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Minimum bond incident degree indices of unicyclic graphs with fixed girth and maximum degree

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Abstract: For a graph G, its bond incident degree index is given by

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

in which $f(x,y) = f(y,x)$ is a real-valued symmetric function. In this paper, we establish three sufficient conditions respectively for the minimum bond incident degree (BID) index of unicyclic graphs with given girth and those with given maximum degree. As applications, we verify that seven topological indices, including the recently proposed hyperbolic Sombor index and diminished Sombor index satisfy these sufficient conditions. This work provides a theoretical foundation for further investigations into the extremal values of topological indices.

Keywords: bond incident degree index; girth; maximum degree; unicyclic graphs
Mathematics Subject Classification: 05C05, 05C09, 05C92

1. Introduction

Let $G = (V(G), E(G))$ be a simple and connected graph, where $V(G)$ denotes its vertex set and $E(G)$ represents its edge set. For any vertex $u \in V(G)$, let $d_G(u)$ (or $d(u)$ for brevity) signify the degree of u, and let $N_G(u)$ stand for the neighborhood of u. The maximum degree is written as Δ. Specifically, a vertex u satisfying $d(u) = 1$ is referred to as a pendant vertex or a leaf. We denote the n-vertex path graph as P_n and the n-vertex cycle graph as C_n. A connected graph G that contains precisely one cycle is defined as a unicyclic graph, and as such, it satisfies the relation $|V(G)| = |E(G)|$. For any unicyclic graph, girth is defined as the length of its sole cycle C. We use $\mathbb{U}_{n,g}$ and $\mathbb{U}_{n,\Delta}$ to stand for the families of all unicyclic graphs with n-vertex, where $\mathbb{U}_{n,g}$ consists of those with fixed girth g and $\mathbb{U}_{n,\Delta}$ comprises those with fixed maximum degree Δ. Undefined notions and terminologies follow the graph theory work [1].

Chemical graph theory stands as a prominent subfield within mathematical chemistry that mathematically models molecular structures and represents chemical information. In chemical graph theory, topological indices are a class of important molecular descriptors: They capture the structural characteristics of molecules in a mathematical manner and reveal the relationships between molecular structures and various physicochemical properties [2, 3]. Their predictive power can reduce experimental redundancy, and topological indices are widely applied in drug screening, the development of new chemical products, and other related fields [4, 5].

As an important class of topological indices, the bond incident degree index dominates the research within chemical graph theory [6–8]. A bond incident degree index of G is defined as

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

in which $f(x, y) = f(y, x)$ serves as a real-valued symmetric function. Specifically, let $m_{x,y}$ denote the number of edges where $(x, y) = (d(u), d(v))$, then BID can be expressed alternatively by

$$BID = \sum_{1\leq x\leq y\leq\Delta} m_{x,y} f(x, y).$$

In 2021, Gutman [9] first introduced a geometric-distance-based bond incident degree index known as the Sombor index, which is expressed as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d(u)^2 + d(v)^2}.$$

In other words, let $f(x, y) = \sqrt{x^2 + y^2}$ in the formula for BID, and it follows that $BID(G) = SO(G)$.

Subsequently, various modified versions of the Sombor index have been introduced, such as the average Sombor index [9], the Euler Sombor index [10, 11], and the elliptic Sombor index [12], among others. Very recently, Barman et al. [13] and Movahedi et al. [14] independently put forward the hyperbolic Sombor index (HSO) and diminished Sombor index (DSO), which are given by

$$HSO(G) = \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 + d(v)^2}}{min\{d(u), d(v)\}} \text{ and } DSO(G) = \sum_{\mathrm{uv}\in \mathrm{E(G)}} \frac{\sqrt{d(u)^2 + d(v)^2}}{\mathrm{d(u) + d(v)}}.$$

Other bond incident degree indices that have attracted extensive research attention include the Lanzhou index [15], the harmonic-arithmetic index [16], the general sum-connectivity index [17], and so forth.

Unicyclic graphs, as an important class of chemical structural graphs, have long been the subject of extensive research. In 2021, Zhou et al. [18] determined the minimum Sombor index of trees as well as unicyclic graphs having prescribed maximum degree. In 2022, Liu et al. [19] characterized the orderings of the Sombor index and reduced Sombor index for unicyclic graphs and other graph classes. In 2023, Nithya et al. [20] identified the ranking corresponding to the first through fourth smallest atom-bond sum-connectivity (ABS) index among all unicyclic graphs having a predefined girth g. In 2024, Cui et al. [21] established the smallest Lanzhou index of unicyclic graphs having given maximum degree. In the same year, Chen et al. [22] characterized the smallest and largest Sombor indices among unicyclic graphs having prescribed girth and among chemical unicyclic graphs. In 2025, Zhang et al. [23] established the unicyclic graphs that attain the largest and smallest ABS indices with a fixed diameter. Very recently, Das et al. [24] determined the minimum Euler Sombor index of unicyclic graphs possessing a prescribed girth, along with the maximum Euler Sombor index of connected graphs having a predetermined count of pendant vertices.

Inspired by [18] and [24], we aim to solve extremal problems for bond incident degree indices among unicyclic graphs in a unified manner. In Section 2, two sufficient conditions for the minimum BID index of unicyclic graphs having fixed girth are established by analyzing structural properties of graphs. In Section 3, via several graph transformations, a sufficient condition for the smallest BID index for all unicyclic graphs having fixed maximum degree is presented. In Section 4, as applications of these sufficient conditions, we verify that seven bond incident degree indices meet the corresponding conditions for the two families of unicyclic graphs mentioned above.

2. Minimum $BID(G)$ among unicyclic graphs with fixed girth

This section presents two sufficient conditions that serve to characterize the minimum BID index of unicyclic graphs having fixed girth. First, we define two special families of unicyclic graphs, as illustrated in Figure 1.

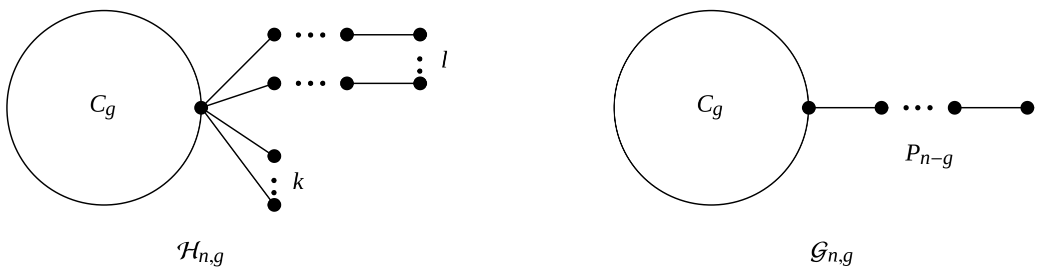

Figure 1. Graphs of $\mathcal{H}_{n,g}$ and $\mathcal{G}_{n,g}$.

Let $\mathcal{H}_{n,g} \in \mathbb{U}_{n,g}$ be the graph obtained by attaching k pendant edges and l pendant paths each of length at least 2 to a single common vertex of the cycle C_g (where $g \leq n-2$), and its maximum degree equals $k+l+2$.

Let $\mathcal{G}_{n,g} \in \mathbb{U}_{n,g}$ be the graph obtained by attaching a single pendant path P_{n-g} to one vertex of the cycle C_g.

Based on the structural properties of these graphs, we derive the following expressions:

$$BID(\mathcal{H}_{n,g}) = (l+2)f(k+l+2,2) + kf(k+l+2,1) + lf(2,1) + (n-k-2l-2)f(2,2), \tag{2.1}$$

$$BID(\mathcal{G}_{n,g}) = f(2,1) + 3f(3,2) + (n-4)f(2,2).$$

Lemma 2.1. *Let $G \in \mathcal{H}_{n,g}$. If $f(x,y)$ satisfies the following conditions:*

(i) Both $f(x,2)$ and $f(x,1)$ are strictly increasing for $x \geq 2$;

(ii) $f(3,2) < f(4,1)$ *and* $2f(2,2) < f(2,4) + f(2,1)$,
then

$$BID(G) \geq BID(\mathcal{G}_{n,g}) = 3f(3,2) + f(2,1) + (n-4)f(2,2),$$

with equality iff $G \cong \mathcal{G}_{n,g}$.

Proof. From the structure of $\mathcal{H}_{n,g}$ and the condition $g \leq n-2$, it follows immediately that $k + l \geq 1$. We first consider the case $k + l = 1$. The condition $g \leq n-2$ implies $l = 1$ and $k = 0$, so $G \cong \mathcal{G}_{n,g}$. Thus,

$$BID(G) = BID(\mathcal{G}_{n,g}) = 3f(3,2) + f(2,1) + (n-4)f(2,2).$$

Next, we consider $k + l \geq 2$. For $l = 0$, from condition (i), we obtain $f(k+2,2) \geq f(4,2)$ and $f(k+2,1) \geq f(4,1)$. Combined with (ii), we have $2f(4,2) + 2f(4,1) \geq 3f(3,2) + f(2,1)$. Therefore, from (2.1), it follows that

$$\begin{aligned} BID(G) &= 2f(k+2,2) + kf(k+2,1) + (n-k-2)f(2,2) \\ &\geq 2f(4,2) + 2f(4,1) + (n-4)f(2,2) \\ &> 3f(3,2) + f(2,1) + (n-4)f(2,2). \end{aligned}$$

For $l \geq 1$, the conditions (i) and (ii) imply that $f(2,2)$ is less than both $f(4,1)$ and $f(4,2)$. Using (2.1) and the inequality $2f(2,2) < f(4,2) + f(2,1)$ from condition (ii), we obtain

$$\begin{aligned} BID(G) = {} & 3f(k+l+2,2) + f(2,1) + kf(k+l+2,1) \\ & + (n-k-2l-2)f(2,2) + (l-1)(f(k+l+2,2) + f(2,1)) \\ & \geq 3f(4,2) + f(2,1) + kf(4,1) + (n-k-2l-2)f(2,2) + (l-1)(f(4,2) + f(2,1)) \\ & > 3f(3,2) + f(2,1) + (n-4)f(2,2). \end{aligned}$$

Therefore, combining all cases above, the lemma follows. □

Theorem 2.1. *Let* $G \in \mathbb{U}_{n,g}$. *If* $f(x,y)$ *satisfies the following conditions:*
(i) $f(x,y)$ *is strictly increasing for all* $x \geq 1$*;*
(ii) $f(x-1,2) < f(x,1)$ *holds for all* $x \geq 3$*;*
(iii) $2f(2,2) < f(2,3) + f(2,1)$ *holds,*
then

$$BID(G) \geq \begin{cases} 3f(3,2) + (n-4)f(2,2) + f(2,1), & g \leq n-2, \\ 2f(3,2) + (n-3)f(2,2) + f(3,1), & g = n-1, \\ nf(2,2), & g = n, \end{cases}$$

with equality iff $G \cong \mathcal{G}_{n,g}$ *when* $g \leq n-2$, $G \cong G_{n,n-1}$ *when* $g = n-1$, *and* $G \cong C_n$ *when* $g = n$.

Proof. First, when $g = n-1$ and $g = n$, G is isomorphic to $G_{n,n-1}$ and C_n, respectively. From the structure of G, it is straightforward to obtain

$$BID(C_n) = nf(2,2),$$

$$BID(G_{n,n-1}) = 2f(3,2) + f(3,1) + (n-3)f(2,2).$$

Thus, it remains to prove the case $g \leq n-2$.

Denote by s the count of vertices in G with degree at least 3. Since $g \leq n-2$, it immediately follows that $s \geq 1$. We now consider two cases depending on the value of s.

Case 1. $s = 1$. G contains precisely one vertex with degree at least 3, while every other vertex is of degree either 1 or 2, which implies $G \in \mathcal{H}_{n,g}$. Clearly, the conditions of the theorem satisfy those of Lemma 2.1. Therefore, by Lemma 2.1, we deduce

$$BID(G) \geq BID(\mathcal{G}_{n,g}) = 3f(3,2) + f(2,1) + (n-4)f(2,2).$$

Equality is attained iff $G \cong \mathcal{G}_{n,g}$.

Case 2. $s \geq 2$. We partition all pendant paths of G into two types: those of length 1 and those with length no less than 2. For any pendant edge vv_i with length 1, by conditions (i) and (ii), we have

$$f(d(v), d(v_i)) = f(d(v), 1) \geq f(3,1) > f(2,2).$$

For any pendant path $P : vv_1v_2 \cdots v_k$ with length no less than 2, by conditions (i) and (iii), we obtain

$$\begin{aligned}\sum_{v_iv_j \in E(P)} f(d(v_i), d(v_j)) &= f(d(v), 2) + (k-2)f(2,2) + f(2,1)\\ &\geq f(3,2) + f(2,1) + (k-2)f(2,2)\\ &> kf(2,2).\end{aligned}$$

Let A denote the collection of all pendant paths. From the inequalities established above, it follows that

$$\sum_{v_iv_j \in A} f(d(v_i), d(v_j)) > |A| \cdot f(2,2). \tag{2.2}$$

For any edge $v_iv_j \in E(G)\backslash A$, we have $d(v_i), d(v_j) \geq 2$. By condition (i),

$$f(d(v_i), d(v_j)) \geq f(2,2).$$

Let $B = \{v_iv_j \in E(G)\backslash A \mid d(v_i) \geq 3, d(v_j) \geq 2\}$. Since $s \geq 2$, it follows that $|B| \geq 3$. Therefore, together with condition (i), we obtain

$$\begin{aligned}\sum_{v_iv_j \in E(G)\backslash A} f(d(v_i), d(v_j)) &= \sum_{v_iv_j \in B} f(d(v_i), d(v_j)) + \sum_{v_iv_j \in E(G)\backslash(A\cup B)} f(d(v_i), d(v_j))\\ &\geq |B|f(3,2) + (n-|A|-|B|)f(2,2)\\ &\geq 3f(3,2) + (n-|A|-3)f(2,2).\end{aligned} \tag{2.3}$$

Combining inequalities (2.2), (2.3) and the result $f(2,1) < f(2,2)$ from condition (i), we further derive

$$\begin{aligned}TI_f(G) &= \sum_{v_iv_j \in A} f(d(v_i), d(v_j)) + \sum_{v_iv_j \in E(G)\backslash A} f(d(v_i), d(v_j))\\ &> |A| \cdot f(2,2) + 3f(3,2) + (n-|A|-3)f(2,2)\\ &= 3f(3,2) + (n-3)f(2,2)\\ &> 3f(3,2) + f(2,1) + (n-4)f(2,2).\end{aligned}$$

This finishes the proof of the theorem. □

Analogous to Theorem 2.1, we adjust the relevant assumptions to establish Theorem 2.2, a counterpart of Theorem 2.1. In Section 4 below, we verify that these two theorems apply to different topological indices, respectively.

Theorem 2.2. *Let $G \in \mathbb{U}_{n,g}$. If $f(x, y)$ satisfies the following conditions:*
(i) Both $f(x, 2)$ and $f(x, 1)$ are strictly increasing functions for $x \geq 2$;
(ii) $f(3, 2) < f(4, 1)$ and $2f(2, 2) < f(4, 2) + f(2, 1)$;
(iii) $f(2, 2) \leq f(x, y)$ for all $x, y \geq 1$ but $(x, y) \neq (1, 1)$;
(iv) $3f(3, 2) < f(3, 1) + 2f(2, 2)$ and $3f(3, 2) < 2f(2, 1) + f(2, 2)$,
then

$$BID(G) \geq \begin{cases} 3f(3,2) + (n-4)f(2,2) + f(2,1), & g \leq n-2, \\ 2f(3,2) + (n-3)f(2,2) + f(3,1), & g = n-1, \\ nf(2,2), & g = n, \end{cases}$$

with equality iff $G \cong \mathcal{G}_{n,g}$ when $g \leq n-2$, $G \cong G_{n,n-1}$ when $g = n-1$, and $G \cong C_n$ when $g = n$.

Proof. First, when $g = n$ and $g = n - 1$, it follows that $G \cong C_n$ and $G \cong G_{n,n-1}$, respectively. Thus,

$$BID(C_n) = nf(2, 2),$$

$$BID(G_{n,n-1}) = 2f(3, 2) + f(3, 1) + (n - 3)f(2, 2).$$

We now consider the case $g \leq n-2$. Denote by s the count of vertices in G with degree at least 3. Then $s \geq 1$.

If $s = 1$, then similarly to Theorem 2.1, we obtain $G \in \mathcal{H}_{n,g}$. Therefore, by Lemma 2.1, we deduce

$$BID(G) \geq BID(\mathcal{G}_{n,g}) = 3f(3, 2) + f(2, 1) + (n - 4)f(2, 2).$$

Equality is attained precisely when $G \cong \mathcal{G}_{n,g}$.

Therefore, $s \geq 2$. Let A denote the collection of all pendant paths. For any edge $v_iv_j \in E(G)\backslash A$, by condition (iii), we have

$$f(d(v_i), d(v_j)) \geq f(2, 2). \tag{2.4}$$

Within A, for a pendant edge vv_i of length 1, by condition (i), we deduce

$$f(d(v), d(v_i)) = f(d(v), 1) \geq f(3, 1).$$

For any pendant path $P : vv_1v_2 \cdots v_k$ with length no less than 2, it follows from condition (i) that

$$\begin{aligned} \sum_{v_iv_j \in E(P)} f(d(v_i), d(v_j)) &= f(d(v), 2) + (k-2)f(2, 2) + f(2, 1) \\ &\geq f(3, 2) + f(2, 1) + (k-2)f(2, 2) \\ &> (k-1)f(2, 2) + f(2, 1). \end{aligned}$$

Since $s \geq 2$, G contains at least two pendant paths. We now distinguish two cases according to whether G has pendant edges.

Case 1. G contains at least one pendant edge. Since G has at least two pendant paths,

$$\sum_{v_iv_j\in A} f(d(v_i),d(v_j)) > f(3,1)+f(2,1)+(|A|-2)f(2,2).$$

Combining this with condition (iv), we obtain

$$\begin{aligned}
BID(G) &= \sum_{v_iv_j\in A} f(d(v_i),d(v_j)) + \sum_{v_iv_j\in E(G)\setminus A} f(d(v_i),d(v_j))\\
&> (f(3,1)+f(2,1)+(|A|-2)f(2,2)) + (n-|A|)f(2,2)\\
&= f(3,1)+f(2,1)+(n-2)f(2,2)\\
&> 3f(3,2)+f(2,1)+(n-4)f(2,2).
\end{aligned}$$

Case 2. All pendant paths of G have length at least 2.
Subcase 2.1. Exactly two pendant paths. Let them be $P_1 = vv_1v_2\cdots v_i$ and $P_2 = ww_1w_2\cdots w_k$, where $d(v), d(w) \geq 3$, $d(v_1) = \cdots = d(v_{i-1}) = d(w_1) = \cdots = d(w_{k-1}) = 2$, and $d(v_i) = d(w_k) = 1$. From condition (i), we have

$$\sum_{v_iv_j\in A} f(d(v_i),d(v_j)) \geq 2f(3,2)+2f(2,1)+(|A|-4)f(2,2). \tag{2.5}$$

On the other hand, it follows from conditions (iii) and (iv) that

$$3f(3,2) < 2f(2,1)+f(2,2) < 3f(2,1),$$

which implies $f(3,2) < f(2,1)$. Combining (2.4) and (2.5), we obtain

$$\begin{aligned}
BID(G) &= \sum_{v_iv_j\in A} f(d(v_i),d(v_j)) + \sum_{v_iv_j\in E(G)\setminus A} f(d(v_i),d(v_j))\\
&> 2f(3,2)+2f(2,1)+(|A|-4)f(2,2)+(n-|A|)f(2,2)\\
&= 2f(3,2)+2f(2,1)+(n-4)f(2,2)\\
&> 3f(3,2)+f(2,1)+(n-4)f(2,2).
\end{aligned}$$

Subcase 2.2. At least three pendant paths. Then there are at least three edges v_iv_j, such that $d(v_i) = 2$ and $d(v_j) = 1$. By condition (iii), we deduce

$$\sum_{v_iv_j\in A} f(d(v_i),d(v_j)) \geq 3f(2,1)+(|A|-3)f(2,2). \tag{2.6}$$

Combining (2.4), (2.6) and the inequality $3f(2,3) < 2f(1,2)+f(2,2)$ given in condition (iv), we obtain

$$\begin{aligned}
BID(G) &= \sum_{v_iv_j\in A} f(d(v_i),d(v_j)) + \sum_{v_iv_j\in E(G)\setminus A} f(d(v_i),d(v_j))\\
&\geq 3f(2,1)+(|A|-3)f(2,2)+(n-|A|)f(2,2)\\
&= 3f(2,1)+(n-3)f(2,2)\\
&> 3f(3,2)+f(2,1)+(n-4)f(2,2).
\end{aligned}$$

Combining all cases above, the proof of the theorem is complete. □

3. Minimum $BID(G)$ among unicyclic graphs with fixed maximum degree

Lemma 3.1. *Let P_{wu} be a path in $G \in \mathbb{U}_{n,\Delta}$ connecting w and u, where $d_G(u) = \Delta$, $w \in V(C)$, and $u \notin V(C)$. Suppose that either $v \in V(G)\backslash(V(C) \cup P_{wu})$ with $d_G(v) \geq 3$; or $v \in V(C) \cup P_{wu}\backslash\{w, u\}$ with $d_G(v) \geq 4$. If $f(x, y)$ meets the conditions listed below:*

(i) $f(x, y)$ is strictly increasing with respect to x;

(ii) $f(x-1, 2) < f(x, 1)$ is valid for all $x \geq 3$;

(iii) $f(x, 2)$ is strictly convex as a function of x,

then there exists $G' \in \mathbb{U}_{n,\Delta}$ such that $BID(G') < BID(G)$.

Proof. (1) We first consider the case where $v \in V(G)\backslash(V(C) \cup P_{wu})$ and $d_G(v) \geq 3$. Let $d_G(v) = r \geq 3$ and $N_G(v) = \{v_1, v_2, \cdots, v_r\}$, where v_r is the vertex at the maximum distance from u to v. Since $d_G(v) = r \geq 3$, there exist at least two more paths $vv_1v_1^2 \cdots v_1^p$ and $vv_2v_2^2 \cdots v_2^q$ attached at v other than v_r, where we may assume $p \leq q$, as illustrated in Figure 2. Here, the cycle C is connected to some vertex $u_i (1 \leq i \leq \Delta)$ by a path. We now construct a new graph $G' \in \mathbb{U}_{n,\Delta}$ by Transformation 1, and distinguish three cases according to whether vv_1 and vv_2 are leaves.

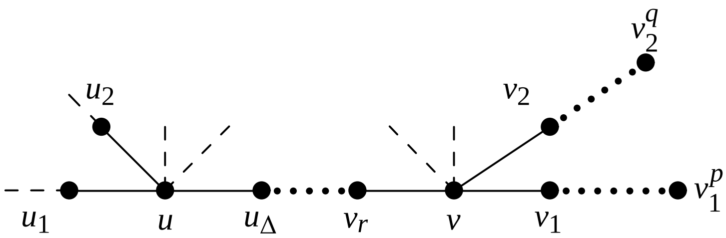

Figure 2. Graph G in Transformation 1.

Transformation 1: $G' = G - vv_1 + v_1v_2^q$.

Case 1. Both vv_1 and vv_2 are leaves. By conditions (i), (ii), and $r \geq 3$, we deduce

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=3}^{r}[f(r-1, d_G(v_i)) - f(r, d_G(v_i))] + f(2,1) - f(r,1) + f(r-1,2) - f(r,1) \\ &< f(2,1) - f(r,1) + f(r-1,2) - f(r,1) \\ &< f(r-1,2) - f(r,1) < 0. \end{aligned}$$

Thus $BID(G') < BID(G)$.

Case 2. vv_1 is a leaf, while vv_2 is not (the symmetric case where vv_2 is a leaf and vv_1 is not can be treated similarly). Then $d_{G'}(v) = d_G(v) - 1 = r - 1$ and $d_{G'}(v_2^q) = d_G(v_2^q) + 1 = 2$. By conditions (i), (ii), and $r \geq 3$, we have

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=2}^{r}[f(r-1, d_G(v_i)) - f(r, d_G(v_i))] + f(2,2) - f(r,1) \\ &< f(2,2) - f(3,1) < 0. \end{aligned}$$

Hence, $BID(G') < BID(G)$.

Case 3. Neither vv_1 nor vv_2 is a leaf. Analogously to Case 2, by conditions (i), (iii), and $r \geq 3$, we deduce

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=2}^{r}[f(r-1, d_{G'}(v_i)) - f(r, d_G(v_i))] + 2f(2,2) - f(r,2) - f(2,1) \\ &< 2f(2,2) - f(3,2) - f(2,1) < 0. \end{aligned}$$

Therefore $BID(G') < BID(G)$.

(2) Now suppose that $v \in V(C) \cup P_{wu} \backslash \{w, u\}$ and $d_G(v) \geq 4$. It follows that some vertex v contained in the path P_{wu} such that $d_G(v) \geq 4$. Let $d_G(v) = r \geq 4$ and $N_G(v) = \{v_1, v_2, \cdots, v_r\}$, where $v_{r-1}, v_r \in V(C)$ or $v_{r-1}, v_r \in V(P_{wu})$. Since $d_G(v) = r \geq 4$, there exist at least two additional paths $vv_1v_1^2 \cdots v_1^p$ and $vv_2v_2^2 \cdots v_2^q$ attached at v, other than v_{r-1} and v_r. Applying the same method as in (1), we can construct a new graph $G' \in \mathbb{U}_{n,\Delta}$ by Transformation 1, and the desired result also holds. □

Lemma 3.2. *Let P_{wu} be a path in $G \in \mathbb{U}_{n,\Delta}$ connecting w and u, where $d_G(u) = \Delta$, $w \in V(C)$, and $u \notin V(C)$. Suppose that $d_G(v) \geq 3$ for every vertex $v \in V(G) \backslash \{w, u\}$. If $f(x, y)$ meets the conditions listed below:*

(i) $f(x, y)$ is strictly increasing with respect to the variable x;

(ii) $f(x-1, 2) < f(x, 1)$ holds for all $x \geq 3$;

(iii) $f(x, 2)$ is strictly convex with respect to x.

(iv) $f(x, 2) - f(x, 1)$ is strictly decreasing with respect to x,

then there exists $G' \in \mathbb{U}_{n,\Delta}$, such that $BID(G') < BID(G)$.

Proof. By the given conditions, assume that $d_G(u) = \Delta$ and $N_G(u) = \{u_1, u_2, \cdots, u_\Delta\}$. Let another vertex whose degree is larger than 2 be v such that $d_T(v) = r \geq 3$ and $N_T(v) = \{v_1, v_2, \cdots, v_r\}$, where v_r is the vertex at maximum length from u to v. Given that G is a unicyclic graph, we can find a vertex $w \in V(C)$ with $d_G(w) \geq 3$.

On one hand, if there exists $v \in V(G) \backslash (V(C) \cup P_{wu})$ with $d(v) \geq 3$; or $v \in (V(C) \cup P_{wu}) \backslash \{u, w\}$ with $d(v) \geq 4$, then the result follows from Lemma 3.1. Therefore, it is enough to verify that if $v \in (V(C) \cup P_{wu}) \backslash \{u, w\}$ with $d(v) = 3$, then there exists $G' \in \mathbb{U}_{n,\Delta}$ such that $BID(G') < BID(G)$. We only consider the case $v \in P_{wu}$, since the case $v \in V(C)$ can be proved similarly.

On the other hand, if $d_G(w) \geq 5$, then at least two pendant paths are incident to w. Thus, similarly to Lemma 3.1, we can construct $G' \in \mathbb{U}_{n,\Delta}$ by Transformation 1 such that $BID(G') < BID(G)$.

Combining the above two cases, under the condition $v \in P_{wu}$ and $d(v) = 3$, we conclude the proof by distinguishing the cases $d_G(w) = 3$ or 4.

Case 1. $d_G(w) = 4$. Then there is a pendant path $ww_1w_1^2 \cdots w_1^p$ incident to w, where $d_G(w_1^p) = 1$. Since $N_G(u) = \{u_1, u_2, \cdots, u_\Delta\}$, we may assume that $uu_\Delta u_\Delta^2 \cdots u_\Delta^q$ is a path incident to uu_Δ. Then G is depicted in Figure 3.

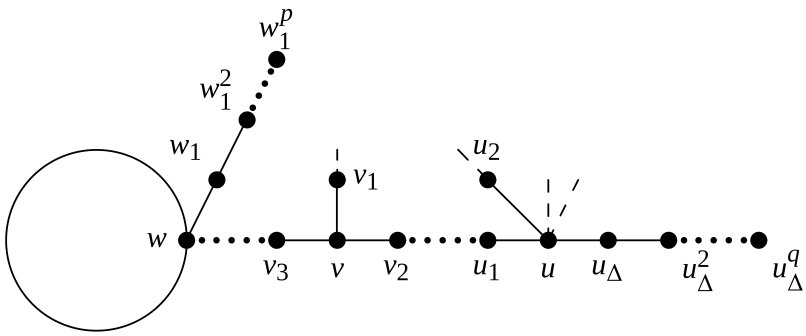

Figure 3. Graph G in Transformation 2.

Transformation 2: $G' = G - ww_1 + w_1u_\Delta^q$.

Then $G' \in \mathbb{U}_{n,\Delta}$. We distinguish four subcases according to whether ww_1 and uu_Δ are leaves.

Case 1.1. Both ww_1 and uu_Δ are leaves. By condition (iv), we have $f(\Delta,2)-f(\Delta,1) \le f(3,2)-f(3,1)$. By condition (ii), $f(3,2) < f(4,1)$. Thus, combined with condition (i), we deduce that

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=2}^{4}[f(3,d_G(w_i)) - f(4,d_G(w_i))] + f(\Delta,2) - f(\Delta,1) + f(2,1) - f(4,1) \\ &< f(3,2) - f(3,1) + f(2,1) - f(4,1) < 0. \end{aligned}$$

Hence $BID(G') < BID(G)$.

Case 1.2. Neither ww_1 nor uu_Δ is a leaf. By Transformation 2 and conditions (i) and (iii), we have

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=2}^{4}[f(3,d_T(w_i)) - f(4,d_T(w_i))] + 2f(2,2) - f(2,1) - f(4,2) \\ &< 2f(2,2) - f(2,1) - f(4,2) \\ &< 2f(2,2) - f(2,1) - f(3,2) < 0. \end{aligned}$$

Thus $BID(G') < BID(G)$.

Case 1.3. ww_1 is not a leaf, and uu_Δ is a leaf. By condition (ii), $f(2,2) < f(3,1)$. By condition (iv), $f(\Delta,2) - f(\Delta,1) \le f(3,2) - f(3,1)$. Thus, combined with condition (i), we deduce that

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=2}^{4}[f(3,d_T(w_i)) - f(4,d_T(w_i))] + f(\Delta,2) - f(\Delta,1) + f(2,2) - f(2,4) \\ &< f(\Delta,2) - f(\Delta,1) + f(2,2) - f(4,2) \\ &\le f(3,2) - f(3,1) + f(2,2) - f(4,2) \\ &< f(3,2) - f(4,2) < 0. \end{aligned}$$

That is, $BID(G') < BID(G)$.

Case 1.4. ww_1 is a leaf, and uu_Δ is not a leaf. By Transformation 2, conditions (i) and (ii), we have

$$\begin{aligned} BID(G') - BID(G) &= \sum_{i=2}^{4}[f(3,d_T(w_i)) - f(4,d_T(w_i))] + f(2,2) - f(4,1) \\ &< f(2,2) - f(4,1) < 0. \end{aligned}$$

Hence, $BID(G') < BID(G)$.

Case 2. $d_G(w) = 3$. Since $d_G(v) = 3$, the three subpaths incident to v are $vv_1v_1^2 \cdots v_1^p$, $vv_2 \cdots u_1u$, and $vv_3 \cdots w$. Since $N_G(u) = \{u_1, u_2, \cdots, u_\Delta\}$, we may assume that $uu_\Delta u_\Delta^2 \cdots u_\Delta^q$ is a path incident to uu_Δ, where $d_G(v_1^p) = d_G(u_\Delta^q) = 1$. The graph G is illustrated in Figure 4.

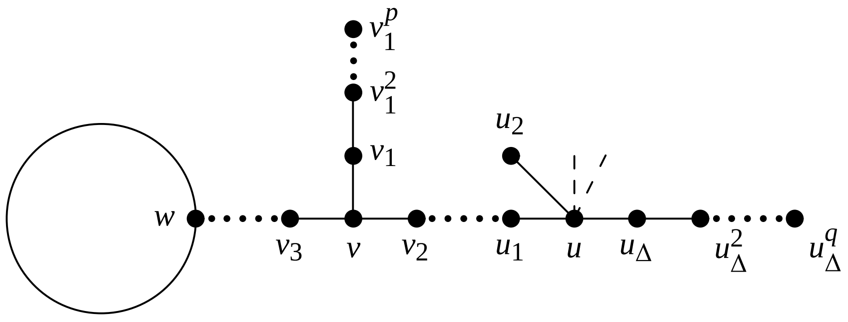

Figure 4. Graph G in Transformation 3.

Transformation 3: $G' = G - vv_1 + v_1u_\Delta^q$.

Then $G' \in \mathbb{U}_{n,\Delta}$. Analogous to Transformation 2 in Case 1, we split into four subcases based on whether vv_1 and uu_Δ are leaf edges. A case-by-case analysis yields $BID(G') < BID(G)$.

Therefore, combining all cases above, the proof of the lemma is complete. □

Let $\mathcal{U}(P^3, P^4, \cdots, P^\Delta) \in \mathbb{U}_{n,\Delta}$ be the graph obtained by attaching $\Delta - 2$ paths $P^3, P^4, \cdots, P^\Delta$ to a common vertex of a cycle C. By the two preceding lemmas, we can further derive the following result.

Lemma 3.3. *Let $G \in \mathbb{U}_{n,\Delta}^{min}$. If $f(x, y)$ meets the conditions listed below:*

(i) $f(x, y)$ is strictly increasing with respect to x;

(ii) $f(x - 1, 2) < f(x, 1)$ holds for all $x \geq 3$;

(iii) $f(x, 2)$ is strictly convex for x;

(iv) $f(x, 2) - f(x, 1)$ is strictly decreasing with x,

then $G \in \mathcal{U}(P^3, P^4, \cdots, P^\Delta)$.

Proof. Let $G \in \mathbb{U}_{n,\Delta}^{min}$. By Lemma 3.2, all vertices are of degree at most 2 other than the maximum-degree vertex u and $w \in V(C)$. We first establish the following claim.

Claim 1. $d(w) = 3$.

Otherwise, if $d(w) = 5$, then similarly to Lemma 3.1, we can apply Transformation 1 to obtain $BID(G') < BID(G)$, which contradicts $G \in \mathbb{U}_{n,\Delta}^{min}$. If $d(w) = 4$, then similarly to Case 1 in Lemma 3.2, Transformation 2 yields $BID(G') < BID(G)$, again contradicting $G \in \mathbb{U}_{n,\Delta}^{min}$. □

Accordingly, $d_G(w) = 3$ and $d_G(u) = \Delta$. For convenience, let $N_G(u) = \{u_1, u_2, \cdots, u_\Delta\}$ and $N_G(w) = \{w_1, w_2, w_3\}$, where w_3 and u_1 lie on the path wu, and w_3 may coincide with u_1.

Claim 2. $u = w$.

Suppose otherwise that $u \neq w$. Then G is depicted in Figure 5. We perform the following Transformation 4.

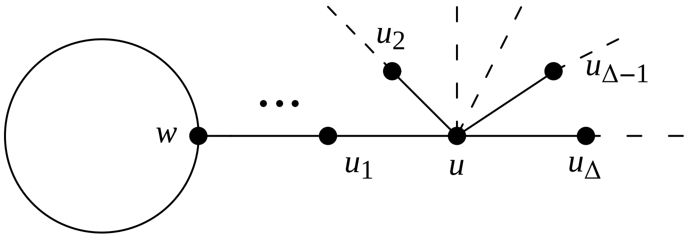

Figure 5. Graph G in Transformation 4.

Transformation 4. $G^* = G - \{uu_i | 2 \le i \le \Delta - 2\} + \{wu_i | 2 \le i \le \Delta - 2\}$.

By Transformation 4, we have

$$BID(G^*) - BID(G) = \sum_{i=\Delta-1}^{\Delta} (f(3, d_G(u_i)) - f(\Delta, d_G(u_i))) + 2f(\Delta, 2) - 2f(3, 2).$$

Since $1 \le d_G(u_i) \le 2$ for $\Delta - 1 \le i \le \Delta$, three cases arise: $d_G(u_\Delta) = d_G(u_{\Delta-1}) = 1$; $d_G(u_\Delta) = d_G(u_{\Delta-1}) = 2$; and $d_G(u_\Delta) = 1$, $d_G(u_{\Delta-1}) = 2$. Substituting these three cases into the above expression, we obtain

$$\begin{aligned} BID(G^*) - BID(G) &= 2(f(\Delta, 2) - f(\Delta, 1) + f(3, 1) - f(3, 2)) < 0, \\ BID(G^*) - BID(G) &= 2(f(\Delta, 2) - f(\Delta, 2) + f(3, 2) - f(3, 2)) = 0, \\ BID(G^*) - BID(G) &= f(\Delta, 2) - f(\Delta, 1) + f(3, 1) - f(3, 2) < 0, \end{aligned}$$

where $f(\Delta, 2) - f(\Delta, 1) + f(3, 1) - f(3, 2) < 0$ follows from condition (iv).

Thus, $BID(G^*) \le BID(G)$, and G^* is isomorphic to the graph G in Lemma 3.1. Similarly to Lemma 3.1, we apply Transformation 1 to the two edges incident to u in G^* to obtain a graph G' such that $BID(G') < BID(G^*)$. Hence,

$$BID(G') < BID(G^*) \le BID(G),$$

which contradicts $G \in \mathbb{U}_{n,\Delta}^{min}$. □

Therefore, in G, the equality $u = w$ implies that there is precisely one vertex with degree at least 3, and simultaneously, this vertex is both the maximum-degree vertex and lies on the cycle C. That is, $G \in \mathcal{U}(P^3, P^4, \cdots, P^\Delta)$. □

Before establishing the subsequent theorem, we define two classes of unicyclic graphs $\mathcal{U}_{n,\Delta}^1, \mathcal{U}_{n,\Delta}^2 \in \mathbb{U}_{n,\Delta}$ as follows:

Let $\mathcal{U}_{n,\Delta}^1$ denote the graph formed by appending $\Delta - 2$ paths P_j (each of length no less than 2) to a common vertex of a cycle C_i with $i \ge 3$.

Let $\mathcal{U}_{n,\Delta}^2$ denote the graph constructed by joining $2\Delta - n + 1$ pendant edges P_2 and $n - \Delta - 1$ paths P_3 of length 2 to a common vertex of a 3-cycle C_3.

Theorem 3.1. *Let $G \in \mathbb{U}_{n,\Delta}$, where $3 \le \Delta \le n - 2$ and $n \ge 5$. If $f(x, y)$ meets the conditions listed below:*

(i) $f(x, y)$ is strictly increasing with respect to x;

(ii) $f(x - 1, 2) < f(x, 1)$ holds for all $x \ge 3$;

(iii) $f(x,2)$ *is strictly convex with respect to x;*

(iv) $f(x,2) - f(x,1)$ *is strictly decreasing in x,*

then the following statements hold:

(1) For $3 \le \Delta \le \lfloor \frac{n+1}{2} \rfloor$,

$$BID(G) \ge \Delta f(\Delta, 2) + (\Delta - 2) f(2,1) + (n + 4 - 2\Delta) f(2,2),$$

and the equality occurs iff $G \cong \mathcal{U}^1_{n,\Delta}$.

(2) For $\lfloor \frac{n+1}{2} \rfloor < \Delta \le n-2$,

$$BID(G) \ge (n + 1 - \Delta) f(\Delta, 2) + (2\Delta - n - 1) f(\Delta, 1) + (n - \Delta - 1) f(2,1) + f(2,2),$$

and the equality occurs iff $G \cong \mathcal{U}^2_{n,\Delta}$.

Proof. Let $G \in \mathbb{U}^{min}_{n,\Delta}$. Using Lemma 3.3, we derive $G \in \mathcal{U}(P^3, P^4, \cdots, P^\Delta)$, where P_i are $\Delta - 2$ paths with lengths k_i. Without loss of generality, assume $k_3 \ge k_4 \ge \cdots \ge k_\Delta$.

(1) For $3 \le \Delta \le \lfloor \frac{n+1}{2} \rfloor$, we claim that $k_\Delta \ge 2$. Otherwise, $k_\Delta = 1$. We distinguish two cases.

Case 1. $k_3 \ge 3$. Let $P_3 = uu_3u_3^2 \cdots u_3^r$ and $P_\Delta = uu_\Delta$, where $r = k_3 \ge 3$.

Transformation 5: $G' = G - u_3^{r-1}u_3^r + u_3^r u_\Delta$.

By condition (iv) and $\Delta \ge 3$, we obtain

$$BID(G') - BID(G) = f(\Delta, 2) - f(\Delta, 1) + f(2,1) - f(2,2) < 0.$$

This contradicts $G \in \mathbb{U}^{min}_{n,\Delta}$.

Case 2. $k_3 = 2$. Immediately, we derive $|E(C)| \ge 4$. Take v_1, v_2, v_3 to be three distinct vertices of cycle C other than u; such that $v_1v_2, v_2v_3 \in E(C)$. We construct the following transformation.

Transformation 6: $G' = G - v_1v_2 - v_2v_3 + v_1v_3 + v_2u_\Delta$.

Similar to Transformation 5, by condition (iv) and $\Delta \ge 3$, we have

$$BID(G') - BID(G) = f(\Delta, 2) - f(\Delta, 1) + f(2,1) - f(2,2) < 0.$$

This contradicts $G \in \mathbb{U}^{min}_{n,\Delta}$.

Therefore, $k_\Delta \ge 2$. From the structure of the graph, we conclude that

$$BID(G) \ge BID(G) \ge \Delta f(2, \Delta) + (n + 4 - 2\Delta) f(2,2) + (\Delta - 2) f(2,1),$$

with equality iff $G \cong \mathcal{U}^1_{n,\Delta}$.

(2) For $\lfloor \frac{n+1}{2} \rfloor < \Delta \le n-2$, we claim that $k_3 \le 2$ and $|E(C)| = 3$. Suppose otherwise. From $\lfloor \frac{n+1}{2} \rfloor < \Delta$, we have $2(\Delta - 2) > n - 3$, which implies $k_3 \ge 3$ or $|E(C)| \ge 4$. Applying Transformations 5 and 6 similarly to part (1), we obtain $BID(G') < BID(G)$, contradicting $G \in \mathbb{U}^{min}_{n,\Delta}$.

Thus, $k_3 \le 2$ and $|E(C)| = 3$. From the structure of the graph, we have

$$BID(G) \ge (n + 1 - \Delta) f(\Delta, 2) + (2\Delta - n - 1) f(\Delta, 1) + (n - \Delta - 1) f(2,1) + f(2,2),$$

and the equality occurs iff $G \cong \mathcal{U}^2_{n,\Delta}$.

Combining (1) and (2), the theorem is proved. □

4. Application

This section is devoted to verifying that the bond incident degree indices satisfy the sufficient conditions for achieving the smallest *BID* value among unicyclic graphs, where the three sufficient conditions were derived in the previous two sections. Direct computation yields the following propositions, and detailed derivations are omitted for brevity.

Proposition 4.1. *The bond incident degree indices numbered 1 to 5 in Table 1 satisfy the following conditions:*
(i) $f(x,y)$ *is strictly increasing in* x*;*
(ii) $f(x-1,2) < f(x,1)$ *holds for all* $x \geq 3$*;*
(iii) $2f(2,2) < f(2,3) + f(2,1)$ *holds.*

Proof. We only verify that the function $f(x,y) = (x^2+y^2)^\alpha$ with $1/2 \leq \alpha < 1$ satisfies conditions (i), (ii), and (iii); and omit the remaining cases.

(i) Fixing y, we have

$$\frac{\partial f}{\partial x} = 2\alpha x(x^2+y^2)^{\alpha-1} > 0,$$

so $f(x,y)$ is strictly increasing with respect to x.

(ii) Since t^α is strictly increasing for $t > 0$ and $\alpha > 0$, we only need to compare the bases

$$x^2 + 1 - ((x-1)^2 + 4) = 2x - 4.$$

For $x \geq 3$, $2x - 4 \geq 2 > 0$, which implies $x^2 + 1 > (x-1)^2 + 4$. Raising both sides to the power α, we obtain $f(x-1,2) < f(x,1)$.

(iii) Substitute $x = 2$ into the the function

$$2f(2,2) = 2 \cdot 8^\alpha, \quad f(2,3) + f(2,1) = 13^\alpha + 5^\alpha.$$

Define $g(t) = 13^t + 5^t - 2 \cdot 8^t$ for $t \in [\frac{1}{2}, 1)$. Direct computation gives $g(1) = 2 > 0$ and $g(\frac{1}{2}) = \sqrt{13} + \sqrt{5} - 4\sqrt{2} > 0$. Its derivative satisfies

$$g'(t) = 13^t \ln 13 + 5^t \ln 5 - 2 \cdot 8^t \ln 8 > 0$$

over this interval, so $g(\alpha) > 0$. Consequently, $2f(2,2) < f(2,3) + f(2,1)$. □

Table 1. The minimum *BID* of some bond incident degree indices.

No.	Indices	$f(x,y)$	$\mathbb{U}_{n,g}^{min}$	$\mathbb{U}_{n,\Delta}^{min}$
1	Sombor index	$\sqrt{x^2+y^2}$	$\mathcal{G}_{n,g}$ [22]	$\mathcal{U}_{n,\Delta}^i$ [18]
2	Reduced Sombor index	$\sqrt{(x-1)^2+(y-1)^2}$	$\mathcal{G}_{n,g}$	$\mathcal{U}_{n,\Delta}^i$
3	Euler Sombor index	$\sqrt{x^2+y^2+xy}$	$\mathcal{G}_{n,g}$ [24]	$\mathcal{U}_{n,\Delta}^i$
4	General Sombor index	$(x^2+y^2)^\alpha$ $(1/2 \leq \alpha < 1)$	$\mathcal{G}_{n,g}$	$\mathcal{U}_{n,\Delta}^i$
5	Elliptic Sombor index	$(x+y)\sqrt{x^2+y^2}$	$\mathcal{G}_{n,g}$	
6	Hyperbolic Sombor index	$\sqrt{x^2+y^2}/min\{x,y\}$	$\mathcal{G}_{n,g}$	
7	Diminished Sombor index	$\sqrt{x^2+y^2}/(x+y)$	$\mathcal{G}_{n,g}$	

Proposition 4.2. *The bond incident degree indices listed as 6 and 7 in Table 1 satisfy the following conditions:*

(i) Both $f(x,2)$ and $f(x,1)$ are strictly increasing in $x \geq 2$;

(ii) $f(3,2) < f(4,1)$ and $2f(2,2) < f(4,2) + f(2,1)$;

(iii) $f(2,2) \leq f(x,y)$ for all $x,y \geq 1$ with $(x,y) \neq (1,1)$;

(iv) $3f(3,2) < f(3,1) + 2f(2,2)$ and $3f(3,2) < 2f(2,1) + f(2,2)$.

Proposition 4.3. *The bond incident degree indices numbered 1 to 4 in Table 1 match the requirements:*

(i) $f(x,y)$ is strictly increasing for x;

(ii) $f(x-1,2) < f(x,1)$ holds for all $x \geq 3$;

(iii) $f(x,2)$ is strictly convex in x;

(iv) $f(x,2) - f(x,1)$ is strictly decreasing for x.

Consequently, combining the results from Properties 4.1, 4.2 and Theorems 2.1, 2.2, we derive the following conclusion regarding the smallest BID value among unicyclic graphs having fixed girth, which is presented in Theorem 4.1. From Property 4.3 and Theorem 3.1, we derive the result on the minimum BID value with fixed maximum degree, as shown in Theorem 4.2.

In particular, References [22] and [24] confirmed that $\mathcal{G}_{n,g}$ attains the minimal Sombor index and minimal Euler Sombor index over the family $\mathbb{U}_{n,g}$, respectively. Meanwhile, Reference [18] proved that $\mathcal{U}^i_{n,\Delta}$ yields the minimum Sombor index among all graphs in $\mathbb{U}_{n,\Delta}$. This paper extends the aforementioned results to the seven Sombor-type indices presented in Table 1.

Theorem 4.1. *Let $G \in \mathbb{U}_{n,g}$. For the bond incident degree indices listed in Table 1, we have*

$$BID(G) \geq \begin{cases} 3f(3,2) + (n-4)f(2,2) + f(2,1), & g \leq n-2, \\ 2f(3,2) + (n-3)f(2,2) + f(3,1), & g = n-1, \\ nf(2,2), & g = n, \end{cases}$$

with equality iff $G \cong \mathcal{G}_{n,g}$ when $g \leq n-2$, $G \cong G_{n,n-1}$ when $g = n-1$, and $G \cong C_n$ when $g = n$.

Theorem 4.2. *Let $G \in \mathbb{U}_{n,\Delta}$, where $3 \leq \Delta \leq n-2$ and $n \geq 5$. For the bond incident degree indices listed from 1 to 4 in Table 1, we have*

(1) For $3 \leq \Delta \leq \lfloor \frac{n+1}{2} \rfloor$,

$$BID(G) \geq \Delta f(\Delta,2) + (\Delta-2)f(2,1) + (n+4-2\Delta)f(2,2),$$

and the equality occurs iff $G \cong \mathcal{U}^1_{n,\Delta}$.

(2) For $\lfloor \frac{n+1}{2} \rfloor < \Delta \leq n-2$,

$$BID(G) \geq (n+1-\Delta)f(\Delta,2) + (2\Delta-n-1)f(\Delta,1) + (n-1-\Delta)f(2,1) + f(2,2),$$

and the equality occurs iff $G \cong \mathcal{U}^2_{n,\Delta}$.

5. Concluding remarks

This paper systematically investigates the minimum bond incident degree indices for two families of unicyclic graphs: unicyclic graphs with fixed girth and those with fixed maximum degree. For the symmetric function $f(x, y)$ appearing in the definition of the BID index, we derive sufficient conditions for extremal values by analyzing structural properties of graphs and employing a variety of graph transformations, and we characterize two types of extremal graphs $\mathcal{G}_{n,g}$ and $\mathcal{U}^i_{n,\Delta}$ that attain the extremal BID values.

As applications, we verify that seven mainstream Sombor-type indices satisfy the sufficient conditions established in this paper, including the general Sombor index with parameter range $\frac{1}{2} \leq \alpha < 1$, the hyperbolic Sombor index, and the diminished Sombor index.

This work unifies the extremal problems of multiple degree-based topological indices within a consistent bond incident degree research framework, laying a theoretical foundation for analyzing extremal structures of chemical molecular graphs. Future research can extend the transformation methods proposed herein to molecular graphs with more complicated structures, such as bicyclic graphs and multicyclic graphs.

Use of Generative-AI tools declaration

The author declares that they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The author declares no conflict of interest.

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