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Research Paper

A Note on the Additively Weighted Mostar Index of Graphs

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Abstract

In this article, we discuss the additively weighted Mostar index, an innovative topological measure that extends the traditional Mostar index by incorporating edge weights computed as the sum of the degrees of their end point vertices. We focus on its application within the set $\mathcal{U}_n$ comprising all unicyclic graphs of order n. Our study rigorously establishes the first two sharp lower and upper bounds for this index across graphs in $\mathcal{U}_n$. Additionally, we analyze the additively weighted Mostar index of Cartesian product graphs and investigate its properties across various graph classes. Furthermore, we demonstrate the practical utility of this index by comparing its effectiveness against eight other distance-based topological indices in predicting chemical properties of octane isomers. Remarkably, we find that the additively weighted Mostar index outperforms or matches the predictive capabilities of other indices in linear models with these chemical properties, highlighting its potential in quantitative structure-property relationships. This research significantly contributes to both graph theory and chemical informatics by showcasing the unique advantages of the additively weighted Mostar index in structural analysis and predictive modeling.

1 Introduction

Let G be a simple connected graph with vertex set V and edge set E. For a vertex $v \in V$, $d(v)$ denotes the degree of the vertex v. A vertex v is a *pendant vertex* if $d(v) = 1$ and the

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corresponding edge e incident on v is a *pendant edge*. Let u, v be two vertices in V, then the *distance* between u and v is the length of the shortest $u - v$ path in G, denoted by $d(u,v)$. For any edge $e = uv$, $N_u(e|G)$ denotes the set of all vertices in G which are closer to u than v and $|N_u(e|G)| = n_u(e|G)$. A graph is distance balanced if $n_u(e|G) = n_v(e|G)$ for all $e \in E$ [1]. Throughout this paper, we consider only simple, finite, connected, undirected graphs.

Molecular graphs translate molecules as graphical structures where atoms are represented as vertices and bonds between atoms as edges. In chemical graph theory, studying molecular graphs is crucial as it provides deeper insights into the structure, composition, and physico-chemical properties of molecules. An essential tool in this analysis is the use of topological indices, numerical values associated with graphs that succinctly describe their structural features and remain unchanged regardless of the specific arrangement of vertices and edges. These indices play a vital role in predicting and understanding various chemical properties solely based on the molecular structure represented by the graph. They are instrumental in establishing quantitative relationships between molecular structure and properties, benefiting fields such as pharmaceuticals, materials science, and environmental chemistry.

The *Wiener index*, the earliest topological index, was introduced in 1947 by H. Wiener. The Wiener index $W(G)$ of a graph [2] $G = (V,E)$ is defined as

$$W(G) = \sum_{\{u,v\} \in V} d(u,v).$$

In the case of acyclic connected graphs this definition can be restated as [3]

$$W(G) = \sum_{e=uv \in E} n_u(e|G) n_v(e|G).$$

This definition was extended to non-tree graphs, which led to the introduction of the Szeged index (Sz) by I. Gutman [4]. The Szeged index was found to be very useful in studying the physico-chemical properties of chemical compounds and drugs [5, 6]. For detailed literature on the Szeged type indices, see [7–11]. In 2018, T. Došlić *et al.* proposed the Mostar index, $Mo(G)$, of a graph $G = (V,E)$ defined as

$$Mo(G) = \sum_{e=uv \in E} |n_u(e|G) - n_v(e|G)|.$$

The Mostar index measures how far a graph deviates from being distance-balanced [12]. For a detailed literature on the Mostar index, see [12–19]. Many more applications and modifications of the Mostar index can be seen in [20–22]. The additively weighted Mostar index [21, 22] ($Mo_A(G)$) is one among the modified versions. Let $G = (V,E)$ be a graph, the additively weighted Mostar index is defined as

$$Mo_A(G) = \sum_{e=uv \in E} (d(u) + d(v)) |n_u(e|G) - n_v(e|G)|.$$

Recently defined, the additively weighted Mostar index has seen limited exploration in literature. In [12], Akbar Ali and Tomislav Došlić computed extremal values of this index for trees. Additionally, in [23], two authors of this paper established upper bounds for the additively weighted Mostar index for distinct classes of cacti.

In this study, we determine extremal values of the additively weighted Mostar index for unicyclic graphs of specified order. Furthermore, we investigate the relationship between this index and the chemical properties of octane isomers and benzenoid hydrocarbons. This paper is structured as follows: Sections 1 and 2 focus on deriving the first two lower bounds and the first two upper bounds of $Mo_A(G)$ for unicyclic graphs, and exploring its correlation with various degree-based topological indices. In Section 3, we examine the correlation between the additively weighted Mostar index and chemical properties of octane isomers.

2 Main results

In this section, we derive the initial two lower bounds and upper bounds for $Mo_A(G)$ specifically for unicyclic graphs. Additionally, we discuss various properties associated with the additively weighted Mostar index. For every edge $e = uv$ in G, let $Mo_A(e|G) = (d(u) + d(v))|n_u(e|G) - n_v(e|G)|$ denotes the contribution by the edge e to the additively weighted Mostar index of G. We have the following lemmas, the proofs of which follow from the definition of $Mo_A(e|G)$.

Lemma 2.1. *Let $G = (V, E)$ be a connected graph and $e = uv \in E$. Then $Mo_A(e|G) \geq 0$ and the equality holds if and only if $n_u(e|G) = n_v(e|G)$.*

Lemma 2.2. *Let $G = (V, E)$ be a connected graph of order $n \geq 3$ and $e = uv \in E$. If e is a pendant edge then $Mo_A(e|G) > 0$.*

Lemma 2.3. *Let G be a connected graph. Then $Mo_A(G) \geq 0$ and the equality holds if and only if G is distance balanced.*

The following discussions on lower bounds are based on Lemmas 2.1 to 2.3.

Theorem 2.4. *Let $G \in \mathcal{U}_n$. Then $Mo_A(G) \geq 0$ and the equality holds if and only if $G \cong C_n$.*

Proof. According to Lemma 2.3, for any graph $G \in \mathcal{U}_n$, it holds that $Mo_A(G) \geq 0$. Consider a graph $G \in \mathcal{U}_n$ where $Mo_A(G) = 0$. This implies that G does not contain any bridge. If G did contain a bridge e, then e would belong to an induced subtree T within G, and consequently, T would include a pendant edge e'. However, by Lemma 2.2, this would lead to $Mo_A(e'|G) > 0$, which contradicts the assumption that $Mo_A(G) = 0$. Therefore, every edge of G must be part of a cycle, indicating that G is isomorphic to C_n, a cycle of length n.
Conversely, if $G = C_n$, then it is straightforward that $Mo_A(G) = 0$ since C_n does not contain any bridges. ■

Next, we establish the second smallest lower bound for the additively weighted Mostar index concerning unicyclic graphs. Consider the unicyclic graph denoted as $C_{r,p}$, which is constructed by connecting a vertex of a cycle C_r with a pendant vertex of a path of length p.
Let G_1^0 represent a unicyclic graph of order n (where n is even), comprising a cycle C_{n-2} along with two pendant edges attached at diametrically opposite vertices of the cycle C_{n-2}.

Proposition 2.5. *If $n \geq 6$, then*

(a.) $$Mo_A(C_{n-1,1}) = \begin{cases} 8n - 10, & \text{if } n \text{ is odd,} \\ 8n - 14, & \text{if } n \text{ is even,} \end{cases}$$

(b.) $Mo_A(G_1^0) = 8n - 16$, *where n is even.*

Proof. (a.) For the pendant edge e, its contribution to the additively weighted Mostar index is given by $Mo_A(e \mid C_{n-1,1}) = 4n - 8$.

If n is odd, then in the cycle C_{n-1} with $n - 1$ edges: $Mo_A(e \mid C_{n-1,1}) = 4$ for $n - 3$ edges, $Mo_A(e \mid C_{n-1,1}) = 5$ for the remaining two edges that connect C_{n-1} to the pendant edge.

Therefore, the additively weighted Mostar index $Mo_A(C_{n-1,1})$ is $8n-10$.

If n is even, then: $Mo_A(e \mid C_{n-1,1}) = 4$ for $n-4$ edges of C_{n-1} and $Mo_A(e \mid C_{n-1,1}) = 5$ for the two additional edges connecting C_{n-1} to the pendant vertex. The contribution from the remaining one edge is zero.

Thus, the additively weighted Mostar index $Mo_A(C_{n-1,1})$ in this case is $8n-14$.

(b.) In G_1^0, all edges except the pendant edges contribute zero to the additively weighted Mostar index. Hence, $Mo_A(G_1^0) = 4(n-2)+4(n-2) = 8n-16$. ∎

Let $\mathcal{U}_n|\{H\}$ denotes the collection of all unicyclic graphs of order n other than the graph H.

Corollary 2.6. *If G is a unicyclic graph in $\mathcal{U}_n|\{C_n\}$ with $n \geq 6$ which attains the minimum value of additively weighted Mostar index, then $Mo_A(G) \leq 8n-10$ if n is odd and $Mo_A(G) \leq 8n-16$ if n is even.*

Theorem 2.7. *Let $n \geq 6$. Then $C_{n-1,1}, G_1^0$ are the graphs in $\mathcal{U}_n|\{C_n\}$ with minimum value of additively weighted Mostar index for odd and even orders respectively.*

Proof. Let G be a graph which attains minimum value of additively weighted Mostar index in $\mathcal{U}_n|\{C_n\}$, $n \geq 6$. Then by Corollary 2.6, $Mo_A(G) \leq 8n-10$ if n is odd and $Mo_A(G) \leq 8n-16$ if n is even. It is evident that a pendant edge $e = uv \in G$ contributes at least $(d(u)+d(v))(n-2)$ to $Mo_A(G)$. Based on this observation, we propose the following claims about G:

Claim I: G has one or two pendant edges.

On the contrary assume that G has three or more pendant edges.

1. If at least one of these pendant edges is incident on a cycle, then $Mo_A(G) > 10n-20$. This contradicts the bound $Mo_A(G) \leq 8n-10$ for $n \geq 6$.

2. If none of the pendant edges are incident on a cycle, then there exist at most three edges $f_i, i = 1,2,3$ such that $Mo_A(f_i \mid G) \geq 4n-16$. Thus, $Mo_A(G) > 13n-34$. However, $13n-34 > 8n-10$ when $n \geq 6$, which is impossible given the upper bound provided by the corollary.

Therefore, G cannot have three or more pendant edges. Hence Claim I is established.

Consider the case where G has exactly two pendant edges e_1 and e_2. Let's analyse the following possibilities.

1. **One pendant edge is incident on a bridge:**

If one of e_1 or e_2 is incident on a bridge, there exists another edge f such that $Mo_A(f \mid G) \geq 4n-16$. Additionally, there are two more edges contributing at least 4 each. Therefore, $Mo_A(G) \geq 4(n-2)+3(n-2)+4(n-4)+8 = 11n-22$. However, $11n-22 > 8n-10$ when $n \geq 6$, which is impossible.

2. **Both pendant edges incident on the same bridge:**

If both e_1 and e_2 are incident on the same bridge f, $Mo_A(f \mid G) \geq 5(n-6)$. Additionally, two more edges contribute at least 4 each. Thus, $Mo_A(G) > 8n-16+5n-30+8 = 13n-38$. Similarly, $13n-38 > 8n-10$ when $n \geq 6$, which is impossible.

3. **Pendant edges incident on different bridges:**

If e_1 and e_2 are incident on different bridges f_1 and f_2, respectively, then $Mo_A(f_i \mid G) \geq 4n-16$ for $i = 1,2$. Therefore, $Mo_A(G) > 14n-44$. Again, $14n-44 > 8n-10$ when $n \geq 6$, which is impossible.

4. **Pendant edges incident on the cycle at the same vertex:**

If e_1 and e_2 are incident on the cycle at the same vertex, $Mo_A(G) > 10n-20$. Now $10n-20 > 8n-10$ when $n \geq 6$, which is impossible.

5. **Pendant edges incident on different vertices of the cycle with distance less than $\lfloor \frac{n-2}{2} \rfloor$:**

If e_1 and e_2 are incident on different vertices of the cycle with distance $d(e_1,e_2) < \lfloor \frac{n-2}{2} \rfloor$, then there are two more edges contributing at least 4 each to $Mo_A(G)$. Thus, $Mo_A(G) \geq 8n-8$. Again, $8n-8 > 8n-10$ is impossible.

6. **Case when n is odd and $d(e_1, e_2) = \lfloor \frac{n-2}{2} \rfloor$:**
There are no such graphs because $d(e_1, e_2) = \lfloor \frac{n-2}{2} \rfloor$ cannot be satisfied for odd n.

7. **Case when n is even and $d(e_1, e_2) = \lfloor \frac{n-2}{2} \rfloor$:**
This implies $G \cong G_1^0$, the specific unicyclic graph described earlier.
Thus we have considered all the case having at least 2 pendant edges. If G has no pendant edges, then $G \cong C_n$, which is impossible. Now consider the case that G has exactly one pendant edge and is of the form $C_{r,p}$ where $r + p = n$.

Claim II: $r = n - 1$.

Suppose $r = n - m$ where $m \geq 2$. If n and m are of the same parity, then we have

1. **Contribution from the cycle C_{n-m}:**
The $n-m-2$ edges of the cycle C_{n-m} each contribute at least $4m$ to $Mo_A(G)$. The remaining two edges in C_{n-m} incident to the path P_{m+1} contribute $5m$.

2. **Contribution from the path P_{m+1}:**
Among the m edges on the path P_{m+1}, $m-2$ edges contribute at least 4 each. The pendant edge attached to P_{m+1} contributes $3(n-2)$.

Thus, the minimum additively weighted Mostar index $Mo_A(G)$ satisfies:

$$\begin{aligned} Mo_A(G) &\geq 4m(n-m-2) + 10m + 4(m-2) + 3(n-2) \\ &\geq 8(n-m-2) + 14m + 3n - 14 \\ &= 11n + 6m - 30 \end{aligned}$$

Now, $11n + 6m - 30 \geq 11n - 18 > 8n - 10$ when $n \geq 6$ (since $m \geq 2$). This contradiction arises because $Mo_A(G)$ cannot exceed $8n - 10$ as per the given bound. Therefore, this configuration for G is impossible under the assumption that n and m have the same parity.

Suppose $r = n - m$ where n and m are of different parity: Then we have

1. **Contribution from the cycle C_{n-m}:**
At least $n - m - 3$ edges of the cycle C_{n-m} each contribute $4m$ to $Mo_A(G)$. Two edges that share a common vertex with the path P_{m+1} contribute $5m$.

2. **Contribution from the path P_{m+1}:**
Among the m edges on the path P_{m+1}, $m - 3$ edges contribute at least 4 each. One edge on P_{m+1} contributes at least 5.

3. **Contribution from the pendant edge:**
The pendant edge attached contributes $3(n - 2)$. Thus, the additively weighted Mostar index $Mo_A(G)$ satisfies:

$$\begin{aligned} Mo_A(G) &\geq 4m(n-m-3) + 10m + 4(m-3) + 5 + 3(n-2) \\ &\geq 8(n-m-3) + 14m + 3n - 13 \\ &= 11n + 6m - 37. \end{aligned}$$

Now, $11n + 6m - 37 \geq 11n - 25 > 8n - 10$ when $n \geq 6$ (since $m \geq 2$). This contradiction arises because $Mo_A(G)$ cannot exceed $8n - 10$ as per the given bound. Thus $m \geq 2$ is impossible and consequently $r = n - 1$, implying $G \cong C_{n-1,1}$. According to Proposition 2.5, $G = C_{n-1,1}$ specifically when n is odd. ■

Next, we will derive the first two upper bounds of the additively weighted Mostar index for unicyclic graphs. In the context of this discussion, a bridge that is distinct from a pendant edge is referred to as a non-trivial bridge.

Lemma 2.8. *([12]). Let $e = uv$ be a non trivial bridge of G. Let G' be the graph obtained from G by deleting the edge e, identifying its end vertices u and v to a new vertex z and adding a new vertex w connected to z by the edge e'. Then*

$$Mo_A(G') > Mo_A(G).$$

Let $U_{r,p}$ denote the unicyclic graph consisting of a cycle C_r of length r along with p pendant edges that are incident at some vertex v of C_r.

Proposition 2.9. *For $n \geq 6, r \geq 3$,*

$$Mo_A(U_{r,n-r}) = \begin{cases} n^3 - 2n^2r + 3n^2 + nr^2 + nr - 6n - 4r^2 + 6r, & \text{if } r \text{ is even,} \\ n^3 - 2n^2r + 3n^2 + nr^2 + nr - 10n - 4r^2 + 10r, & \text{if } r \text{ is odd.} \end{cases}$$

Proof. For each pendant edge e in $U_{r,n-r}$, the contribution to the additively weighted Mostar index is given by $Mo_A(e \mid U_{r,n-r}) = (n-r+3)(n-2)$. When r is even, the $r-2$ edges in the cycle C_r contribute $4(n-r)$ each and the remaining two edges contribute $2(n-r+4)(n-r)$. Thus, the additively weighted Mostar index $Mo_A(U_{r,n-r})$ is:

$$\begin{aligned} Mo_A(U_{r,n-r}) &= (n-r)(n-r+3)(n-2) + (r-2)\cdot 4(n-r) + 2(n-r+4)(n-r) \\ &= n^3 - 2n^2r + 3n^2 + nr^2 + nr - 6n - 4r^2 + 6r. \end{aligned}$$

When r is odd, except for one edge in the cycle whose contribution is zero, all other edges have the same contributions as in the previous case. Therefore, $Mo_A(U_{r,n-r})$ when r is odd is:

$$\begin{aligned} Mo_A(U_{r,n-r}) &= (n-r)(n-r+3)(n-2) + (r-3)\cdot 4(n-r) + 2(n-r+4)(n-r) \\ &= n^3 - 2n^2r + 3n^2 + nr^2 + nr - 10n - 4r^2 + 10r. \end{aligned}$$

Hence, the proof is completed. ■

Lemma 2.10. *Let $G = C_r[T_1, T_2, \ldots, T_r]$ be a unicyclic graph of order n obtained from a cycle $C_r = v_1v_2\ldots v_rv_1$ by attaching the trees T_i at the vertex v_i for $i = 1, 2, \ldots, r$. Then*

(a.) $Mo_A(G) \leq n^3 - 2n^2r + 3n^2 + nr^2 + nr - 6n - 4r^2 + 6r$, *if r is even,*

(b.) $Mo_A(G) \leq n^3 - 2n^2r + 3n^2 + nr^2 + nr - 10n - 4r^2 + 10r$, *if r is odd,*

and equality holds if and only if $G \cong U_{r,n-r}$.

Proof. By sequentially applying Lemma 2.8, we know that $Mo_A(G') \geq Mo_A(G)$, where G' is the graph obtained by attaching $|E(T_i)|$ pendant edges at vertex v_i for $i = 1, 2, \ldots, r$. Now, we aim to prove that $Mo_A(G_1) \geq Mo_A(G')$ where $G_1 = U_{r,n-r}$.

Let d_i denote the number of pendant edges attached to vertex v_i in G', and let $d = \sum_{i=1}^{r} d_i$. Suppose v_1 is the vertex in G_1 where d pendant edges are attached. Define n_i as the number of vertices in T_i, including v_i, then $n = \sum_{i=1}^{r} n_i$. We categorize the edges of G into two groups: Those edges that belong to T_i for $i = 1, 2, \ldots, r$. and those edges that belong to the cycle C_r, denoted as $e = uv \in T_i$ for $i = 1, 2, \ldots, r$ and $e = v_iv_{i+1} \in C_r$ for $i = 1, 2, \ldots, r$. Then

$$\begin{aligned} Mo_A(G') = &\sum_{i=1}^{r} \sum_{e=uv\in T_i} (d(u) + d(v))|n_u(e|G') - n_v(e|G')| \\ &+ \sum_{\substack{i=1 \\ e\in C_r}}^{r} (d(v_i) + d(v_{i+1}))|n_{v_i}(e|G') - n_{v_{i+1}}(e|G')|. \end{aligned}$$

For each edge $e = uv \in T_i, i = 1, 2, \ldots, r$, $|n_u(e|G') - n_v(e|G')| = |n_u(e|G_1) - n_v(e|G_1)| = n - 2$. Also for $e = uv_i \in T_i \cap G'$, $d(u) + d(v_i) = d_i + 3$ and for $e = uv_i \in T_i \cap G_1$, $d(u) + d(v_i) = \sum_{i=1}^{r} d_i + 3 = d + 3$. Thus

$$\sum_{i=1}^{r} \sum_{e=uv \in T_i} (Mo_A(e|G_1) - Mo_A(e|G')) = (d^2 + 3d)(n-2) - \sum_{i=1}^{r} (d_i^2 + 3d_i)(n-2)$$
$$= 2 \sum_{\substack{i,j=1 \\ i \neq j}}^{r} d_i d_j (n-2) > 0. \quad (1)$$

For $e = v_i v_{i+1} \in C_r$, we consider the following two different cases.

Case I : $r = 2k$ **is even:** For every edge $e = v_i v_{i+1} \in C_{2k}$, $|n_{v_i}(e|G') - n_{v_{i+1}}(e|G')| = (n - n_e)$, where n_e denote the diminishing factor and $|n_{v_i}(e|G_1) - n_{v_{i+1}}(e|G_1)| = (n - 2k)$, clearly $n_e \geq 2k \ \forall i = 1, 2, \ldots, 2k$, thus

$$|n_{v_i}(e|G') - n_{v_{i+1}}(e|G')| = (n - n_e) \leq |n_{v_i}(e|G_1) - n_{v_{i+1}}(e|G_1)| = (n - 2k).$$

Also $d(v_i) + d(v_{i+1}) = d_i + d_{i+1} + 4$ in G' and in G_1, $d(v_i) + d(v_{i+1}) = 4$ for $i \neq 1, 2k$ and $(d(v_i) + d(v_{i+1})) = \sum_{i=1}^{2k} d_i + 4 = d + 4$ for $i = 1, 2k$. Now, let $n - n_e^* = max\{n - n_e : e \in C_{2k}\}$. Thus

$$\sum_{\substack{i=1 \\ e=v_i v_{i+1} \in C_{2k}}}^{2k} (Mo_A(e|G_1) - Mo_A(e|G'))$$
$$= \sum_{\substack{i=2 \\ e=v_i v_{i+1}}}^{2k-1} 4(n-2k) + 2(d+4)(n-2k) - \sum_{\substack{i=1 \\ e=v_i v_{i+1}}}^{2k} (d_i + d_{i+1} + 4)(n - n_e)$$
$$\geq 8k(n-2k) + 2d(n-2k) - 2d(n - n_e^*) - 8k(n - n_e^*) \geq 0. \quad (2)$$

Since $n - 2k \geq n - n_e^* \ \forall e \in C_{2k}$. Thus from (1) and (2), $Mo_A(G_1) - Mo_A(G') \geq 0$ and $Mo_A(G) = n^3 - 2n^2 r + 3n^2 + nr^2 + nr - 6n - 4r^2 + 6r$, whenever $G \cong G_1$.

Case II: $r = 2k+1$ **is odd:** Now, for every edge $e = v_i v_{i+1} \in C_{2k+1}$, $|n_{v_i}(e|G') - n_{v_{i+1}}(e|G')| = (n - n_e - n_0)$ where n_0 denotes the number of vertices equidistant from both v_i and v_{i+1} in G' and $n_e + n_0 \geq 2k+1 \ \forall i = 1, 2, \ldots, 2k+1$. Also, $|n_{v_i}(e|G_1) - n_{v_{i+1}}(e|G_1)| = \begin{cases} (n-2k-1), & i \neq k, \\ 0, & i = k. \end{cases}$

Thus,

$$|n_{v_i}(e|G') - n_{v_{i+1}}(e|G')| = (n - n_e - n_0) \leq |n_{v_i}(e|G_1) - n_{v_{i+1}}(e|G_1)| = (n - 2k - 1).$$

Now, in G', $d(v_i) + d(v_{i+1}) = d_i + d_{i+1} + 4$ and in G_1, $d(v_i) + d(v_{i+1}) = \begin{cases} 4, & \text{for } i \neq 1, 2k+1, \\ d+4, & \text{for } i = 1, 2k+1. \end{cases}$

Also, let $n - \bar{n_e} = max\{n - n_e - n_0 : e \in C_{2k+1}\}$. Thus

$$\sum_{\substack{i=1 \\ e=v_i v_{i+1} \in C_{2k}}}^{2k+1} (Mo_A(e|G_1) - Mo_A(e|G'))$$
$$= \sum_{\substack{i=1 \\ e=v_i v_{i+1}, i \neq k}}^{2k+1} 4(n-2k-1) + 2(d+4)(n-2k-1)$$

$$
\begin{aligned}
&- \sum_{\substack{i=1 \\ e=v_i v_{i+1}}}^{2k+1} (d_i + d_{i+1} + 4)(n - n_e - n_0) \\
&\geq 8k(n-2k-1) + 2d(n-2k-1) - 2d(n-\bar{n_e}) - (8k+4)(n-\bar{n_e}) \\
&\geq -4(n-2k-1). \qquad (3)
\end{aligned}
$$

Thus, from (1) and (3), $Mo_A(G_1) - Mo_A(G') \geq 2\sum_{\substack{i,j=1 \\ i\neq j}}^{r} d_i d_j (n-2) - 4(n-2k-1) > 0$, if $d > 2$. When $d = 2$, $Mo_A(G_1) - Mo_A(G') \geq 2n > 0$, thus $Mo_A(G_1) - Mo_A(G) \geq 0$ and $Mo_A(G) = n^3 - 2n^2 r + 3n^2 + nr^2 + nr - 10n - 4r^2 + 10r$, whenever $G \cong G_1$. ■

Theorem 2.11. *Let $G \in \mathcal{U}_n$, $n \geq 4$. Then $Mo_A(G) \leq n^3 - 3n^2 + 2n - 6$ and the equality holds if and only if $G \cong U_{3,n-3}$.*

Proof. Let $G \in \mathcal{U}_n$ be the graph with the maximum additively weighted Mostar index. According to Lemma 2.8, all the bridges of G must be pendant edges. Additionally, Lemma 2.10 states that all pendant edges should be attached to a single vertex. Therefore, after applying these transformations iteratively, the resulting unicyclic graph G_1 must take the form $G_1 = U_{r,p}$. Let $G_2 = U_{r-2,p+2}$ denote the graph obtained by transforming two cyclic edges into pendant edges. It follows that $|V(G_1)| = |V(G_2)| = n$.

In simpler terms, starting from G, which has the highest additively weighted Mostar index in its class of unicyclic graphs with n vertices, we can transform it step by step and ultimately, this process leads us to graph G_1, which is of the form $U_{r,p}$, and then to graph G_2, which is of the form $U_{r-2,p+2}$. When $r = 2k$ is even, we have

$$
\begin{aligned}
Mo_A(G_2) - Mo_A(G_1) &= (p+2)(n-2)(p+5) + 4(n-p-4)(p+2) + 2(p+2)(p+6) \\
&\quad - p(n-2)(p+3) - 4(n-p-2)(p) - 2(p+4)(p) \\
&= 4np + 18n - 16p - 28 > 0.
\end{aligned}
$$

When $r = 2k+1$ is odd, then

$$
\begin{aligned}
Mo_A(G_2) - Mo_A(G_1) &= (p+2)(n-2)(p+5) + 4(n-p-5)(p+2) + 2(p+2)(p+6) \\
&\quad - p(n-2)(p+3) - 4(n-p-3)(p) - 2(p+4)(p) \\
&= 4np + 18n - 16p - 36 > 0.
\end{aligned}
$$

Thus, $Mo_A(G_2) - Mo_A(G_1) > 0$. Therefore, by repeatedly applying this transformation, we get either the graph $G_3 = U_{4,n-4}$ or $G_4 = U_{3,n-3}$ having the maximum additively weighted Mostar index. Now, if $|V(G_3)| = |V(G_4)| = n$, then

$$
\begin{aligned}
Mo_A(G_4) - Mo_A(G_3) &= (n)(n-2)(n-3) + 8(n-4) + 2(n+1)(n-3) \\
&\quad - 8(n-4) - 2n(n-4) - (n-1)(n-2)(n-4) \\
&= 2n^2 - 12n + 34 > 0.
\end{aligned}
$$

Thus, $Mo_A(G_4) - Mo_A(G_3) > 0$. So, if $G \in \mathcal{U}_n$, then $Mo_A(G) \leq Mo_A(U_{3,n-3}) = n^3 - 3n^2 + 2n - 6$. ■

Consider the graph G', which is formed by attaching $n-5$ pendant edges and a path of length 2 to a vertex v of the cycle C_3. By using the earlier findings, we aim to determine the second highest value of the additively weighted Mostar index among unicyclic graphs.

Theorem 2.12. *Let $G \in \mathcal{U}_n | \{U_{3,n-3}\}$, $n \geq 7$. Then $Mo_A(G) \leq n^3 - 5n^2 + 14n - 40$ and the equality holds if and only if $G \cong U_{4,n-4}$.*

Proof. Let $G \in \mathcal{U}_n | \{U_{3,n-3}\}$, $n \geq 7$ be a graph with the maximum additively weighted Mostar index. According to Lemma 2.10, all the pendant edges of G must be attached to a single vertex. Applying the transformation outlined in Theorem 2.11, the cycle in G cannot exceed a length of 5. Therefore, G must be one of the three graphs: $G_1 = U_{4,n-4}$, $G_2 = U_{5,n-5}$, or G'. Evaluating the differences in their additively weighted Mostar indices, we find:

$$\begin{aligned} Mo_A(G_1) - Mo_A(G') &= 4n - 24 > 0, \\ Mo_A(G_1) - Mo_A(G_2) &= 2n^2 - 6n + 10 > 0. \end{aligned}$$

Thus, $Mo_A(G) \leq n^3 - 5n^2 + 14n - 40$, and equality holds if and only if $G \cong U_{4,n-4}$.

In summary, the graph G, which maximizes the additively weighted Mostar index among unicyclic graphs of n vertices, is $U_{4,n-4}$. ■

Now, let's explore some mathematical properties of the additively weighted Mostar index for various classes of graphs. A variant of the cut method can be employed to calculate the additively weighted Mostar index of lattice grids and other nanostructures. However, we aim to establish a more general expression by determining the additively weighted Mostar index of the Cartesian product of graphs.

Theorem 2.13. *Let $G_1 = (n_1, m_1)$ and $G_2 = (n_2, m_2)$ be two connected graphs. Then,*

$$Mo_A(G_1 \times G_2) = n_1^2 Mo_A(G_2) + 4n_1 m_1 Mo(G_2) + n_2^2 Mo_A(G_1) + 4n_2 m_2 Mo(G_1).$$

Proof. By the definition of additively weighted Mostar index,

$$\begin{aligned} Mo_A(G_1 \times G_2) &= \sum_{\substack{(u,v)\in E(G_1\times G_2)\\ u=(u_1,v_1),v=(u_2,v_2)}} (d(u)+d(v))|n_u(e|G_1\times G_2) - n_v(e|G_1\times G_2)| \\ &= \sum_{\substack{(u,v)\in E(G_1\times G_2)\\ u=(u_1,v_1),v=(u_1,v_2)}} (d(u)+d(v))|n_u(e|G_1\times G_2) - n_v(e|G_1\times G_2)| \\ &+ \sum_{\substack{(u,v)\in E(G_1\times G_2)\\ u=(u_1,v_1),v=(u_2,v_1)}} (d(u)+d(v))|n_u(e|G_1\times G_2) - n_v(e|G_1\times G_2)| \\ &= \sum_{\substack{(u,v)\in E(G_1\times G_2)\\ u=(u_1,v_1),v=(u_1,v_2)}} (2d(u_1)+d(v_1)+d(v_2))(n_1|n_{v_1}(e|G_2) - n_{v_2}(e|G_2)|) \\ &+ \sum_{\substack{(u,v)\in E(G_1\times G_2)\\ u=(u_1,v_1),v=(u_2,v_1)}} (d(u_1)+d(u_2)+2d(v_1))(n_2|n_{u_1}(e|G_1) - n_{u_2}(e|G_1)|) \\ &= n_1 \sum_{v_1v_2\in E(G_2)} (d(v_1)+d(v_2))(n_1|n_{v_1}(e|G_2) - n_{v_2}(e|G_2)|) \\ &+ \sum_{\substack{v_1v_2\in E(G_2)\\ u_1\in G_1}} (2d(u_1))(n_1|n_{v_1}(e|G_2) - n_{v_2}(e|G_2)|) \end{aligned}$$

$$+ n_2 \sum_{u_1u_2 \in E(G_1)} (d(u_1) + d(u_2))(n_2|n_{u_1}(e|G_1) - n_{u_2}(e|G_1)|)$$
$$+ \sum_{\substack{u_1u_2 \in E(G_1) \\ v_1 \in G_2}} (2d(v_1))(n_2|n_{u_1}(e|G_1) - n_{u_2}(e|G_1)|)$$
$$= n_1^2 Mo_A(G_2) + 4n_1m_1Mo(G_2) + n_2^2 Mo_A(G_1) + 4n_2m_2Mo(G_1).$$

■

Now, we determine the relationship between the additively weighted Mostar index and some other degree-based graph invariants.

Theorem 2.14. *Let G be a graph with diameter at most two. Then*

$$Mo_A(G) = \sum_{uv \in E(G)} |d(u)^2 - d(v)^2|.$$

Proof. For every edge $e = uv$ in G, we have $n_u(e|G) = d(u) - |N_u(e|G) \cap N_v(e|G)|$. Therefore,

$$Mo_A(G) = \sum_{uv \in E(G)} (d(u) + d(v))|n_u(e|G) - n_v(e|G)|$$
$$= \sum_{uv \in E(G)} (d(u) + d(v))|d(u) - |N_u(e|G) \cap N_v(e|G)| - (d(v) - |N_u(e|G) \cap N_v(e|G)|)|$$
$$= \sum_{uv \in E(G)} (d(u) + d(v))|d(u) - d(v)| = \sum_{uv \in E(G)} |d(u)^2 - d(v)^2|.$$

■

Theorem 2.15. *Let T be a tree on n vertices. Then $Mo_A(T) \geq \sum_{e=uv \in E(T)} |d(u)^2 - d(v)^2|$, with equality if and only if T is isomorphic with S_n.*

Proof. For every edge $e = uv$ on T, $N_u(e|G)$ must have at least as many vertices as the degree of the vertex u. Thus, $|n_u(e|T) - n_v(e|T)| \geq |d(u) - d(v)|$. Therefore,

$$Mo_A(T) = \sum_{e=uv \in E(T)} (d(u) + d(v))|n_u(e|T) - n_v(e|T)|$$
$$\geq \sum_{e=uv \in E(T)} (d(u) + d(v))|d(u) - d(v)|$$
$$= \sum_{e=uv \in E(T)} |d(u)^2 - d(v)^2|.$$

Now, the equality holds iff $|n_u(e|G) - n_v(e|G)| = |d(u) - d(v)|$ for every edge $e \in T$, which which is equivalent to every edge being a pendant edge. Therefore, $G \cong S_n$. ■

Theorem 2.16. *For a bipartite graph $G = (V, E)$, $0 \leq Mo_A(G) \leq (n - 2)M_1(G)$ and the equality holds if and only if $G \cong C_{2k}$ and $G \cong S_n$, respectively.*

Proof. Let $|G| = n$, since $G = (V, E)$ is a bipartite graph for every edge $e = uv$, $n_u(e|G) + n_v(e|G) = n$. For convenience, take $n_u(e|G) \geq n_v(e|G)$ for every edge $e = uv$. Therefore, $|n_u(e|G) - n_v(e|G)| = n - 2n_v(e|G)$.

$$\begin{aligned} Mo_A(G) &= \sum_{e=uv\in E} (d(u)+d(v))|n_u(e|G) - n_v(e|G)| \\ &= \sum_{e=uv\in E} (d(u)+d(v))(n - 2n_v(e|G)) \\ &= n \sum_{e=uv\in E} (d(u)+d(v)) - 2 \sum_{e=uv\in E} (d(u)+d(v))n_v(e|G)) \\ &= nM_1(G) - 2 \sum_{e=uv\in E} (d(u)+d(v))n_v(e|G)). \end{aligned}$$

We know, $1 \leq n_v(e|G) \leq \dfrac{n}{2}$. Therefore,

$$\begin{aligned} nM_1(G) - 2 \sum_{e=uv\in E} (d(u)+d(v))\frac{n}{2} \leq & Mo_A(G) \leq nM_1(G) - 2 \sum_{e=uv\in E} (d(u)+d(v))1 \\ nM_1(G) - 2\frac{n}{2}M_1(G) \leq & Mo_A(G) \leq nM_1(G) - 2M_1(G) \\ 0 \leq & Mo_A(G) \leq (n-2)M_1(G). \end{aligned}$$

The equality on the right-hand side holds if and only if $n_v(e|G) = 1$, for every edge $e = uv$ in G. Similarly, the equality on the left-hand side holds if and only if $n_v(e|G) = \frac{n}{2}$, for every edge $e = uv$ in G. Therefore, the left-hand side equality holds if and only if G is the cycle graph C_{2k}, and the right-hand side equality holds if and only if $G = S_n$. ■

We now examine the properties of the additively weighted Mostar index across various classes of graphs.

Theorem 2.17. *([24]). For every tree T, the Zagreb index of T is even.*

Theorem 2.18. *For every tree T, the additively weighted Mostar index of T is even.*

Proof. Let T be a tree of order n. For every edge $e = uv \in E(T)$, $n_u(e|T) + n_v(e|T) = n$. Assume that $n_u(e|T) \geq n_v(e|T)$, then $|n_u(e|T) - n_v(e|T)| = n - 2n_v(e|T)$. Thus

$$\begin{aligned} Mo_A(T) &= \sum_{e=uv\in E(T)} (d(u)+d(v))|n_u(e|T) - n_v(e|T)| \\ &= \sum_{e=uv\in E(T)} (d(u)+d(v))(n - 2n_v(e|T)) \\ &= n \sum_{e=uv\in E(T)} (d(u)+d(v)) - 2 \sum_{e=uv\in E(T)} (d(u)+d(v))n_v(e|T) \\ &= nM_1(T) - 2 \sum_{e=uv\in E(T)} (d(u)+d(v))n_v(e|T), \end{aligned}$$

since the first Zagreb index ($M_1(T)$) of a tree is even. The result follows. ■

We can extend this result onto the class of connected bipartite graphs.

Theorem 2.19. *([24]). The Zagreb index of a connected bipartite graph is even.*

Theorem 2.20. *Let G be a connected bipartite graph. Then the additively weighted Mostar index of G is even.*

Proof. Let G be a connected bipartite graph of order n. For every edge $e = uv \in E(G)$, $n_u(e|G) + n_v(e|G) = n$. Without loss of generality, assume that $n_u(e|T) \geq n_v(e|T)$, then $|n_u(e|T) - n_v(e|T)| = n - 2n_v(e|T)$. Thus

$$\begin{aligned} Mo_A(G) &= \sum_{e=uv\in E(G)} (d(u)+d(v))|n_u(e|G) - n_v(e|G)| \\ &= \sum_{e=uv\in E(G)} (d(u)+d(v))(n - 2n_v(e|G)) \\ &= n \sum_{e=uv\in E(G)} (d(u)+d(v)) - 2 \sum_{e=uv\in E(G)} (d(u)+d(v))n_v(e|G) \\ &= nM_1(G) - 2 \sum_{e=uv\in E(G)} (d(u)+d(v))n_v(e|G), \end{aligned}$$

since the first Zagreb index ($M_1(G)$) of a connected bipartite graph is even. The result follows. ■

3 Application of additively weighted Mostar index

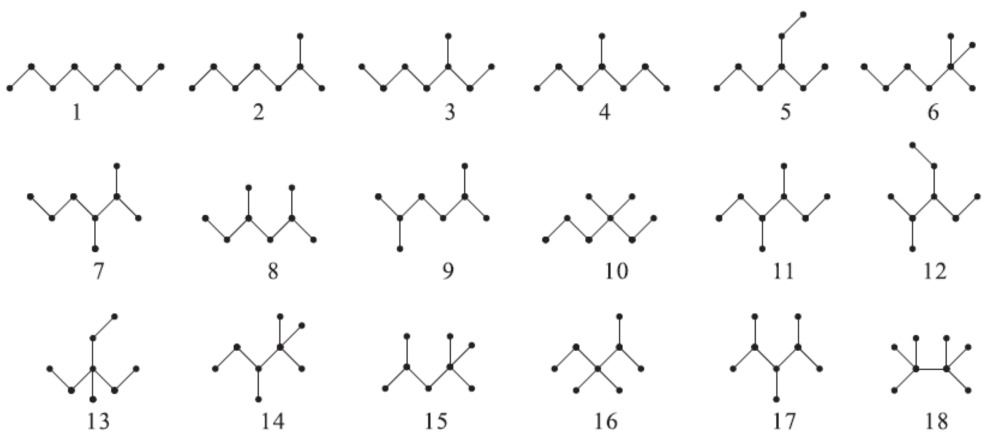

Figure 1: Octane Isomers.

In this section, we examine the relationship between the additively weighted Mostar index and various chemical properties of octane isomers exhibited in Figure 1. All experimental values of the chemical compounds are sourced from [16]. Using the data from Table 1, we can establish relationships among the acentric factor, total surface area (TSA), enthalpy of vaporization

(HVAP), standard enthalpy of vaporization (DHVAP), and entropy with the additively weighted Mostar indices of the octane isomers.

The correlations between the additively weighted Mostar index and the acentric factor, TSA, HVAP, DHVAP, and entropy are approximately -0.9835, -0.6005, -0.7706, -0.8514, and -0.9174, respectively. These results indicate a strong linear relationship between the additively weighted Mostar index and both the acentric factor and entropy of the octane isomers.

Additionally, we present a comparative study of the additively weighted Mostar index with other distance-based topological indices, such as the Szeged index (Sz), Mostar index (Mo), edge Mostar index (Mo_e), first eccentric connectivity index (S_1), second eccentric connectivity index (S_2), first status connectivity index (ζ_1), second status connectivity index (ζ_2), and weighted Szeged index (wSz). Our findings suggest that the additively weighted Mostar index is a superior predictor of the acentric factor and entropy of octane isomers compared to other topological indices; see Tables 2 and 3.

Table 1: Acentric factor, total surface area (TSA), enthalpy of vaporizatian (HVAP), standard enthalpy of vaporization (DHVAP), entropy, additively weighted Mostar index and other distance-based topological indices of the numbered octane isomers.

No	Acent Factor	TSA	HVAP	DHVAP	Entropy	Mo_A	Sz	Mo	Mo_e	S_1	S_2	ζ_1	ζ_2	wSz
1	0.4	415.3	73.19	9.915	111.67	84	84	24	24	280	2856	74	200	322
2	0.38	407.85	70.30	9.484	109.84	100	79	26	26	260	2441	65	154	324
3	0.37	397.34	71.30	9.521	111.26	104	76	28	28	248	2224	63	144	318
4	0.37	396.04	70.91	9.483	109.32	112	75	30	30	244	2157	61	136	316
5	0.36	379.04	71.7	9.476	109.43	120	72	32	32	228	1865	56	113	306
6	0.34	405.11	67.7	8.915	103.42	132	71	30	30	224	1796	54	105	330
7	0.35	384.93	70.2	9.272	108.02	128	70	32	32	228	1853	54	105	318
8	0.34	388.11	68.5	9.029	106.98	120	71	30	30	240	2052	56	113	320
9	0.36	395.08	68.6	9.051	105.72	116	74	28	28	212	1609	52	97	326
10	0.32	389.79	68.5	8.973	104.74	148	67	34	34	216	1664	52	97	322
11	0.34	376.91	70.2	9.316	106.59	124	68	32	32	232	1940	54	105	314
12	0.33	368.10	69.7	9.209	106.06	136	67	34	34	196	1349	43	66	308
13	0.31	366.99	69.3	9.081	101.48	156	64	36	36	208	1520	45	72	314
14	0.30	371.75	67.3	8.826	101.31	152	63	34	34	192	1292	41	60	326
15	0.31	392.19	64.87	8.402	104.09	148	66	32	32	204	1461	43	66	332
16	0.29	377.40	68.1	8.897	102.06	164	62	36	36	212	1597	43	66	324
17	0.32	368.93	68.37	9.014	102.39	144	65	34	34	200	1420	41	60	320
18	0.26	390.47	66.2	8.41	93.06	180	58	36	36	176	1060	34	40	338

Table 2: Correlation coefficient (R), coefficient of determination(R^2) and standard error of estimates (SEE) between chemical properties of octane isomers and their distance-based topological indices.

	Acentric Factor			TSA			HVAP		
	R	R^2	SEE	R	R^2	SEE	R	R^2	SEE
Mo_A	-0.9835	0.9674	0.0065	-0.6005	0.3606	11.7285	-0.7706	0.5938	1.3312
Sz	0.9732	0.9471	0.0083	0.7210	0.5199	10.1632	0.7381	0.5447	1.409
Mo	-0.8874	0.7874	0.0166	-0.8139	0.6624	8.5226	0.5499	0.3024	1.7444
Mo_e	-0.8874	0.7874	0.0166	-0.8139	0.6624	8.5226	-0.5499	0.3024	1.7444
S_1	0.8823	0.7785	0.0170	0.6653	0.4426	10.9508	0.7612	0.5794	1.3545
S_2	0.8787	0.7721	0.0172	0.6835	0.4672	10.7067	0.7665	0.5875	1.3414
ζ_1	0.9328	0.8701	0.0130	0.7032	0.4945	10.4287	0.6141	0.3772	1.2825
ζ_2	0.9157	0.8384	0.0145	0.7303	0.5333	10.0201	0.7893	0.6230	1.2824
wSz	-0.4161	0.1732	0.0328	0.4273	0.1826	13.2608	-0.6840	0.4679	1.5236

Table 3: Correlation coefficient (R), coefficient of determination(R^2) and standard error of estimates (SEE) between chemical properties of octane isomers and their distance-based topological indices.

	DHVAP			Entropy		
	R	R^2	SEE	R	R^2	SEE
Mo_A	-0.8514	0.7249	0.2072	-0.9174	0.8415	1.8537
Sz	0.8202	0.6727	0.2261	0.8778	0.7705	2.2308
Mo	-0.6531	0.4266	0.2992	-0.7549	0.5699	3.0539
Mo_e	-0.6531	0.4266	0.2992	-0.7549	0.5699	3.0539
S_1	0.8300	0.6890	0.2204	0.8545	0.7301	2.4193
S_2	0.8343	0.6961	0.2178	0.8382	0.7026	2.5395
ζ_1	0.8517	0.7254	0.2071	0.8779	0.7707	2.2300
ζ_2	0.7893	0.6230	0.2080	0.8458	0.7153	2.4845
wSz	-0.6840	0.4679	0.3041	-0.5597	0.3133	3.8588

4 Conclusion

In this paper, we computed the first two lower and upper bounds of the additively weighted Mostar index for unicyclic graphs of a given order. We established several properties of the additively weighted Mostar index for different classes of graphs. Additionally, we determined the correlation between the additively weighted Mostar index and the chemical properties of octane isomers as well as benzenoid hydrocarbons. We also propose the following problems for further study.

Problem 4.1. Investigate the inverse problem of the additively weighted Mostar index for trees, bipartite graphs, and connected graphs.

Problem 4.2. Determine the bounds of the additively weighted Mostar index for connected graphs and bipartite graphs.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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References

[1] J. Jerebic, S. Klavžar and D. F. Rall, Distance-balanced graphs, *Ann. Comb.* **12** (2008) 71–79, https://doi.org/10.1007/s00026-008-0337-2.

[2] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20, https://doi.org/10.1021/ja01193a005.

[3] I Gutman, L Popović, P. V. Khadikar, S. Karmarkar, S. Joshi and M. Mandloi, Relations between Wiener and Szeged indices of monocyclic molecules, *MATCH Commun. Math. Comput. Chem.* **35** (1997) p. 103.

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

[5] T. Al-Fozan, P. Manuel, I. Rajasingh and R. S. Rajan, Computing Szeged index of certain nanosheets using partition technique, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 339–353.

[6] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, J. Singh, A. Shrivastava, I. Lukovits and M. V. Diudea, Szeged index-applications for drug modeling, *Lett. Drug Des. Discov.* **2** (2005), 606–624, https://doi.org/10.2174/157018005774717334.

[7] G. Indulal, L. Alex and I. Gutman, On graphs preserving PI index upon edge removal, *J. Math. Chem.* **59** (2021) 1603–1609, https://doi.org/10.1007/s10910-021-01255-1.

[8] P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. Dobrynin, I. Gutman and G. Domotor, The Szeged index and an analogy with the Wiener index, *J. Chem. Inf. Comput. Sci.* **35** (1995) 547–550, https://doi.org/10.1021/ci00025a024.

[9] S. Klavžar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, *Appl. Math. Lett.* **9** (1996) 45–49, https://doi.org/10.1016/0893-9659(96)00071-7.

[10] S. Simić, I. Gutman and V. Baltić, Some graphs with extremal Szeged index, *Math. Slovaca* **50** (2000) 1–15.

[11] B. Zhou, X. Cai and Z. Du, On Szeged indices of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 113–132.

[12] A. Ali and T. Došlić, Mostar index: results and perspectives, *Appl. Math. Comput.* **404** (2021) p. 126245, https://doi.org/10.1016/j.amc.2021.126245.

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

[14] L. Alex and I. Gutman, On the inverse mostar index problem for molecular graphs, *Trans. Combi.* **14** (2024) 65–77, https://doi.org/10.22108/toc.2024.139474.2115.

[15] K. Deng and S. Li, Chemical trees with extremal Mostar index, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 161–180.

[16] K. Deng and S. Li, On the extremal values for the Mostar index of trees with given degree sequence, *Appl. Math. Comput.* **390** (2021) p. 125598, https://doi.org/10.1016/j.amc.2020.125598.

[17] T. Došlić, I. Martinjak, R. Skrekovski, S. T. Spužević and I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018) 2995–3013, https://doi.org/10.1007/s10910-018-0928-z.

[18] H. Liu, On the maximal Mostar index of tree-type phenylenes, *Polycyclic aromatic compounds* **42** (2022) 3829–3843, https://doi.org/10.1080/10406638.2021.1873151.

[19] L. Wei, H. Bian, H. Yu and G. Lin, Extremal cata-condensed benzenoids with two full-hexagons with respect to the Mostar indices, *Polycyclic aromatic compounds* **44** (2024) 5624–5639, https://doi.org/10.1080/10406638.2023.2266182.

[20] L. Alex and I. Gopalapillai, On a conjecture on edge Mostar index of bicyclic graphs, *Iranian J. Math. Chem.* **14** (2023) 97–108, https://doi.org/10.22052/IJMC.2023.248632.1680.

[21] S. Brezovnik and N. Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, *Int. J. Quantum Chem.* **121** (2021) e26530, https://doi.org/10.1002/qua.26530.

[22] T. Réti, A. Ali and I. Gutman, On bond-additive and atoms-pair-additive indices of graphs, *Electron. J. Math.* **2** (2021) 52–61, https://doi.org/10.47443/ejm.2021.0033.

[23] L. Alex and G. Indulal, Sharp bounds on additively weighted Mostar index of cacti, *Commun. Comb. Optim.* In press (2024), https://doi.org/10.22049/CCO.2024.28757.1702.

[24] A. Yurtas, M. Togan, V. Lokesha, I. N. Cangul and I. Gutman, Inverse problem for Zagreb indices, *J. Math. Chem.* **57** (2019) 609–615, https://doi.org/10.1007/s10910-018-0970-x.