

Article

On Bond Incident Degree Indices of Chemical Graphs

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Abstract: By swapping out atoms for vertices and bonds for edges, a graph may be used to model any molecular structure. A graph G is considered to be a chemical graph in graph theory if no vertex of G has a degree of 5 or greater. The bond incident degree (BID) index for a chemical graph G is defined as the total of contributions $f(d_G(u), d_G(v))$ from all edges uv of G , where $d_G(w)$ stands for the degree of a vertex w of G , $E(G)$ is the set of edges of G , and f is a real-valued symmetric function. This paper addresses the problem of finding graphs with extremum BID indices over the class of all chemical graphs of a fixed number of edges and vertices.

Keywords: molecular descriptors; topological indices; bond incident degree indices; extremal problem; chemical graph theory

MSC: 05C07; 05C09; 05C92



Citation: Albalahi, A.M.; Ali, A.; Du, Z.; Bhatti, A.A.; Alraqad, T.; Iqbal, N.; Hamza, A.E. On Bond Incident Degree Indices of Chemical Graphs. *Mathematics* **2023**, *11*, 27. <https://doi.org/10.3390/math11010027>

Academic Editor: Andrea Scozzari

Received: 13 November 2022

Revised: 8 December 2022

Accepted: 15 December 2022

Published: 21 December 2022



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1. Introduction

Every molecular structure can be viewed as a graph, usually referred to as a chemical graph, in which vertices correspond to atoms and edges represent bonds of the considered compound [1]. In graph-theoretical notion, a graph in which no vertex has a degree of 5 or greater is referred to as a chemical graph [2]. Chemical graph theory [1,2], the part of graph theory having some chemical applications, provides useful tools in QSAR and QSPR research [3]. Such tools include topological indices [4,5]; a topological index of a chemical graph is a number that remains unchanged under graph isomorphism. Various existing well-known topological indices are defined via edge contributions of the considered chemical graph [6], and many of them have the following form:

$$BID(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)),$$

where $d_G(w)$ represents the degree of a vertex $w \in V(G)$ of a graph G , $E(G)$ is the set of edges of G , and f is a real-valued symmetric function. These indices are named as bond incident degree indices [7,8] (for short, BID indices [8]); it is this class of topological indices with which we deal in this paper. Details regarding some of the existing properties of BID indices can be found in [9–14]. For some particular BID indices, we refer the reader to [15–18] (see also [19,20], where a novel BID index has been studied).

In the rest of this paper, by a graph we mean a connected, finite, simple, and undirected graph. We use (chemical) graph-theoretical notation and terminology from standard books, such as [1,2,21,22].

2. Statements of Main Results

Let $n_i(G)$ be the number of those vertices of a graph G that have degree i . Denote by $m_{i,j}(G)$ the number of those edges of a graph G whose end vertices have degrees i and j . In the remainder of this paper, for the sake of simplicity, we drop “ (G) ” from the notations $n_i(G)$ and $m_{i,j}(G)$.

For a graph G , its *BID* indices can be defined as

$$BID(G) = \sum_{\delta(G) \leq i \leq j \leq \Delta(G)} m_{i,j}(G) \cdot \beta_{i,j}, \quad (1)$$

where $\beta_{i,j}$ is a non-negative real-valued (symmetric) function depending on i and j , $\delta(G)$ is the minimum degree of G , and $\Delta(G)$ is the maximum degree of G .

If G is a chemical graph of order $n \geq 5$ and size m , then the following equations hold:

$$\sum_{i=1}^4 n_i = n, \quad (2)$$

$$\sum_{i=1}^4 i \cdot n_i = 2m, \quad (3)$$

$$\sum_{\substack{1 \leq i \leq 4 \\ i \neq j}} m_{j,i} + 2m_{j,j} = j \cdot n_j, \quad (4)$$

where $j = 1, 2, 3, 4$. The following values of $m_{1,4}$ and $m_{4,4}$ are obtained (see also [23]) from Equations (2)–(4):

$$m_{1,4} = \frac{4n}{3} - \frac{2m}{3} - \frac{10}{9}m_{1,3} - \frac{4}{3}m_{1,2} - \frac{2}{3}m_{2,2} - \frac{1}{3}m_{2,4} - \frac{4}{9}m_{2,3} - \frac{1}{9}m_{3,4} - \frac{2}{9}m_{3,3}, \quad (5)$$

$$m_{4,4} = -\frac{4n}{3} + \frac{5m}{3} + \frac{1}{9}m_{1,3} + \frac{1}{3}m_{1,2} - \frac{1}{3}m_{2,2} - \frac{2}{3}m_{2,4} - \frac{5}{9}m_{2,3} - \frac{8}{9}m_{3,4} - \frac{7}{9}m_{3,3}. \quad (6)$$

Using Equations (5) and (6) in Equation (1), we obtain

$$BID(G) = \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + m_{1,2}B_{1,2} + m_{1,3}B_{1,3} + m_{2,2}B_{2,2} + m_{2,3}B_{2,3} + m_{2,4}B_{2,4} + m_{3,3}B_{3,3} + m_{3,4}B_{3,4}, \quad (7)$$

where

$$B_{1,2} = \beta_{1,2} - \frac{4}{3}\beta_{1,4} + \frac{1}{3}\beta_{4,4}, \quad B_{1,3} = \beta_{1,3} - \frac{10}{9}\beta_{1,4} + \frac{1}{9}\beta_{4,4},$$

$$B_{2,2} = \beta_{2,2} - \frac{2}{3}\beta_{1,4} - \frac{1}{3}\beta_{4,4}, \quad B_{2,3} = \beta_{2,3} - \frac{4}{9}\beta_{1,4} - \frac{5}{9}\beta_{4,4},$$

$$B_{2,4} = \beta_{2,4} - \frac{1}{3}\beta_{1,4} - \frac{2}{3}\beta_{4,4}, \quad B_{3,3} = \beta_{3,3} - \frac{2}{9}\beta_{1,4} - \frac{7}{9}\beta_{4,4},$$

$$B_{3,4} = \beta_{3,4} - \frac{1}{9}\beta_{1,4} - \frac{8}{9}\beta_{4,4}.$$

The substitution

$$\Gamma_{BID}(G) = m_{1,2}B_{1,2} + m_{1,3}B_{1,3} + m_{2,2}B_{2,2} + m_{2,3}B_{2,3} + m_{2,4}B_{2,4} + m_{3,3}B_{3,3} + m_{3,4}B_{3,4} \quad (8)$$

in Equation (7) gives

$$BID(G) = \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + \Gamma_{BID}(G). \quad (9)$$

Theorem 1. Let G be a chemical graph of order n and size m such that $n - 1 \leq m \leq 2n$ and $n \geq 13$. Consider Equation (1) and let $\beta_{i,j}$ be a given function. Additionally, consider $B_{i,j}$ defined in Equation (7). Let all $B_{i,j}$ be positive, and let the following inequalities hold:

$$\min\{6B_{3,4}, 3B_{3,3}, B_{2,3} + B_{3,4}, B_{3,3} + B_{3,4}, 2B_{1,2}, B_{2,2} + B_{2,4}, 2B_{2,3}\} > 2B_{2,4},$$

$$\min\{3B_{1,3}, 4B_{2,4}, 2B_{2,2}, B_{2,2} + B_{2,4}, 2B_{2,3}, B_{2,3} + B_{2,4}, B_{3,3} + B_{3,4}\} > 3B_{3,4}.$$

(i) If $n + m \equiv 0 \pmod{3}$, then

$$BID(G) \geq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 4\}$.

(ii) If $n + m \equiv 1 \pmod{3}$, then

$$BID(G) \geq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + 3B_{3,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 3, 4\}$ and G has only one vertex of degree 3, which has neighbors of degree 4 only.

(iii) If $n + m \equiv 2 \pmod{3}$, then

$$BID(G) \geq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + 2B_{2,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 2, 4\}$ and G has only one vertex of degree 2, which has neighbors of degree 4 only.

Remark 1. If we take $\beta_{i,j} = 2\sqrt{ij}(i+j)^{-1}$, $\beta_{i,j} = 2(i+j)^{-1}$, or $\beta_{i,j} = (i+j)^{-1/2}$ in Equation (1), we obtain the harmonic index, the geometric-arithmetic index, or the sum-connectivity index, respectively. After elementary calculations, one deduces that for each of the aforementioned choices of $\beta_{i,j}$, all the conditions of Theorem 1 concerning $B_{i,j}$ are satisfied. Thus, if BID is any of the aforementioned three indices, then the conclusion of Theorem 1 holds.

Theorem 2. Let G be a chemical graph of size m and order n such that $n - 1 \leq m \leq 2n$ and $n \geq 13$. Consider Equation (1) and let $\beta_{i,j}$ be a given function. Additionally, consider $B_{i,j}$ defined in Equation (7). Let all $B_{i,j}$ be negative and the following inequalities hold:

$$\max\{6B_{3,4}, 3B_{3,3}, B_{2,3} + B_{3,4}, B_{3,3} + B_{3,4}, 2B_{1,2}, B_{2,2} + B_{2,4}, 2B_{2,3}\} < 2B_{2,4}$$

and

$$\max\{3B_{1,3}, 4B_{2,4}, 2B_{2,2}, B_{2,2} + B_{2,4}, 2B_{2,3}, B_{2,3} + B_{2,4}, B_{3,3} + B_{3,4}\} < 3B_{3,4}.$$

(i) If $n + m \equiv 0 \pmod{3}$, then

$$BID(G) \leq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m,$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 4\}$.

(ii) If $n + m \equiv 1 \pmod{3}$, then

$$BID(G) \leq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + 3B_{3,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 3, 4\}$ and G has only one vertex of degree 3, which has neighbors of degree 4 only.

(iii) If $n + m \equiv 2 \pmod{3}$, then

$$BID(G) \leq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + 2B_{2,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 2, 4\}$ and G has only one vertex of degree 2, which has neighbors of degree 4 only.

Remark 2. If we take $\beta_{i,j} = i(j)^{-1} + j(i)^{-1}$, $\beta_{i,j} = \sqrt{i^2 + j^2}$, $\beta_{i,j} = \sqrt{(i-1)^2 + (j-1)^2}$, $\beta_{i,j} = (i+j)(4ij)^{-1/2}$, $\beta_{i,j} = (i+j)(4ij)^{-1/2} - 2\sqrt{ij}(i+j)^{-1}$, $\beta_{i,j} = \ln(i+j)$, or $\beta_{i,j} = 1 - 2(i+j)^{-1/2}$ in Equation (1), we obtain the symmetric division deg index, the Sombor index, the reduced Sombor index, the arithmetic-geometric index, the difference between arithmetic-geometric index and geometric-arithmetic index, the natural logarithm of the multiplicative sum Zagreb index, or the atom-bond sum-connectivity index, respectively. After elementary calculations, one deduces that for each of the aforementioned choices of $\beta_{i,j}$, all the conditions of Theorem 2 concerning $B_{i,j}$ are satisfied, and hence if BID is any of these graph invariants, then the conclusion of Theorem 2 holds.

Example 1. Let us consider the class $\mathcal{T}$ of graphs representing all octane isomers. Certainly, the class $\mathcal{T}$ consists of 18 chemical graphs, each having 8 vertices and 7 edges. Note that there is only one graph in $\mathcal{T}$ having the degree set $\{1, 4\}$, and that graph corresponds to the chemical compound 2,2,3,3-tetramethylbutane. As indicated in Remark 2, the conclusion of Theorem 2 holds also for the atom-bond sum-connectivity (ABS) index. Therefore, by Theorem 2(i), we conclude that the chemical compound 2,2,3,3-tetramethylbutane has the maximum value of the ABS index among all octane isomers.

Theorem 3. Let G be a chemical graph of size m and order n such that $4 \leq n-1 \leq m \leq 2n$. Consider Equation (1) and let $\beta_{i,j}$ be a given function. Additionally, consider $B_{i,j}$ defined in Equation (7). Let all $B_{i,j}$ be negative and the following inequalities hold:

$$\max\{B_{2,4} + B_{3,4}, 2B_{3,4}, 2B_{2,4}, 3B_{3,3}, B_{1,3} + B_{3,3}, B_{1,2} + B_{2,2}, 2B_{2,2}\} < \min\{B_{1,2} + B_{2,4}, 2B_{1,3} + B_{3,4}\}, \quad (10)$$

$$\max\{2B_{2,3}, B_{1,2} + B_{2,3}\} < B_{1,2} + B_{2,4}, \quad (11)$$

$$\max\{3B_{2,3}, B_{1,3} + B_{2,3}\} < 2B_{1,3} + B_{3,4}, \quad (12)$$

$$\max\{B_{2,2}, B_{2,3}, B_{2,4}\} < B_{1,2}, \quad (13)$$

and

$$\max\{B_{2,3}, B_{3,3}, B_{3,4}\} < B_{1,3}. \quad (14)$$

(i) If $n + m \equiv 0 \pmod{3}$, then

$$BID(G) \leq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m,$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 4\}$.

(ii) If $n + m \equiv 1 \pmod{3}$, then

$$BID(G) \leq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + 2B_{1,3} + B_{3,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 3, 4\}$ and G possesses exactly one vertex of degree 3, which has one neighbor of degree 4 and two neighbors of degree 1.

(iii) If $n + m \equiv 2 \pmod{3}$, then

$$BID(G) \leq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + B_{1,2} + B_{2,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 2, 4\}$ and G possesses only one vertex of degree 2, which has one neighbor of degree 4 and one neighbor of degree 1.

Remark 3. The choice $\beta_{i,j} = (i + j)^2$ in Equation (1) gives the hyper Zagreb index. It can be easily checked that all the conditions of Theorem 3 concerning $B_{i,j}$ are satisfied for the choice $\beta_{i,j} = (i + j)^2$. Thus, if BID is the hyper Zagreb index, then the conclusion of Theorem 3 holds.

Theorem 4. Let G be a chemical graph of order n and size m such that $4 \leq n - 1 \leq m \leq 2n$. Consider Equation (1) and let $\beta_{i,j}$ be a given function. Additionally, consider $B_{i,j}$ defined in Equation (7). Let all $B_{i,j}$ be positive and the following inequalities hold:

$$\begin{aligned} \min\{B_{2,4} + B_{3,4}, 2B_{3,4}, 2B_{2,4}, 3B_{3,3}, B_{1,3} + B_{3,3}, B_{1,2} + B_{2,2}, 2B_{2,2}\} &> \max\{B_{1,2} + B_{2,4}, 2B_{1,3} + B_{3,4}\}, \\ \min\{2B_{2,3}, B_{1,2} + B_{2,3}\} &> B_{1,2} + B_{2,4}, \\ \min\{3B_{2,3}, B_{1,3} + B_{2,3}\} &> 2B_{1,3} + B_{3,4}, \\ \min\{B_{2,2}, B_{2,3}, B_{2,4}\} &> B_{1,2}, \end{aligned}$$

and

$$\min\{B_{2,3}, B_{3,3}, B_{3,4}\} > B_{1,3}.$$

(i) If $n + m \equiv 0 \pmod{3}$, then

$$BID(G) \geq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m,$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 4\}$.

(ii) If $n + m \equiv 1 \pmod{3}$, then

$$BID(G) \geq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + 2B_{1,3} + B_{3,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 3, 4\}$ and G possesses only one vertex of degree 3, which has one neighbor of degree 4 and two neighbors of degree 1.

(iii) If $n + m \equiv 2 \pmod{3}$, then

$$BID(G) \geq \frac{4(\beta_{1,4} - \beta_{4,4})}{3}n + \frac{5\beta_{4,4} - 2\beta_{1,4}}{3}m + B_{1,2} + B_{2,4},$$

where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 2, 4\}$ and G possesses only one vertex of degree 2, which has one neighbor of degree 4 and one neighbor of degree 1.

3. Proofs

We start this section by proving the following lemma, which is useful in proving Theorem 1.

Lemma 1. Let G be a chemical graph such that $n_2 + n_3 \geq 2$.

(a). If Γ_{BID} is a graph invariant defined in Equation (8) such that every $B_{i,j}$ used there is positive and that the inequalities

$$\min\{6B_{3,4}, 3B_{3,3}, B_{2,3} + B_{3,4}, B_{3,3} + B_{3,4}, 2B_{1,2}, B_{2,2} + B_{2,4}, 2B_{2,3}\} > 2B_{2,4} \quad (15)$$

and

$$\min\{3B_{1,3}, 4B_{2,4}, 2B_{2,2}, B_{2,2} + B_{2,4}, 2B_{2,3}, B_{2,3} + B_{2,4}, B_{3,3} + B_{3,4}\} > 3B_{3,4} \quad (16)$$

hold, then

$$\Gamma_{BID}(G) > 2B_{2,4} \quad \text{and} \quad \Gamma_{BID}(G) > 3B_{3,4}. \quad (17)$$

(b). If Γ_{BID} is a graph invariant defined in Equation (8) such that every $B_{i,j}$ used there is negative and that the inequalities

$$\max\{6B_{3,4}, 3B_{3,3}, B_{2,3} + B_{3,4}, B_{3,3} + B_{3,4}, 2B_{1,2}, B_{2,2} + B_{2,4}, 2B_{2,3}\} < 2B_{2,4}$$

and

$$\max\{3B_{1,3}, 4B_{2,4}, 2B_{2,2}, B_{2,2} + B_{2,4}, 2B_{2,3}, B_{2,3} + B_{2,4}, B_{3,3} + B_{3,4}\} < 3B_{3,4}$$

hold, then the inequalities' signs in (17) are reversed.

Proof. Since the proofs of two parts are similar to each other, we provide the proof of part (a) only. We prove the desired result by considering the four possible cases: (i) $m_{2,2} \geq 1$, (ii) $m_{2,3} \geq 1$, (iii) $m_{3,3} \geq 1$, (iv) $m_{2,2} = m_{2,3} = m_{3,3} = 0$.

Case (i). $m_{2,2} \geq 1$.

From Equations (8) and (15), it follows that

$$\Gamma_{BID}(G) \geq m_{2,2}B_{2,2} + (m_{1,2} + m_{2,3} + m_{2,4})B_{2,4}. \quad (18)$$

Equation (4) with $j = 2$ this becomes $m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2$, which gives the following two possibilities (because $n_2 \geq 2$ in this case):

- $m_{2,2} = 1$ and $m_{1,2} + m_{2,3} + m_{2,4} > 1$;
- $m_{2,2} \geq 2$.

If $m_{2,2} = 1$ and $m_{1,2} + m_{2,3} + m_{2,4} > 1$, then by using (15) and (16) in (18), we obtain

$$\Gamma_{BID}(G) > B_{2,2} + B_{2,4} > \begin{cases} 3B_{3,4}, \\ 2B_{2,4}. \end{cases}$$

If $m_{2,2} \geq 2$, then again by using (15) and (16) in (18), we have

$$\Gamma_{BID}(G) \geq 2B_{2,2} > \begin{cases} 3B_{3,4}, \\ 2B_{2,4}. \end{cases}$$

Case (ii). $m_{2,3} \geq 1$.

First, we prove the inequality $\Gamma_{BID}(G) > 2B_{2,4}$. From Equations (8) and (16), it follows that

$$\Gamma_{BID}(G) \geq m_{2,3}B_{2,3} + (m_{1,3} + m_{3,3} + m_{3,4})B_{3,4}. \quad (19)$$

Equation (4) with $j = 3$, this becomes $m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3$, which gives the following two possibilities (as $n_3 \geq 1$ in this case):

- $m_{2,3} = 1$ or 2 , and $m_{1,3} + m_{3,3} + m_{3,4} \geq 1$;
- $m_{2,3} \geq 3$.

If $m_{2,3} = 1$ or 2 , and $m_{1,3} + m_{3,3} + m_{3,4} \geq 1$, then by using (15) in (19), we have

$$\Gamma_{BID}(G) \geq B_{2,3} + B_{3,4} > 2B_{2,4}.$$

If $m_{2,3} \geq 3$, then again by using (15) in (19), we have

$$\Gamma_{BID}(G) \geq 3B_{2,3} > 2B_{2,4}.$$

Next, in the remaining part of this case, we prove the inequality $\Gamma_{BID}(G) > 3B_{3,4}$. From Equations (8) and (15), it follows that

$$\Gamma_{BID}(G) \geq m_{2,3}B_{2,3} + (m_{1,2} + m_{2,2} + m_{2,4})B_{2,4}. \quad (20)$$

Equation (4) with $j = 2$, this becomes $m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2$, which gives the following two possibilities (because $n_2 \geq 1$ in this case):

- $m_{2,3} = 1$ and $m_{1,2} + m_{2,2} + m_{2,4} \geq 1$;
- $m_{2,3} \geq 2$.

If $m_{2,3} = 1$ and $m_{1,2} + m_{2,2} + m_{2,4} \geq 1$, then by using (16) in (20), we have

$$\Gamma_{BID}(G) \geq B_{2,3} + B_{2,4} > 3B_{3,4}.$$

If $m_{2,3} \geq 2$, then again by using (16) in (20), we have

$$\Gamma_{BID}(G) \geq 2B_{2,3} > 3B_{3,4}.$$

Case (iii). $m_{3,3} \geq 1$.

From (8) and (16), it follows that

$$\Gamma_{BID}(G) \geq m_{3,3}B_{3,3} + (m_{1,3} + m_{2,3} + m_{3,4})B_{3,4}. \quad (21)$$

Equation (4) with $j = 3$, this becomes $m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3$. Note that $n_3 \geq 2$ in this case and hence there are two subcases that need to be considered:

- $m_{3,3} = 1$ or 2, and $m_{1,3} + m_{2,3} + m_{3,4} > 1$;
- $m_{3,3} \geq 3$.

If $m_{3,3} = 1$ or 2, and $m_{1,3} + m_{2,3} + m_{3,4} > 1$, then by using (15) and (16) in (21), we have

$$\Gamma_{BID}(G) > B_{3,3} + B_{3,4} > \begin{cases} 3B_{3,4}, \\ 2B_{2,4}. \end{cases}$$

If $m_{3,3} \geq 3$, then again by using (15) and (16) in (21), we have

$$\Gamma_{BID}(G) \geq 3B_{3,3} > \begin{cases} 3B_{3,4}, \\ 2B_{2,4}. \end{cases}$$

Case (iv). $m_{2,2} = m_{2,3} = m_{3,3} = 0$.

By using (15) and (16) in Equation (8), we obtain

$$\Gamma_{BID}(G) \geq (m_{1,2} + m_{2,4})B_{2,4} + (m_{1,3} + m_{3,4})B_{3,4}.$$

Equation (4) with $j = 2, 3$, gives $m_{1,2} + m_{2,4} = 2n_2$ and $m_{1,3} + m_{3,4} = 3n_3$. Thus,

$$\Gamma_{BID}(G) \geq 2n_2B_{2,4} + 3n_3B_{3,4}. \quad (22)$$

The assumption $n_2 + n_3 \geq 2$ gives three possibilities: (i) $n_2 \geq 1$ and $n_3 \geq 1$, (ii) $n_2 = 0$ and $n_3 \geq 2$, (iii) $n_2 \geq 2$ and $n_3 = 0$; for each of these possibilities, by using (15) and (16) in (22), we obtain

$$\Gamma_{BID}(G) > \begin{cases} 2B_{2,4}, \\ 3B_{3,4}. \end{cases}$$

The proof is completed. $\square$

Lemma 1 has now enabled us to prove Theorem 1.

Proof of Theorem 1. The following congruence follows from Equations (2) and (3) (see also the paper [23]):

$$n + m \equiv n_3 - n_2 \pmod{3}. \quad (23)$$

(i) In this part, we have $n + m \equiv 0 \pmod{3}$. From Equation (8), it follows that $\Gamma_{\text{BID}}(G) \geq 0$, where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 4\}$ and hence from Equation (9) the desired conclusion is deduced.

(ii) In this part, we have $n + m \equiv 1 \pmod{3}$.

If $n_2 + n_3 \geq 2$, then Lemma 1 guarantees that $\Gamma_{\text{BID}}(G) > 3B_{3,4}$.

Next, assume that $n_2 + n_3 \leq 1$. Then, Equation (23) yields $n_2 = 0$ and $n_3 = 1$. Thereby, Equation (4) (with $j = 3$) gives $m_{1,3} + m_{3,4} = 3n_3 = 3$ and hence by using (16) in Equation (8) we obtain

$$\Gamma_{\text{BID}}(G) = m_{1,3}B_{1,3} + m_{3,4}B_{3,4} \geq m_{1,3}B_{3,4} + m_{3,4}B_{3,4} = 3B_{3,4}.$$

The equality $\Gamma_{\text{BID}}(G) = 3B_{3,4}$ holds if and only if $m_{1,3} = 0$; that is, the unique vertex of degree 3 is adjacent to three vertices of degree 4.

Now, by combining the conclusions of both cases considered in this part and by using Equation (9), we arrive at the desired result.

(iii) In this part, we have $n + m \equiv 2 \pmod{3}$.

If $n_2 + n_3 \geq 2$, then Lemma 1 guarantees that $\Gamma_{\text{BID}}(G) > 2B_{2,4}$.

Now, suppose that $n_2 + n_3 \leq 1$. Then, Equation (23) yields $n_2 = 1$ and $n_3 = 0$. Thereby, Equation (4) (with $j = 2$) gives $m_{1,2} + m_{2,4} = 2n_2 = 2$, and hence by using (15) in Equation (8) we obtain

$$\Gamma_{\text{BID}}(G) = m_{1,2}B_{1,2} + m_{2,4}B_{2,4} \geq m_{1,2}B_{2,4} + m_{2,4}B_{2,4} = 2B_{2,4}.$$

The equality $\Gamma_{\text{BID}}(G) = 2B_{2,4}$ holds if and only if $m_{1,2} = 0$; that is, the unique vertex of degree 2 has two neighbors of degree 4.

By combining the conclusions of both cases considered in this part and by using Equation (9), we arrive at the desired result. $\square$

The proof of Theorem 2 is fully analogous to that of Theorem 1, and is hence omitted. In order to prove Theorem 3, we prove the following lemma first.

Lemma 2. Let G be a chemical graph such that $n_2 + n_3 \geq 2$.

(a). If Γ_{BID} is a graph invariant defined in Equation (8) such that every $B_{i,j}$ used there is negative and that the inequalities

$$\max\{B_{2,4} + B_{3,4}, 2B_{3,4}, 2B_{2,4}, 3B_{3,3}, B_{1,3} + B_{3,3}, 3B_{2,3}, B_{1,3} + B_{2,3}, 2B_{2,2}, B_{1,2} + B_{2,2}\} < 2B_{1,3} + B_{3,4}, \quad (24)$$

$$\max\{B_{2,4} + B_{3,4}, 2B_{3,4}, 2B_{2,4}, 2B_{2,2}, B_{1,2} + B_{2,2}, 2B_{2,3}, B_{1,2} + B_{2,3}, 3B_{3,3}, B_{1,3} + B_{3,3}\} < B_{1,2} + B_{2,4}, \quad (25)$$

$$\max\{B_{2,2}, B_{2,3}, B_{2,4}\} < B_{1,2}, \quad (26)$$

and

$$\max\{B_{2,3}, B_{3,3}, B_{3,4}\} < B_{1,3} \quad (27)$$

hold, then

$$\Gamma_{\text{BID}}(G) < 2B_{1,3} + B_{3,4} \quad \text{and} \quad \Gamma_{\text{BID}}(G) < B_{1,2} + B_{2,4}. \quad (28)$$

(b). If Γ_{BID} is a graph invariant defined in Equation (8) such that every $B_{i,j}$ used there is positive and that the inequalities

$$\min\{4B_{1,2}, 6B_{1,3}, 2B_{1,2} + 3B_{1,3}, 3B_{3,3}, B_{1,3} + B_{3,3}, 3B_{2,3}, B_{1,3} + B_{2,3}, B_{2,2}\} > 2B_{1,3} + B_{3,4},$$

$$\min\{4B_{1,2}, 6B_{1,3}, 2B_{1,2} + 3B_{1,3}, 2B_{2,2}, B_{1,2} + B_{2,2}, 2B_{2,3}, B_{1,2} + B_{2,3}, B_{3,3}\} > B_{1,2} + B_{2,4},$$

$$\min\{B_{2,2}, B_{2,3}, B_{2,4}\} > B_{1,2},$$

and

$$\min\{B_{2,3}, B_{3,3}, B_{3,4}\} > B_{1,3}$$

hold, then the inequalities' signs in (28) are reversed.

Proof. Since the proof of two parts are similar to each other, we prove only part (a). We prove the desired result by considering the four possible cases: (i) $m_{2,2} \geq 1$, (ii) $m_{2,3} \geq 1$, (iii) $m_{3,3} \geq 1$, (iv) $m_{2,2} = m_{2,3} = m_{3,3} = 0$.

Case (i). $m_{2,2} \geq 1$.

From (8) and (26), it follows that

$$\Gamma_{BID}(G) \leq m_{2,2}B_{2,2} + (m_{1,2} + m_{2,3} + m_{2,4})B_{1,2}. \quad (29)$$

Equation (4) with $j = 2$ becomes $m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2$, which gives the following two possibilities (because $n_2 \geq 2$ in this case):

- $m_{2,2} = 1$ and $m_{1,2} + m_{2,3} + m_{2,4} > 1$;
- $m_{2,2} \geq 2$.

If $m_{2,2} = 1$ and $m_{1,2} + m_{2,3} + m_{2,4} > 1$, then from (24), (25), and (29), we have

$$\Gamma_{BID}(G) < B_{2,2} + B_{1,2} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

If $m_{2,2} \geq 2$, then again from (24), (25), and (29), we obtain

$$\Gamma_{BID}(G) \leq 2B_{2,2} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

Case (ii). $m_{2,3} \geq 1$.

First, we prove the inequality $\Gamma_{BID}(G) < 2B_{1,3} + B_{3,4}$. From (8) and (27), it follows that

$$\Gamma_{BID}(G) \leq m_{2,3}B_{2,3} + (m_{1,3} + m_{3,3} + m_{3,4})B_{1,3}. \quad (30)$$

Equation (4) with $j = 3$ becomes $m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3$, which gives the following two possibilities (as $n_3 \geq 1$ in this case):

- $m_{2,3} = 1$ or 2, and $m_{1,3} + m_{3,3} + m_{3,4} \geq 1$;
- $m_{2,3} \geq 3$.

If $m_{2,3} = 1$ or 2, and $m_{1,3} + m_{3,3} + m_{3,4} \geq 1$, then from (24) and (30) it follows that

$$\Gamma_{BID}(G) \leq B_{2,3} + B_{1,3} < 2B_{1,3} + B_{3,4}.$$

If $m_{2,3} \geq 3$, then again from (24) and (30), we have

$$\Gamma_{BID}(G) \leq 3B_{2,3} < 2B_{1,3} + B_{3,4}.$$

Next, in the remaining part of this case, we prove the inequality $\Gamma_{\text{BID}}(G) < B_{1,2} + B_{2,4}$. From (8) and (26), it follows that

$$\Gamma_{\text{BID}}(G) \leq m_{2,3}B_{2,3} + (m_{1,2} + m_{2,2} + m_{2,4})B_{1,2}. \quad (31)$$

Equation (4) with $j = 2$ becomes $m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2$, which gives the following two possibilities (because $n_2 \geq 1$ in this case):

- $m_{2,3} = 1$ and $m_{1,2} + m_{2,2} + m_{2,4} \geq 1$;
- $m_{2,3} \geq 2$.

If $m_{2,3} = 1$ and $m_{1,2} + m_{2,2} + m_{2,4} \geq 1$, then from (25) and (31), it follows that

$$\Gamma_{\text{BID}}(G) \leq B_{2,3} + B_{1,2} < B_{1,2} + B_{2,4}.$$

If $m_{2,3} \geq 2$, then again from (25) and (31), we obtain

$$\Gamma_{\text{BID}}(G) \leq 2B_{2,3} < B_{1,2} + B_{2,4}.$$

Case (iii). $m_{3,3} \geq 1$.

From (8) and (27), we have

$$\Gamma_{\text{BID}}(G) \leq m_{3,3}B_{3,3} + (m_{1,3} + m_{2,3} + m_{3,4})B_{1,3}. \quad (32)$$

Equation (4) with $j = 3$ becomes $m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3$. Note that $n_3 \geq 2$ in this case and hence there are two subcases that need to be considered:

- $m_{3,3} = 1$ or 2, and $m_{1,3} + m_{2,3} + m_{3,4} > 1$;
- $m_{3,3} \geq 3$.

If $m_{3,3} = 1$ or 2, and $m_{1,3} + m_{2,3} + m_{3,4} > 1$, then from (24), (25), and (32), it follows that

$$\Gamma_{\text{BID}}(G) < B_{3,3} + B_{1,3} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

If $m_{3,3} \geq 3$, then again from (24), (25), and (32), we have

$$\Gamma_{\text{BID}}(G) \leq 3B_{3,3} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

Case (iv). $m_{2,2} = m_{2,3} = m_{3,3} = 0$.

In this case, Equation (8) becomes

$$\Gamma_{\text{BID}}(G) = m_{1,2}B_{1,2} + m_{1,3}B_{1,3} + m_{2,4}B_{2,4} + m_{3,4}B_{3,4}. \quad (33)$$

In this case, note also that $m_{1,2} \leq m_{2,4}$ and $m_{1,3} \leq 2m_{3,4}$. Moreover, Equation (4) with $j = 2, 3$ gives $m_{1,2} + m_{2,4} = 2n_2$ and $m_{1,3} + m_{3,4} = 3n_3$. Thus,

$$m_{2,4} \geq n_2 \quad \text{and} \quad m_{3,4} \geq n_3. \quad (34)$$

If $n_2 \geq 1$ and $n_3 \geq 1$, then from (34) one obtains $\min\{m_{2,4}, m_{3,4}\} \geq 1$, and hence from (24), (25), and (33), one obtains

$$\Gamma_{\text{BID}}(G) \leq B_{2,4} + B_{3,4} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

If $n_2 = 0$ and $n_3 \geq 2$, then from (34) the inequality $m_{3,4} \geq 2$ follows, and hence from (24), (25), and (33), it follows that

$$\Gamma_{BID}(G) \leq 2B_{3,4} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

Finally, if $n_2 \geq 2$ and $n_3 = 0$, then from (34) we have $m_{2,4} \geq 2$, and hence by using (24), (25), and (33), we have

$$\Gamma_{BID}(G) \leq 2B_{2,4} < \begin{cases} 2B_{1,3} + B_{3,4}, \\ B_{1,2} + B_{2,4}. \end{cases}$$

The proof is completed. $\square$

Now, we are in position to prove Theorem 3.

Proof of Theorem 3. (i) In this part, we have $n + m \equiv 0 \pmod{3}$. From Equation (8), it follows that $\Gamma_{BID}(G) \leq 0$, where the necessary and sufficient condition for the equality is that the degree set of G is $\{1, 4\}$, and hence from Equation (9) the desired conclusion is deduced.

(ii) In this part, we have $n + m \equiv 1 \pmod{3}$.

If $n_2 + n_3 \geq 2$, then Lemma 2 guarantees that $\Gamma_{BID}(G) < 2B_{1,3} + B_{3,4}$ (because the system of inequalities (10)–(14) is equivalent to the system of inequalities (24)–(27)).

Next, assume that $n_2 + n_3 \leq 1$. Then, Equation (23) yields $n_2 = 0$ and $n_3 = 1$. Thereby, Equation (4) (with $j = 3$) gives $m_{1,3} + m_{3,4} = 3n_3 = 3$. Additionally, Equation (8) becomes

$$\Gamma_{BID}(G) = m_{1,3}B_{1,3} + m_{3,4}B_{3,4}.$$

Note that $m_{3,4} \geq 1$ (because $n \geq 5$), and hence by using (14) we have

$$\Gamma_{BID}(G) = m_{1,3}B_{1,3} + m_{3,4}B_{3,4} \leq 2B_{1,3} + B_{3,4}.$$

The equality $\Gamma_{BID}(G) = 2B_{1,3} + B_{3,4}$ holds if and only if $m_{1,3} = 2$ and $m_{3,4} = 1$; that is, the unique vertex of degree 3 has one neighbor of degree 4 and two neighbors of degree 1.

Now, by combining the conclusions of both cases considered in this part and by using Equation (9), we arrive at the desired result.

(iii) In this part, we have $n + m \equiv 2 \pmod{3}$.

If $n_2 + n_3 \geq 2$, then Lemma 2 guarantees that $\Gamma_{BID}(G) < B_{1,2} + B_{2,4}$ (because the system of inequalities (10)–(14) is equivalent to the system of inequalities (24)–(27)).

Now, suppose that $n_2 + n_3 \leq 1$. Then, Equation (23) yields $n_2 = 1$ and $n_3 = 0$. Thereby, Equation (4) (with $j = 2$) gives $m_{1,2} + m_{2,4} = 2n_2 = 2$. Additionally, Equation (8) gives

$$\Gamma_{BID}(G) = m_{1,2}B_{1,2} + m_{2,4}B_{2,4}.$$

Note that $m_{2,4} \geq 1$ (because $n \geq 4$), and hence by using (13) we have

$$\Gamma_{BID}(G) = m_{1,2}B_{1,2} + m_{2,4}B_{2,4} \leq B_{1,2} + B_{2,4}.$$

The equality $\Gamma_{BID}(G) = B_{1,2} + B_{2,4}$ holds if and only if $m_{1,2} = m_{2,4} = 1$ (i.e., the unique vertex of degree 2 has one neighbor of degree 4 and one neighbor of degree 1).

By combining the conclusions of both cases considered in this part and by using Equation (9), we arrive at the desired result. $\square$

The proof of Theorem 4 is fully analogous to that of Theorem 3, and is hence omitted.

4. Concluding Remarks

If we take $\beta_{i,j} = (ij)^{-1/2}$ or $\beta_{i,j} = ij$ in Equation (1), we obtain the Randić index or the second Zagreb index, respectively. Although Theorems 1–4 cover several well-known topological indices, there are some renowned topological indices for which the conclusions of these theorems hold but the conditions of the theorems are not fully satisfied—for example, the Randić index obeys the conclusion of Theorem 2 (see [23]) but not its conditions completely, and the second Zagreb index obeys the conclusion of Theorem 3 (see [24]) but not its conditions completely. Thereby, as a future work, it would be interesting to relax the conditions of Theorems 1–4 provided that their conclusions remain unchanged (that is, to give stronger versions of these theorems) so that some additional indices may also be covered.

Author Contributions: Conceptualization, A.M.A., A.A. and Z.D.; Methodology, A.M.A., A.A., Z.D. and A.A.B.; Software, N.I.; Validation, A.A. and Z.D.; Formal analysis, A.M.A., Z.D., A.A.B. and N.I.; Investigation, A.M.A., Z.D. and A.E.H.; Resources, T.A. and N.I.; Data curation, T.A. and A.E.H.; Writing—original draft, A.M.A.; Writing—review & editing, A.A., Z.D. and T.A.; Visualization, A.E.H.; Supervision, A.A.B.; Project administration, A.A.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Scientific Research Deanship at University of Ha'il-Saudi Arabia through project RG-22 002.

Data Availability Statement: Data about this study may be requested from the authors.

Conflicts of Interest: The authors do not have any conflict of interest.

References

- Trinajstić, N. *Chemical Graph Theory*; CRC Press: Boca Raton, FL, USA, 1992.
- Wagner, S.; Wang, H. *Introduction to Chemical Graph Theory*; CRC Press: Boca Raton, FL, USA, 2018.
- Zanni, R.; Galvez-Llompart, M.; Garcia-Domenech, R.; Galvez, J. What place does molecular topology have in today's drug discovery? *Expert Opin. Drug Discov.* **2020**, *15*, 1133–1144. [\[CrossRef\]](#)
- Ivanov, J.; Polshakov, D.; Kato-Weinstein, J.; Zhou, Q.; Li, Y.; Granet, R.; Garner, L.; Deng, Y.; Liu, C.; Albaiu, D.; et al. Quantitative structure-activity relationship machine learning models and their applications for identifying viral 3CLpro- and RdRp-targeting compounds as potential therapeutics for COVID-19 and related viral infections. *ACS Omega* **2020**, *5*, 27344–27358. [\[CrossRef\]](#) [\[PubMed\]](#)
- Liu, A.L.; Venkatesh, R.; McBride, M.; Reichmanis, E.; Meredith, J.C.; Grover, M.A. Small data machine learning: Classification and prediction of poly(ethylene terephthalate) stabilizers using molecular descriptors. *ACS Appl. Polym. Mater.* **2020**, *2*, 5592–5601. [\[CrossRef\]](#)
- Vukičević, D.; Gašperov, M. Bond additive modeling 1. Adriatic indices. *Croat. Chem. Acta* **2010**, *83*, 243–260.
- Vukičević, D.; Đurđević, J. Bond additive modeling 10. Upper and lower bounds of bond incident degree indices of catacondensed fluoranthenes. *Chem. Phys. Lett.* **2011**, *515*, 186–189. [\[CrossRef\]](#)
- Ali, A.; Raza, Z.; Bhatti, A.A. Bond incident degree (BID) indices of polyomino chains: A unified approach. *Appl. Math. Comput.* **2016**, *287–288*, 28–37. [\[CrossRef\]](#)
- Ali, A.; Bhatti, A.A. Extremal triangular chain graphs for bond incident degree (BID) indices. *Ars Comb.* **2018**, *141*, 213–227.
- Ali, A.; Dimitrov, D. On the extremal graphs with respect to bond incident degree indices. *Discret. Appl. Math.* **2018**, *238*, 32–40. [\[CrossRef\]](#)
- Liu, J.B.; Baig, A.Q.; Imran, M.; Khalid, W.; Saeed, M.; Farahani, M.R. Computation of bond incident degree (BID) indices of complex structures in drugs. *Eurasian Chem. Commun.* **2020**, *2*, 672–679. [\[CrossRef\]](#)
- Rao, Y.; Aslam, A.; Noor, M.U.; Almatroud, A.O.; Shao, Z. Bond incident degree indices of catacondensed pentagonal systems. *Complexity* **2020**, *2020*, 4935760. [\[CrossRef\]](#)
- Rizwan, M.; Bhatti, A.A.; Javaid, M.; Jarad, F. Some bounds on bond incident degree indices with some parameters. *Math. Probl. Eng.* **2021**, *2021*, 8417486. [\[CrossRef\]](#)
- Ye, J.; Liu, M.; Yao, Y.; Das, K.C. Extremal polygonal cacti for bond incident degree indices. *Discrete Appl. Math.* **2019**, *257*, 289–298. [\[CrossRef\]](#)
- Gao, F.; Xu, K. On the reduced second Zagreb index of graphs. *Rocky Mt. J. Math.* **2020**, *50*, 975–988. [\[CrossRef\]](#)
- Xu, K.; Das, K.C. Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index. *MATCH Commun. Math. Comput. Chem.* **2012**, *68*, 257–272.
- Xu, K.; Das, K.C. Some extremal graphs with respect to inverse degree. *Discret. Appl. Math.* **2016**, *203*, 171–183. [\[CrossRef\]](#)

18. Xu, K.; Gao, F.; Das, K.C.; Trinajstić, N. A formula with its applications on the difference of Zagreb indices of graphs. *J. Math. Chem.* **2019**, *57*, 1618–1626. [[CrossRef](#)]
19. Ali, A.; Furtula, B.; Redžepović, I.; Gutman, I. Atom-bond sum-connectivity index. *J. Math. Chem.* **2022**, *60*, 2081–2093. [[CrossRef](#)]
20. Ali, A.; Gutman, I.; Redžepović, I. Atom-bond sum-connectivity index of unicyclic graphs and some applications. *Electron. J. Math.* **2023**, *5*, 1–7.
21. Bondy, J.A.; Murty, U.S.R. *Graph Theory*; Springer: London, UK, 2008.
22. Chartrand, G.; Lesniak, L.; Zhang, P. *Graphs & Digraphs*; CRC Press: Boca Raton, FL, USA, 2016.
23. Gutman, I.; Miljković, O. Molecules with smallest connectivity indices. *MATCH Commun. Math. Comput. Chem.* **2000**, *41*, 57–70.
24. Raza, Z.; Ali, A. Bounds on the Zagreb indices for molecular (n, m) -graphs. *Int. J. Quantum. Chem.* **2020**, *120*, e26333. [[CrossRef](#)]

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