MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **96** (2026) 753–775
ISSN: 0340–6253
doi: 10.46793/match.96-2.19725

On the Difference between Bond Additive Indices and Their Edge Versions

Liju Alex[a], **Muhammad Imran**[b,*]

[a] *Bishop Chulaparambil Memorial College, Kottayam-686001, India*
[b] *Department of Electrical Engineering,*
Prince Mohammad Bin Fahd University (PMU),
P.O. Box 1664, Al Khobar 31952, Saudi Arabia
lijualex0@gmail.com, imrandhab@gmail.com

(Received August 18, 2025)

Abstract

Bond additive indices are a special class of topological indices (TI) that are determined by the sum of the edge contributions of graphs. The Szeged index, PI index, Mostar index, and their edge versions are among the most extensively studied bond additive indices. In this paper, we investigate the difference between bond additive indices and their respective edge versions, denoted by ΔTI. Specifically, we study this problem for the Szeged index, PI index, and Mostar index. We obtain upper and lower bounds for ΔTI for different classes of graphs such as trees, unicyclic graphs, and bicyclic graphs, and identify the graphs that attain these bounds. Furthermore, we characterize the graphs that satisfy the property $\Delta TI = 0$ within these graph classes.

1 Introduction

Topological indices are numerical quantities associated with graphs that provide physical information about the chemical compounds derived from

*Corresponding author.

the underlying graph structures. Since the introduction of the first topological index, the Wiener index ($W(G)$) [27], a large number of topological indices have been studied and analyzed.

Bond additive indices form a major subclass of topological indices, where the index is computed as the sum of edge contributions. Several bond additive indices are available in the literature. For further reading, see [3, 8, 16, 23, 26].

Let $G = (V(G), E(G))$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For each edge $e = uv$ in G, define the following sets:

$$N_u(e|G) = \{w \in V(G) : d(u, w) < d(v, w)\}$$
$$N_v(e|G) = \{w \in V(G) : d(v, w) < d(u, w)\}$$
$$M_u(e|G) = \{e' \in E(G) : d(u, e') < d(v, e')\}$$
$$M_v(e|G) = \{e' \in E(G) : d(v, e') < d(u, e')\}$$

Here, $d(u, v)$ denotes the distance between vertices u and v, and $d(u, e)$ denotes the distance between a vertex u and an edge $e = xy$, defined as $d(u, e) = \min\{d(u, x), d(u, y)\}$. The cardinalities of these sets are denoted by $n_u(e|G)$, $n_v(e|G)$, $m_u(e|G)$, and $m_v(e|G)$ respectively.

Using these parameters, Gutman [15], Khadikar *et al.* [22], and Došlić *et al.* [14] proposed three different bond additive indices: the Szeged index, PI index, and Mostar index. They are defined as follows:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e|G) \cdot n_v(e|G)$$
$$PI(G) = \sum_{e=uv \in E(G)} (n_u(e|G) + n_v(e|G))$$
$$Mo(G) = \sum_{e=uv \in E(G)} |n_u(e|G) - n_v(e|G)|$$

Analogous edge-based versions of these indices were introduced and studied more recently [9, 17, 24]. They are defined as:

$$Sz_e(G) = \sum_{e=uv \in E(G)} m_u(e|G) \cdot m_v(e|G)$$

$$PI_e(G) = \sum_{e=uv\in E(G)} (m_u(e|G) + m_v(e|G))$$

$$Mo_e(G) = \sum_{e=uv\in E(G)} |m_u(e|G) - m_v(e|G)|$$

For more on these bond additive indices and related concepts, see [1–4, 8, 11–13, 16, 21, 26].

Several such indices and their edge versions exist in the literature. For certain classes of graphs, the vertex and edge versions of these bond additive indices may coincide. The present study is focused on analyzing the difference between the vertex and edge versions of topological indices. The investigation also includes identifying classes of graphs where these versions coincide, along with determining bounds on the difference for various graph families.

Throughout this paper, TI_v and TI_e denote the vertex and edge versions of a topological index, respectively. The difference in the contribution of an edge e in the vertex and edge versions is represented by $\Delta TI(e) = TI_v(e) - TI_e(e)$.

To proceed further, the following definitions are proposed.

Definition 1. Let TI_v denote the vertex version and TI_e the corresponding edge version of a topological index. The difference between them is denoted by ΔTI, and is defined as:

$$\Delta TI(G) = TI_v(G) - TI_e(G) = \sum_{e\in E(G)} \Delta TI(e)$$

For the PI index, Mostar index, and Szeged index, this is denoted by ΔPI, ΔMo, and ΔSz, respectively.

The absolute difference of these quantities is defined as follows:

Definition 2. Let $G = (V(G), E(G))$ be a connected graph. For each edge $e = uv$, let $TI_v(e)$ and $TI_e(e)$ denote its contribution in the vertex and edge versions of a topological index, respectively. Then:

$$\Delta TI'(G) = \sum_{e\in E(G)} |TI_v(e) - TI_e(e)| = \sum_{e\in E(G)} |\Delta TI(e)|$$

For PI, Mostar, and Szeged indices, these are denoted as $\Delta PI'$, $\Delta Mo'$, and $\Delta Sz'$, respectively.

Definition 3. An edge $e = uv$ of a graph G is called a *distance balanced edge* if $Mo_v(e) = 0$, and is called a *distance edge-balanced edge* if $Mo_e(e) = 0$.

The study primarily addresses the following problems:

- Determining the relationship between $TI_v(G)$ and $TI_e(G)$ for various classes of graphs.
- Establishing upper and lower bounds for ΔTI and $\Delta TI'$ across different graph classes.
- Characterizing graphs for which $TI_v(G) = TI_e(G)$ for various bond additive indices.

Only simple, finite, undirected, and connected graphs are considered throughout. Let $\mathcal{T}_n$ and $\mathcal{U}_n$ denote the sets of all trees and unicyclic graphs of order n, respectively. Let Φ_n denote the class of all bicyclic graphs of order n in which the cycles are edge-disjoint. Bounds on the quantities ΔTI and $\Delta TI'$ are established for trees, unicyclic graphs, and certain classes of bicyclic graphs of fixed order.

2 Main results

In this section, the explicit bounds of $\Delta TI(G)$ for different classes of graphs are determined. First, consider the problem in the case of trees.

Theorem 1. *For a tree T, $\Delta Mo(T) = \Delta Mo'(T) = 0$.*

Proof. For every edge $e = uv \in E(T)$, $Mo_v(e) = |n_u(e|T) - n_v(e|T)| = |n_u(e|T) - 1 - n_v(e|T) + 1| = |m_u(e|T) - m_v(e|T)| = Mo_e(e)$, therefore the result follows. ■

We extend this onto Szeged and PI indices, we have the following results.

Theorem 2. *Let $T \in \mathcal{T}_n$, then $\Delta PI(T) = \Delta PI'(T) = 2(n-1)$.*

Proof. For every edge $e = uv \in E(T)$, $PI_v(e) = n_u(e|T) + n_v(e|T) = n$ and $PI_e(e) = m_u(e|T) + m_v(e|T) = n - 2$. Clearly, for every edge $e = uv$, $PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)|$. Thus,

$$\begin{aligned}\Delta PI(T) &= \sum_{e=uv\in E(T)} PI_v(e) - \sum_{e=uv\in E(T)} PI_e(e)\\ &= \sum_{e=uv\in E(T)} n - \sum_{e=uv\in E(T)} (n-2) = \sum_{e=uv\in E(T)} 2\\ &= 2(n-1)\end{aligned}$$

■

Corollary. *For every tree T of order $n > 1$, $PI_v(T) > PI_e(T)$.*

Theorem 3. *Let $T \in \mathcal{T}_n$, then $\Delta Sz(T) = (n-1)^2$.*

Proof. Let P denote the collection of pendant edges in T and $|P| = p$. For every $e \in P$, $Sz_v(e) = n - 1$ and $Sz_e(e) = 0$. For every $e = uv \notin P$, if u is closer to $n_u(e|T)$ vertices in T than v then u must be closer to $n_u(e|T) - 1$ edges in T than v. Thus, for $e = uv \notin P$ $Sz_e(e) = (n_u(e|T) - 1)(n_v(e|T) - 1)$ or $Sz_v(e) = (m_u(e|T) + 1)(m_v(e|T) + 1)$. Thus,

$$\begin{aligned}\Delta Sz(T) &= \sum_{e=uv\in T} Sz_v(e) - \sum_{e=uv\in T} Sz_e(e)\\ &= \sum_{e=uv\in P} (n-1) + \sum_{e=uv\notin P} (m_u(e|T)+1)(m_v(e|T)+1)\\ &\quad - \sum_{e=uv\notin P} (m_u(e|T))(m_v(e|T))\\ &= p(n-1) + \sum_{e=uv\notin P} (m_u(e|T) + m_v(e|T)) + \sum_{e=uv\notin P} 1\\ &= p(n-1) + (n-1-p)(n-1) = (n-1)^2\end{aligned}$$

Since

$$\sum_{e=uv\notin P} (m_u(e|T) + m_u(e|T)) = (n-1-p)(n-2).$$

■

Corollary. *For every tree T of order $n > 1$, $Sz_v(T) > Sz_e(T)$.*

Theorem 4. *Let $T \in \mathcal{T}_n$, then $\Delta Sz'(T) = (n-1)^2$.*

Proof. For every non pendant edge $e = uv \in E(T)$

$$\begin{aligned} Sz_v(e) - Sz_e(e) &= (m_u(e|T)+1)(m_v(e|T)+1) - (m_u(e|T))(m_v(e|T)) \\ &= (m_u(e|T) + m_v(e|T)) + 1 = |(m_u(e|T) + m_v(e|T)) + 1| \\ &= |Sz_v(e) - Sz_e(e)| \end{aligned}$$

for every pendant edge $e = uv \in E(T)$

$$Sz_v(e) - Sz_e(e) = (n-1) = |Sz_v(e) - Sz_e(e)|$$

Therefore, the result follows. ■

Now, we study the difference and absolute difference of topological indices on unicyclic graphs.

Theorem 5. *Let $G \in \mathcal{U}_n$, then $\Delta Mo'(G) = b$, where b is the number of bridges in G.*

Proof. On G, let C_r be the cycle and let B denote the collection of bridges with $|B| = b$.

Case I: r is even: For every $e = uv \in B$, let u denote the vertex which is closer to the cycle than v, then $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$. Thus, for every bridge $e = uv$

$$\begin{aligned} |Mo_v(e) - Mo_e(e)| &= ||n_u(e|G) - n_v(e|G)| - |m_u(e|G) - m_v(e|G)|| \\ &= ||n_u(e|G) - n_v(e|G)| - |n_u(e|G) - n_v(e|G) + 1|| = 1 \end{aligned}$$

For every edge $e = uv \notin B$, then one edge other than the edge e in the cycle C_r is not part of the set $M_u(e|G)$ and $M_v(e|G)$(the edge diametrically opposite to e). Therefore, it does not contribute to both $m_u(e|G)$ and $m_v(e|G)$ and all the vertices are either part of $N_u(e|G)$ or $N_v(e|G)$. Thus $n_u(e|G) = m_u(e|G) + 1$ and $n_v(e|G) = m_v(e|G) + 1$. Thus, for every edge

$e = uv \notin B$.

$$
\begin{aligned}
|Mo_v(e) - Mo_e(e)| &= \Big|\, |n_u(e|G) - n_v(e|G)| - |m_u(e|G) - m_v(e|G)| \,\Big| \\
&= \Big|\, |n_u(e|G) - n_v(e|G)| \\
&\quad - |\, n_u(e|G) - 1 - n_v(e|G) + 1| \,\Big| = 0
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\Delta Mo'(G) &= \sum_{e=uv\in E} |Mo_v(e) - Mo_e(e)| \\
&= \sum_{e=uv\in B} |Mo_v(e) - Mo_e(e)| + \sum_{e=uv\notin B} |Mo_v(e) - Mo_e(e)| \\
&= \sum_{e=uv\in B} 1 + \sum_{e=uv\notin B} 0 = b
\end{aligned}
$$

Case II: r is odd: For every $e = uv \in B$, let u denote the vertex which is closer to the cycle than v, then $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$. Therefore, $|Mo_v(e) - Mo_e(e)| = 1$. Now, for every edge $e = uv \notin B$, all the edges of the cycle C_r other than $e = uv$ are part of either $M_u(e|G)$ or $M_v(e|G)$. Also, if w is the vertex on the cycle which is equi-distant from both the end vertices u and v, then all the vertices and edges of the tree T_w attached at w must of equal distance from both u and v. Therefore, corresponding to each vertex which is closer to u(or v) than v (or u) there exist an edge which closer to u(or v) than v (or u). Therefore, $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G)$. Thus, $|Mo_v(e) - Mo_e(e)| = 0$. Therefore,

$$
\begin{aligned}
\Delta Mo'(G) &= \sum_{e=uv\in E} |Mo_v(e) - Mo_e(e)| \\
&= \sum_{e=uv\in B} |Mo_v(e) - Mo_e(e)| + \sum_{e=uv\notin B} |Mo_v(e) - Mo_e(e)| \\
&= \sum_{e=uv\in B} 1 + \sum_{e=uv\notin B} 0 = b
\end{aligned}
$$

■

Let $\mathcal{C}_3$ denote the collection of all unicyclic graphs having cycle C_3.

Corollary. *For any $G \in \mathcal{U}_n$, $0 \leq \Delta Mo'(G) \leq n-3$ and the equality holds if and only if $G \cong C_n$ and $G \in \mathcal{C}_3$ respectively.*

Proof. By Theorem 5, $\Delta Mo'(G) = b$, where b is number of bridges of G. Therefore, $\Delta Mo'(G)$ is maximum when b is maximum (or the cycle length is minimum) and it is minimum when b is minimum (or the cycle length is maximum). Hence the result. ∎

Let $\mathcal{C}_3'$ denote the collection of all unicyclic graph with cycle C_3 along with no distance balanced bridges as well as no distance edge balanced bridges.

Theorem 6. *Let $G \in \mathcal{U}_n$. Then $-(n-3) \leq \Delta Mo(G) \leq 0$ and the equality holds if and only if $G \in \mathcal{C}_3'$ and $G \cong C_n$ respectively.*

Proof. Let G be the unicyclic graph with cycle C_r. Let B denote the collection of all bridges in G. Using Theorem 5, for everey edge $e = uv$, the difference $Mo_v(e) - Mo_e(e)$ is either zero or ± 1. We divide the edges of G into three categories

$$\begin{aligned}
\Delta Mo_0 &= |\{e \in E(G) : Mo_v(e) = Mo_e(e)\}| \\
\Delta Mo_1 &= |\{e \in E(G) : Mo_v(e) = Mo_e(e) + 1\}| \\
\Delta Mo_{-1} &= |\{e \in E(G) : Mo_v(e) = Mo_e(e) - 1\}|
\end{aligned}$$

Therefore, for every graph $G \in \mathcal{U}_n$

$$\Delta Mo(G) = (0).\Delta Mo_0 + (1).\Delta Mo_1 + (-1).\Delta Mo_{-1}$$

Now, by the arguments in Theorem 5, $\Delta Mo_0 = r$. The remaining $n - r$ edges are counted either in ΔMo_1 or in ΔMo_{-1}. We divide the rest into three cases.

Case I: *n is even and there exists a bridge $e = uv$ with $n_u(e|G) = n_v(e|G)$.*

For every bridge $e = uv$, $n_u(e|G) + n_v(e|G) = n$. Thus, $n_u(e|G) = n_v(e|G)$ implies $n_u(e|G) = n_v(e|G) = \frac{n}{2}$. Let u be the vertex in the edge $e = uv$ which is closer to the cycle than v. Then the $\frac{n}{2} - 1$ bridges of G closer to v and the remaining $\frac{n}{2}$ edges except the edge $e = uv$ is closer to u, therefore, the value $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$ and $n_u(e|G) > n_v(e|G)$. Thus

$$\begin{aligned} Mo_v(e) - Mo_e(e) &= |n_u(e|G) - n_v(e|G)| - |m_u(e|G) - m_v(e|G)| \\ &= n_u(e|G) - n_v(e|G) - (n_u(e|G) - (n_v(e|G) - 1)) = -1 \end{aligned}$$

Now for the remaining $\frac{n}{2} - r$ bridges closer to u than v, the value $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$ and $n_u(e|G) < n_v(e|G)$. Thus

$$\begin{aligned} Mo_v(e) - Mo_e(e) &= |n_u(e|G) - n_v(e|G)| - |m_u(e|G) - m_v(e|G)| \\ &= n_v(e|G) - n_u(e|G) - (n_v(e|G) - 1 - n_u(e|G)) = 1 \end{aligned}$$

Thus,

$$\Delta Mo(G) = (0).r + (1).(\frac{n}{2} - r) + (-1).\frac{n}{2} = -r$$

Case II: *n is odd and there exists a bridge $e = uv$ with $m_u(e|G) = m_v(e|G)$.*

For every bridge $e = uv$, $m_u(e|G) + m_v(e|G) = n - 1$. Thus, $m_u(e|G) = m_v(e|G)$ implies $m_u(e|G) = m_v(e|G) = \frac{n-1}{2}$. Let u be the vertex in the edge $e = uv$ which is closer to the cycle than v. Then the $\frac{n-1}{2} - 1$ bridges of G closer to v and the remaining $\frac{n-1}{2}$ edges except the edge $e = uv$ is closer to u, therefore, the value $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$ and $n_u(e|G) \geq n_v(e|G)$. Thus

$$Mo_v(e) - Mo_e(e) = -1$$

Now for the remaining $\frac{n+1}{2} - r$ bridges closer to u than v, the value $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$ and $n_u(e|G) < n_v(e|G)$. Thus

$$Mo_v(e) - Mo_e(e) = 1$$

Thus,

$$\Delta Mo(G) = (0).r + (1).(\frac{n+1}{2} - r) + (-1).(\frac{n-1}{2}) = -r + 1$$

Case III: There exist no bridge $\mathbf{e = uv}$ with $\mathbf{n_u(e|G) = n_v(e|G)}$ or $\mathbf{m_u(e|G) = m_v(e|G)}$: Then for every bridge $e = uv$, the value $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$ (where u is closer to the cycle than v) and $n_u(e|G) \geq n_v(e|G)$. Thus

$$Mo_v(e) - Mo_e(e) = -1$$

Therefore,

$$\Delta Mo(G) = (-1)(n - r) = -(n - r) = -n + r$$

Therefore, the maximum value ΔMo is zero and $\Delta Mo(G) = 0$ if and only if G does not have any bridges, i.e, $G \cong C_n$. Since the girth r is $3 \leq r \leq n$, $\Delta Mo(G)$ is minimum when r is minimum, thus $-(n-3) \leq \Delta Mo(G) \leq 0$.

Now, $\Delta Mo(G) = -(n-3)$ implies $r = 3$, also the graph does not have any bridge $e = uv$ with $n_u(e|G) = n_v(e|G)$ and $m_u(e|G) = m_v(e|G)$, that is $G \in \mathcal{C}_3'$ ∎

As a consequence of the theorem, we have the following results

Corollary. *For any unicyclic graph G, $\Delta Mo(G) = 0$ if and only if $G \cong C_n$.*

Corollary. *For any unicyclic graph G, $Mo_v(G) \leq Mo_e(G)$ and the equality holds if and only if $G \cong C_n$.*

Now, we study the difference and absolute difference of PI index on unicyclic graphs.

Theorem 7. *Let $G \in \mathcal{U}_n$ be a unicyclic graph with cycle C_r. Then*

$$\Delta PI(G) = \Delta PI'(G) = \begin{cases} n + r, & \text{if } r \text{ is even} \\ n - r, & \text{if } r \text{ is odd} \end{cases}$$

.

Proof. Let C_r be the cycle in G and B denote the collection of bridges in G with $|B| = b = n - r$. .

Case I: r is even: For every $e = uv \in B$, let u denote the vertex which is closer to the cycle than v, then $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$. For every edge $e = uv \notin B$, then one edge other that the edge e in the cycle C_r does not contribute to both $m_u(e|G)$ and $m_v(e|G)$ and all the vertices are either part of $N_u(e|G)$ or $N_v(e|G)$. Thus $n_u(e|G) = m_u(e|G) + 1$ and $n_v(e|G) = m_v(e|G) + 1$. Thus,

$$PI_v(e) = PI_e(e) + 1 \text{ when } e \in B$$
$$PI_v(e) = PI_e(e) + 2 \text{ when } e \notin B$$

or

$$PI_v(e) - PI_e(e) = 1 = |PI_v(e) - PI_e(e)| \text{ when } e \in B$$
$$PI_v(e) - PI_e(e) = 2 = |PI_v(e) - PI_e(e)| \text{ when } e \notin B$$

Therefore,

$$\begin{aligned}\Delta PI(G) = \Delta PI'(G) &= \sum_{e=uv\in B} PI_v(e) - PI_e(e) + \sum_{e=uv\notin B} PI_v(e) - PI_e(e) \\ &= \sum_{e=uv\in B} 1 + \sum_{e=uv\notin B} 2 = b + 2r = n + r\end{aligned}$$

Case II: r is odd: For every $e = uv \in B$, let u denote the vertex which is closer to the cycle than v, then $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$. For every edge $e = uv \notin B$, all the edge of the cycle C_r are part of either $M_u(e|G)$ or $M_v(e|G)$ and all except one vertex of the cycle is part of $N_u(e|G)$ or $N_v(e|G)$. Also, all the vertices and edges which are part of a tree incident at the vertex which is equi distant from both u and v of the cycle is not part of $N_u(e|G)$ or $N_v(e|G)$ and $M_u(e|G)$ or $M_v(e|G)$. Thus $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G)$. Therefore,

$$PI_v(e) = PI_e(e) + 1 \text{ when } e \in B$$
$$PI_v(e) = PI_e(e) \text{ when } e \notin B$$

or

$$PI_v(e) - PI_e(e) = 1 = |PI_v(e) - PI_e(e)| \text{ when } e \in B$$
$$PI_v(e) - PI_e(e) = 0 = |PI_v(e) - PI_e(e)| \text{ when } e \notin B$$

Therefore,

$$\Delta PI(G) = \Delta PI'(G) = \sum_{e=uv \in B} PI_v(e) - PI_e(e) + \sum_{e=uv \notin B} PI_v(e) - PI_e(e)$$
$$= \sum_{e=uv \in B} 1 = b = n - r \qquad \blacksquare$$

Now, as an application we determine the vertex PI index unicyclic graph of a given order having a given girth r. For convenience, we quote all the results in terms of the order of the graph G.

Theorem 8. *Let G be a unicyclic graph with n vertices and girth r, then:*

$$PI_v(G) = \begin{cases} n^2 & \text{If } r \text{ is even} \\ n^2 - n & \text{If } r \text{ is odd} \end{cases}$$

Using Theorem 7 and Theorem 8 we can directly compute the edge PI index of unicyclic graph of a fixed order [25].

Theorem 9. *Let G be a unicyclic graph with n vertices and girth r, then:*

$$PI_v(G) = \begin{cases} n^2 - n - r & \text{If } r \text{ is even} \\ n^2 - 2n + r & \text{If } r \text{ is odd} \end{cases}$$

Using these results we can directly obtain the unicylic graphs attaining the bounds of vertex PI index. Let $C_{n-1,1}$ denote the unicyclic graph of order n having the cycle C_{n-1} along with a pendant edge attached at some vertex of the cycle C_{n-1}.

Remark. If G is a unicyclic graph of order n. When n is even, then the upper and lower bounds of edge PI index is obtained for the graphs $C_{n-1,1}, C_n$ respectively. When n is odd, the upper bound and lower bounds are obtained by the graphs $C_{n-1,1}$ and C_n respectively.

Theorem 10. *Let $G \in \mathcal{U}_n$ be a unicyclic graph with cycle C_r. Then*

$$0 \leq \Delta Sz(G) = \Delta Sz'(G) \leq \begin{cases} n(n-1), & \text{if } r \text{ is even} \\ (n-r)(n-1), & \text{if } r \text{ is odd} \end{cases}$$

Proof. Divide the edges into three different sets. Let P, B, C denote the collection of all pendant edges, non pendant bridges, and edges which are part of the cycle C_r of the graph G respectively. Assume that $|P| = p$, $|B| = b$ and $|C| = n - b - p$.

Case I: r is even: For every edge $e = uv \in P$, we have $n_e(e|G)n_v(e|G) = n - 1$ and $m_e(e|G)m_v(e|G) = 0$. For every $e = uv \in B$, let u denote the vertex which is closer to the cycle than v, then $n_u(e|G) = m_u(e|G)$ and $n_v(e|G) = m_v(e|G) + 1$. For every edge $e = uv \notin B$, then one edge other that the edge e in the cycle C_r does not contribute to both $m_u(e|G)$ and $m_v(e|G)$ and all the vertices are either part of $N_u(e|G)$ or $N_v(e|G)$. Thus $n_u(e|G) = m_u(e|G) + 1$ and $n_v(e|G) = m_v(e|G) + 1$. Thus,

$$Sz_v(e) - Sz_e(e) = n - 1 = \left|Sz_v(e) - Sz_e(e)\right| \quad \text{when } e \in P$$

$$\begin{aligned} Sz_v(e) - Sz_e(e) &= n_u(e|G)\, n_v(e|G) - m_u(e|G)\, m_v(e|G) \\ &= m_u(e|G)\, m_v(e|G) + m_u(e|G) - m_u(e|G)\, m_v(e|G) \\ &= m_u(e|G) = \left|Sz_v(e) - Sz_e(e)\right| \quad \text{when } e \in B \end{aligned}$$

$$\begin{aligned} Sz_v(e) - Sz_e(e) &= n_u(e|G)\, n_v(e|G) - m_u(e|G)\, m_v(e|G) \\ &= m_u(e|G)\, m_v(e|G) + m_u(e|G) + m_v(e|G) + 1 \\ &\quad - m_u(e|G)\, m_v(e|G) \\ &= m_u(e|G) + m_v(e|G) + 1 = n - 1 = \left|Sz_v(e) - Sz_e(e)\right| \end{aligned}$$

when $e \in C$

Therefore,

$$\Delta Sz(G) = \sum_{e=uv\in P} \big(Sz_v(e) - Sz_e(e)\big) + \sum_{e=uv\in B} \big(Sz_v(e) - Sz_e(e)\big)$$

$$+\sum_{e=uv\in C}\big(Sz_v(e)-Sz_e(e)\big)$$

$$=\sum_{e=uv\in P}(n-1)+\sum_{e=uv\in B}m_u(e|G)+\sum_{e=uv\in C}(n-1) \qquad \text{(I)}$$

$$<(p+r)(n-1)+(n-r-p)(n-1)$$

$$=(p+r)(n-1)+(n-r-p)(n-1)$$

$$=n(n-1)$$

since

$$m_u(e|G)<(n-1)\ \ \forall e\in B$$

Now, the maximum value $\Delta Sz(G) = n(n-1)$ if and only if $\sum_{e=uv\in B} m_u(e|G)=0$ which is if and only if $b=0$, i.e, all the bridges are pendant edges. Also, since all the quantities of (I) are strictly positive, $\Delta Sz(G)>0$.

Case II: r is odd: For every edge $e=uv\in P$, we have $n_e(e|G)n_v(e|G) = n-1$ and $m_e(e|G)m_v(e|G)=0$. For every $e=uv\in B$, let u denote the vertex which is closer to the cycle than v, then $n_u(e|G)=m_u(e|G)$ and $n_v(e|G)=m_v(e|G)+1$. For every edge $e=uv\notin B$, all the edge of the cycle C_r are part of either $M_u(e|G)$ or $M_v(e|G)$ and all except one vertex of the cycle is part of $N_u(e|G)$ or $N_v(e|G)$. Also, all the vertices and edges which are part of a tree incident at the vertex which is equi distant from u and v of the cycle is not part of $N_u(e|G)$ or $N_v(e|G)$ and $M_u(e|G)$ or $M_v(e|G)$. Thus $n_u(e|G)=m_u(e|G)$ and $n_v(e|G)=m_v(e|G)$. Thus,

$$\begin{aligned}
Sz_v(e)-Sz_e(e) &= n-1=|Sz_v(e)-Sz_e(e)| \text{ when } e\in P\\
Sz_v(e)-Sz_e(e) &= n_u(e|G)n_v(e|G)-m_u(e|G)m_v(e|G)\\
&= m_u(e|G)m_v(e|G)+m_u(e|G)-m_u(e|G)m_v(e|G)\\
&= m_u(e|G)=|Sz_v(e)-Sz_e(e)| \text{ when } e\in B\\
Sz_v(e)-Sz_e(e) &= n_u(e|G)n_v(e|G)-m_u(e|G)m_v(e|G)\\
&= m_u(e|G)m_v(e|G)-m_u(e|G)m_v(e|G)\\
&= 0=|Sz_v(e)-Sz_e(e)| \text{ when } e\in C
\end{aligned}$$

Therefore,

$$\Delta Sz(G) = \sum_{e=uv\in P}\big(Sz_v(e) - Sz_e(e)\big) + \sum_{e=uv\in B}\big(Sz_v(e) - Sz_e(e)\big)$$
$$+ \sum_{e=uv\in C}\big(Sz_v(e) - Sz_e(e)\big)$$
$$= \sum_{e=uv\in P}(n-1) + \sum_{e=uv\in B} m_u(e|G) \qquad \text{(II)}$$
$$< (n-r)(n-1)$$

since $m_u(e|G) < (n-1)\ \ \forall e \in B$ Now, the maximum value $\Delta Sz(G) = (n-r)(n-1)$ if and only if $\sum_{e=uv\in B} m_u(e|G) = 0$ which is if and only if $b = 0$, i.e, all the bridges are pendant edges. Also, since all the quantities of (II) are positive, $\Delta Sz(G) \geq 0$. ■

Corollary. *Let G be a unicyclic graph. Then $Sz_v(G) \geq Sz_e(G)$ and the equality holds if and only if $G \cong C_n, n$ is odd.*

Proof. By Theorem 10, $\Delta Sz(G) \geq 0$. Now, $\Delta Sz(G) = 0$ implies $\Delta Sz'(G) = 0$. Thus, $Sz_v(e) = Sz_e(e)$ for every edge e. Which is if and only if $G \cong C_n, n$ odd from the arguments of the Theorem 10. ■

Now we study the value of ΔTI in the case of a special class of bicyclic graphs called Phi graphs Φ_n. Phi graphs are bicyclic graphs in which any two distinct cycles have at most one common vertex and Φ_n denote the collection of all phi graphs [1] of order n.

Theorem 11. *Let $G \in \Phi_n$ with cycles C_a and C_b. Then*

$$\Delta PI(G) = \begin{cases} a+b, & \text{if } a,b \text{ are even} \\ -(a+b)+2, & \text{if } a,b \text{ are odd} \\ a-b+1, & \text{if } a \text{ is even and } b \text{ odd} \\ -a+1+b, & \text{if } a \text{ is odd and } b \text{ is even} \end{cases}$$

and

$$\Delta PI'(G) = \begin{cases} a+b, & \text{if } a,b \text{ are even} \\ (a+b-2), & \text{if } a,b \text{ are odd} \\ a+b-1, & \text{if } a,b \text{ are of different parity} \end{cases}$$

Proof. We divide the edges of Φ_n into four different classes A, B, C, D. Let A denote the collection of all pendant edges of the graph G, B denote the collection of all non pendant bridges of G which belongs to the path connecting the two cycles of Φ_n. Let C denote the collection of all edges which belongs to the cycle in G and D denote the non pendant bridges of G which do not belong to B. Let C_a, C_b denote the cycles in G. Now, for edges $e = uv \in E(G)$, we have the following relations

- If $e = uv \in A$ then $n_u(e|G) = n - 1, n_v(e|G) = 1$ and $m_u(e|G) = n, m_v(e|G) = 0$. Thus,

$$PI_v(e) = n = PI_e(e)$$

  Therefore,

$$PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 0$$

- If $e = uv \in B$ then $n_u(e|G) = m_u(e|G), n_v(e|G) = n_v(e|G)$. Thus,

$$PI_v(e) = PI_e(e)$$

  Therefore,

$$PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 0$$

- If $e = uv \in C$. Without loss of generality, assume that v denote the vertex which is closer to the other cycle than u. When a, b are even then $n_u(e|G) = m_u(e|G) + 1, n_v(e|G) = m_v(e|G)$. Thus,

$$PI_v(e) = PI_e(e) + 1$$

Therefore,

$$PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 1$$

When a, b are odd, except for one edge in each cycle for all the other edges, we have $n_u(e|G) = m_u(e|G), n_v(e|G) = m_v(e|G) - 1$. Thus,

$$PI_v(e) = PI_e(e) - 1$$

Therefore,

$$PI_v(e) - PI_e(e) = -1 \text{ and } |PI_v(e) - PI_e(e)| = 1$$

Now, for the remaining one edge in each cycle, we have

$$n_u(e|G) = m_u(e|G), \qquad n_v(e|G) = m_v(e|G).$$

Therefore,

$$PI_v(e) = PI_e(e) \implies PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 0$$

When a even and b odd, we have,

$$PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 1 \text{ for all } e \in C_a$$

$$\begin{aligned} PI_v(e) - PI_e(e) &= -1, \\ \big|PI_v(e) - PI_e(e)\big| &= 1, \quad \text{for all except one edge in } C_b \end{aligned}$$

and for the remaining one edge,

$$PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 0$$

- If $e = uv \in D$ then $n_u(e|G) = m_u(e|G) - 1, n_v(e|G) = m_v(e|G) + 1$.

Therefore,

$$PI_v(e) - PI_e(e) = |PI_v(e) - PI_e(e)| = 0$$

Thus,

$$\begin{aligned}
\Delta PI(G) &= \sum_{e=uv \in A\cup B\cup C\cup D} \big(PI_v(e) - PI_e(e)\big) \\
&= \sum_{e=uv\in C} \big(PI_v(e) - PI_e(e)\big) \\
&= \begin{cases} a+b, & \text{if } a, b \text{ are even,} \\ -(a+b)+2, & \text{if } a, b \text{ are odd,} \\ a-b+1, & \text{if } a \text{ is even and } b \text{ odd,} \\ -a+1+b, & \text{if } a \text{ is odd and } b \text{ even.} \end{cases}
\end{aligned}$$

and

$$\begin{aligned}
\Delta PI'(G) &= \sum_{e=uv \in A\cup B\cup C\cup D} \big|PI_v(e) - PI_e(e)\big| \\
&= \sum_{e=uv\in C} \big|PI_v(e) - PI_e(e)\big| \\
&= \begin{cases} a+b, & \text{if } a, b \text{ are even,} \\ a+b-2, & \text{if } a, b \text{ are odd,} \\ a+b-1, & \text{if } a, b \text{ are of different parity.} \end{cases}
\end{aligned}$$ ■

As a consequence of the theorem, we can have the following result

Theorem 12. *Let $G \in \Phi_n$ with cycles C_a and C_b. Then*

(a.) $PI_v(G) \geq PI_e(G)$ if and only if a, b are even or a even b odd with $a \geq b+1$ or a odd b even with $b \geq a+1$

(b.) $PI_v(G) < PI_e(G)$ *if and only if* a, b *are odd or* a *even* b *odd with* $a < b + 1$ *or* a *odd* b *even with* $b < a + 1$

we can also classify the graphs in which the vertex and edge versions of PI index are equal on the graphs in Φ_n.

Theorem 13. *Let* $G \in \Phi_n$ *with cycles* C_a *and* C_b*. Then* $PI_v(G) = PI_e(G)$ *if and only*

- a *even,* b *odd with* $b = a + 1$*.*
- a *odd,* b *even with* $a = b + 1$*.*

Now, we study the absolute difference for the case of Mostar indices.

Theorem 14. *Let* $G \in \Phi_n$ *with cycles* C_a *and* C_b*. Then* $\Delta Mo(G) \leq 2b - 2p + a + b$ *and*

$$\Delta Mo'(G) = \begin{cases} 2p + 2b + a + b, & \text{if } a, b \text{ are even} \\ 2p + 2b + (a + b - 2), & \text{if } a, b \text{ are odd} \\ 2p + 2b + a + b - 1, & \text{if } a, b \text{ are of different parity} \end{cases}$$

where p *denote the number of pendant edges of* G *and* b *denote the number of bridges of* G *other than the bridges on the path connecting the two cycles in* G*.*

Proof. As in the previous theorem, the edges are partitioned into four different categories with the following relationships between $|n_u(e|G) - n_v(e|G)|$ and $|m_u(e|G) - m_v(e|G)|$.

- If $e = uv \in A$ then $|n_u(e|G) - n_v(e|G)| = n - 2 = |m_u(e|G) - m_v(e|G)| - 2$. Thus, $Mo_v(e) - Mo_e(e) = -2$ and $|Mo_v(e) - Mo_e(e)| = 2$.
- If $e = uv \in B$ then $|n_u(e|G) - n_v(e|G)| = |m_u(e|G) - m_v(e|G)|$. Thus, $Mo_v(e) - Mo_e(e) = |Mo_v(e) - Mo_e(e)| = 0$.
- If $e = uv \in C$. Without loss of generality, assume that v denote the vertex which is closer to the other cycle than u. When a, b are even

then $n_u(e|G) = m_u(e|G) + 1, n_v(e|G) = m_v(e|G)$. Thus,

$$Mo_v(e) - Mo_e(e) = \pm 1, |Mo_v(e) - Mo_e(e)| = 1.$$

When a, b are odd, except one edge in each cycle for all the other edges, we have $n_u(e|G) = m_u(e|G), n_v(e|G) = m_v(e|G) - 1$. Thus,

$$Mo_v(e) - Mo_e(e) = \pm 1, |Mo_v(e) - Mo_e(e)| = 1.$$

Now, for the remaining one edge in each cycle, we have

$$n_u(e|G) = m_u(e|G), \qquad n_v(e|G) = m_v(e|G).$$

Therefore,

$$Mo_v(e) - Mo_e(e) = |Mo_v(e) - Mo_e(e)| = 0$$

When a even and b odd, we have,

$$\begin{aligned} Mo_v(e) - Mo_e(e) &= \pm 1, \\ \big|Mo_v(e) - Mo_e(e)\big| &= 1, \quad \text{for all except one edge in } C_b \end{aligned}$$

and for the remaining one edge,

$$Mo_v(e) - Mo_e(e) = |Mo_v(e) - Mo_e(e)| = 0$$

- If $e = uv \in D$ then $n_u(e|G) = m_u(e|G) - 1, n_v(e|G) = m_v(e|G) + 1$. Therefore,

$$Mo_v(e) - Mo_e(e) = \pm 2, |Mo_v(e) - Mo_e(e)| = 2$$

Therefore,

$$\Delta Mo(G) = \sum_{e=uv \in A \cup B \cup C \cup D} Mo_v(e) - Mo_e(e)$$

$$\leq \sum_{e=uv\in A} -2 + \sum_{e=uv\in B} 0 + \sum_{e=uv\in C} 1 + \sum_{e=uv\in D} 2$$
$$\leq -2p + a + b + 2b$$

Now,

$$\begin{aligned}
\Delta Mo'(G) &= \sum_{e=uv\in A\cup B\cup C\cup D} |Mo_v(e) - Mo_e(e)| \\
&= \sum_{e=uv\in A} 2 + \sum_{e=uv\in B} 0 + \sum_{e=uv\in C} 1 + \sum_{e=uv\in D} 2 \\
&= \begin{cases} 2p + 2b + a + b, & \text{if } a, b \text{ are even} \\ 2p + 2b + (a + b - 2), & \text{if } a, b \text{ are odd} \\ 2p + 2b + a + b - 1, & \text{if } a, b \text{ are of different parity} \end{cases}
\end{aligned}$$

■

3 Conclusion

In this study we have determined the difference between the vertex and edge versions of some bond additive indices for several classes of graphs. We studied this problem for tree, unicyclic graphs as well as bicyclic graphs. There are lots of other classes of graph, in which this ΔTI hasn't been explored properly. We end our study by proposing some problems for further studies.

Problem 1: Determine the bounds of $\Delta Mo(G), \Delta PI(G), \Delta Sz(G)$ for connected graphs of fixed order and characterize the graphs attaining the bounds.

Problem 2: Determine the bounds of $\Delta Mo(G), \Delta PI(G), \Delta Sz(G)$ for $c-$cyclic graphs of fixed order and characterize the graphs attaining the bounds where $c \geq 3$.

Problem 3: Determine the bounds of $\Delta Mo(G), \Delta PI(G), \Delta Sz(G)$ for cacti of fixed order having fixed number of cycles.

Problem 4: Characterize the graphs for which $\Delta TI(G) = 0$ and $\Delta TI'(G)$ $= 0$ for the case of Mostar, PI and Szeged indices.

References

[1] L. Alex, I. Gopalapillai, On a conjecture on edge Mostar index of bicyclic graphs, *Iran. J. Math. Chem.* **14** (2023) 97–108.

[2] L. Alex, I. Gopalapillai, Sharp bounds on additively weighted Mostar index of cacti, *Commun. Comb. Optim.* (2024), DOI: `https://doi.org/10.22049/cco.2024.28757.1702`.

[3] L. Alex, I. Gopalapillai, J. J. Mulloor, On the inverse problem of some bond additive indices, *Commun. Comb. Optim.* (2024), DOI: `https://doi.org/10.22049/cco.2024.29470.2019`.

[4] L. Alex, I. Gutman, On the inverse Mostar index problem for molecular graphs, *Trans. Comb.* **14** (2025) 65–77.

[5] L. Alex, G. Indulal, J. T. Baby, A note on the additively weighted Mostar index of graphs, *Iran. J. Math. Chem.* **16** (2025) 155–170.

[6] L. Alex, K. C. Das, Resolving the open problem by proving a conjecture on the inverse Mostar index for c-cyclic graphs, *Symmetry* **17** (2025) #291.

[7] S. Akhter, M. Imran, Z. Iqbal, Mostar indices of SiO_2 nanostructures and melem chain nanostructures, *Int. J. Quantum Chem.* **121** (2021) #e26520.

[8] A. Ali, T. Došlić, Mostar index: Results and perspectives, *Appl. Math. Comput.* **404** (2021) #126245.

[9] M. Arockiaraj, J. Clement, N. Tratnik, Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems, *Int. J. Quantum Chem.* **119** (2019) #e26043.

[10] A. Babai, S. Mondal, K. C. Das, Szeged indices of bicyclic graphs with applications as molecular descriptor, *Croat. Chem. Acta* **96** (2023) 153—170.

[11] S. Brezovnik, N. Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, *Int. J. Quantum Chem.* **121** (2021) #e26530.

[12] X. Cai, B. Zhou, Edge Szeged index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 133–144.

[13] K. C. Das, A. R. Ashrafi, A. Ghalavand, Comparison between Szeged indices of graphs, *Quaest. Math.* **43** (2019) 1031–1046.

[14] T. Došlić, I. Martinjak, R. Škrekovski, S. Tipurić Spužević, I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018) 2995—3013.

[15] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes New York* **27** (1994) 9—15.

[16] I. Gutman, A. A. Dobrynin, The Szeged index — a success story, *Graph Theory Notes New York* **34** (1998) 37—44.

[17] I. Gutman, A. R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta* **81** (2008) 263—266.

[18] J. Hao, Some graphs with extremal PI index, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 211—216.

[19] M. Imran, M. A. Malik, R. Javed, On Szeged-type indices of titanium oxide TiO_2 nanotubes, *Int. J. Quantum Chem.* **121** (2021) #e26669.

[20] M. Imran, M. A. Malik, M. Aqib, G. I. H. Aslam, A. Ali, On Zagreb coindices and Mostar index of TiO_2 nanotubes, *Sci. Rep.* **13** (2023) #13672.

[21] G. Indulal, L. Alex, I. Gutman, On graphs preserving PI index upon edge removal, *J. Math. Chem.* **59** (2021) 1603—1609.

[22] P. V. Khadikar, On a novel structural descriptor PI, *Natl. Acad. Sci. Lett.* **23** (2000) 113—118.

[23] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, *J. Chem. Inf. Comput. Sci.* **41** (2001) 934—949.

[24] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, *Discr. Appl. Math.* **156** (2008) 1780—1789.

[25] G. Ma, Q. Bian, J. Wang, Bounds on the PI index of unicyclic and bicyclic graphs with given girth, *Discr. Appl. Math.* **230** (2017) 156—161.

[26] T. Réti, A. Ali, I. Gutman, On bond-additive and atoms-pair-additive indices of graphs, *El. J. Math.* **2** (2021) 52—61.

[27] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17—20.