d(u) - 1$.

$f(d(v), d(u))$	Equation (1) yields
$\sqrt{d(v) + d(u)}$	reciprocal sum-connectivity index [7]
$\sqrt{(d(v))^2 + (d(u))^2}$	Sombor index [15, 20]
$\sqrt{(d'(v))^2 + (d'(u))^2}$	reduced Sombor index [15]
$\sqrt{(d(v))^2 + (d(u))^2 + d(v)d(u)}$	Euler–Sombor index [16, 22]
$\sqrt{(d'(v))^2 + (d'(u))^2 + (d'(v))(d'(u))}$	reduced Euler–Sombor index [4]
$\sqrt{(d(v))^3 + (d(u))^3}$	cubic Sombor index [3, 17, 19, 28]
$(d(v) + d(u))^{-1/2} \left[(d(v))^2 + (d(u))^2\right]$	contraharmonic root-sum index
$\sqrt{(d(v))^2 + (d(u))^2 + d(v) + d(u)}$	Platt–Sombor index [3]

$f(d(v), d(u)) = [d(v) + d(u) - 2]^{-1/2}\sqrt{(d(v))^2 + (d(u))^2}$ or $f(d(v), d(u)) = [(d(v))^2 + (d(u))^2]^{-1/2}\sqrt{d(v) + d(u) - 2}$, respectively.

We observe that condition (i) of Lemma 2 does not hold for the function associated with the RASO index. Consequently, Theorem 2 does not cover the RASO index. Nevertheless, based on a computer-assisted search, we observed that the graphs minimizing the RASO index over the class of all n-order molecular trees possessing perfect matching, for $n \geq 8$, appear to coincide with the extremal graphs characterized in Theorem 2. This observation led us to conjecture that the extremal graphs in Theorem 2 remain optimal for the RASO index despite the failure of condition (i) in Lemma 2. (The validity of this conjecture follows from Theorem 3 because the reverse strict forms of (23)–(27) hold for the function associated with the RASO index.) This phenomenon suggests that the assumptions imposed in Theorems 1 and 2 may be stronger than necessary. Motivated by this observation, we reinvestigated the hypotheses of Theorems 1 and 2 with the aim of identifying weaker conditions that still preserve the same conclusions; in particular, our goal was to formulate assumptions broad enough to include a wider family of BID indices. As a result, we are able

to relax the conditions of Theorems 1 and 2 without altering the conclusions of these theorems.

Let A (A', respectively) denote the collection of conditions appearing in Theorem 1 (Theorem 2, respectively). Also, let B (B', respectively) denote the collection of the following conditions (reverse strict forms of the following conditions, respectively):

$$\sum_{i=1}^{2}[f(a_i,3)-f(a_i,2)]+\sum_{i=1}^{4}[f(b_i,3)-f(b_i,4)]<0, \tag{23}$$

$$\sum_{i=1}^{3}[f(b_i,3)-f(b_i,4))]+f(a_1,3)-f(a_1,2)+f(3,3)-f(2,4)<0, \tag{24}$$

$$\sum_{i=2}^{s}[f(\omega,b_i)-f(\omega+1,b_i)]+f(\omega,2)-f(\omega+1,1)$$
$$+f(b_4,2)-f(b_4,\omega+1)<0, \tag{25}$$

$$\sum_{i=2}^{s}[f(\omega,b_i)-f(\omega+1,b_i)]+f(\omega,4)-f(\omega+1,1)$$
$$+f(b_4,2)-f(b_4,\omega+1)+f(1,2)-f(1,4)<0, \tag{26}$$

$$f(4,4)-f(1,4)-f(4,2)+f(1,2)<0, \tag{27}$$

for all $a_1,b_1\in\{1,2,3,4\}$, $a_2,b_2,b_3,b_4\in\{2,3,4\}$ and $s,\omega\in\{2,3\}$.

We observe that if all conditions in A hold, then each condition in B also holds (due to (3), (4), (7), (8) and (9)); however, the converse is not true in general because the function associated with the ASO index does not satisfy condition (i) of Lemma 1 and this function satisfies every condition in B. Similarly, if all conditions in A' hold, then each condition in B' also holds; but, the converse is not true in general because of the function associated with the RASO index. Fortunately, all conditions in B and B' may still be checked for validity with the aid of a computer for any BID index $\mathscr{B}_f$. Based on these observations, we have the following result.

Theorem 3. *Let $\mathscr{B}_f$ be a BID index such that f satisfies* (23)–(26) *(the reverse strict forms of* (23)–(26)*, respectively). Let T be an n-order molecular tree with perfect matching such that $n \geq 8$.*

(a). *If $n \equiv 0 \pmod 4$, then the conclusion of Theorem 1 (Theorem 2, respectively), concerning the case $n \equiv 0 \pmod 4$, remains true.*

(b). *Assume that $n \equiv 2 \pmod 4$.*

(i). *If* (27) *(reverse strict form of* (27)*, respectively) holds, then the conclusion of Theorem 1 (Theorem 2, respectively), corresponding to the case $n \equiv 2 \pmod 4$, remains true.*

(ii). *When the reverse strict form of* (27) *holds (*(27) *holds, respectively), then $\mathscr{B}_f(T) \leq \Theta_1$ ($\mathscr{B}_f(T) \geq \Theta_1$, respectively) with equality if and only if $m_{1,3} = m_{2,3} = m_{3,4} = 1$, $m_{2,4} + 1 = m_{1,2} = k + 1$, $m_{1,4} = k - 1$, $m_{4,4} = k - 2$ and $m_{i,j} = 0$ for all other possibilities, where Θ_1 is given in* (21) *and $k = (n-2)/4$. An example of trees satisfying $\mathscr{B}_f(T) = \Theta_1$ is given in Figure 2.*

(iii). *When the left-hand side of* (27) *is equal to zero, then $\mathscr{B}_f(T) \leq \Theta_1$ ($\mathscr{B}_f(T) \geq \Theta_1$, respectively) with equality if and only if all $m_{i,j}$ satisfy either the equality conditions given in Theorem 1 for the cases other than $n \equiv 0 \pmod 4$ or the equality conditions given in part (ii) of the present theorem.*

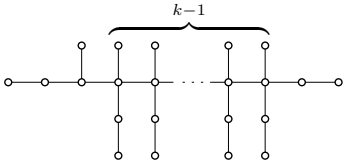

Figure 2. Example of extremal trees characterized in Theorem 3(b)(ii).

Proof. The proof is analogous to that of Theorem 1. For instance, if each of (23)–(27) holds, then each of the two expressions for $\mathscr{B}_f(G) - \mathscr{B}_f(G')$ given in (3) and (4) is negative due to (23) and (24), respectively, whereas the expressions for $\mathscr{B}_f(G) - \mathscr{B}_f(G')$, $\mathscr{B}_f(G) - \mathscr{B}_f(G'')$, $\mathscr{B}_f(G) - \mathscr{B}_f(G''')$

given in (7), (8), (9), respectively, are negative due to (25), (26), (27), respectively. ■

Although Theorem 1 (Theorem 2, respectively) is not applicable to the ASO index (RASO index, respectively), each of the inequalities (23)–(27) (the reverse strict forms of (23)–(27), respectively) holds for the function associated with the ASO index (RASO index, respectively), and therefore, Theorem 3 covers the ASO and RASO indices; the corresponding problem regarding the ASO index has recently been addressed in [29].

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