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ON THE INVERSE MOSTAR INDEX PROBLEM FOR MOLECULAR GRAPHS

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Abstract. Mostar indices are recently proposed distance-based graph invariants, that already have been much investigated and found applications. In this paper, we investigate the inverse problem for Mostar indices of unicyclic and bicyclic molecular graphs. We prove that all positive integers other than 1, 2, 3, and 5 can be the Mostar index of some bicyclic molecular graph. In addition, we resolve the inverse edge Mostar index problem for molecular unicyclic and bicyclic graphs, and in doing so, establish the second and third smallest value of the edge Mostar index of unicyclic graphs.

1. **Introduction**

Topological indices are numerical quantities associated with graphs that are invariant under graph isomorphism, and that reflect certain structural features of the underlying graph. In the mathematical and chemical literature hundreds of such invariants are being studied, see [27, 31]. Recently, Došlić *et al.* proposed a new such graph invariant called Mostar index ($Mo(G)$) [1, 7]. In 2019, a modified edge version, called edge Mostar index ($Mo_e(G)$) was proposed [4]. Let $G = (V, E)$ be a connected graph with vertex set V and edge set E. For every edge $e = uv$, let $n_u(e|G)$ and $m_u(e|G)$ denote the number of vertices and edges, respectively, closer to the vertex u than v. Then, the Mostar index and

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its edge variant are defined as:

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

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

Since their induction, several studies on Mostar indices were reported. In 2020, Liu *et al.* determined bounds for edge Mostar index of trees, unicyclic graphs, and cacti [23]. In [18], Imran *et al.* computed the edge Mostar index of graphs resulting from some graph operations. In [26], Tepeh determined upper and lower bounds on the Mostar index of bicyclic graphs. Alex *et al.* determined upper and lower bounds on the edge Mostar index of bicyclic graphs [2].

The inverse problem of topological indices concerns with the existence or non-existence of a graph with a given number as its topological index. One of the present authors was the first to study this problem for the Wiener index. He proposed a conjecture on the inverse Wiener index problem for trees [14]. Eventually, several studies of this problem were carried out [5, 20]. The conjecture was settled in 2006, independently by Wang *et al.* and Wagner [28]. Wagner also solved the the inverse Wiener index problem for unicyclic graphs [29]. In [21], Li solved the inverse Z-index problem and inverse σ-index problem, whereas the inverse σ index problem was settled in [13]. In 2019, it was proven that all even numbers except 4 and 8 can be the Zagreb indices of some connected graph [33]. Dimitrov and Stevanović studied the inverse irregularity index problem on trees and c-cyclic graphs [6]. A. Y Günes *et al.* solved the inverse Albertson index problem for unicyclic graphs [10]. Indulal and one of the present authors recently settled the inverse Mostar index problem for chemical trees and unicyclic graphs [3]. The present paper is concerned with the inverse Mostar and edge Mostar index problem.

Molecular graphs are simple graphs, representing the carbon-atom skeleton of an organic molecule [12, 31]. Therefore, molecular graphs are simple connected graphs in which the degree of every vertex is at most 4.

2. Notations and Symbols

The notations and symbols used throughout this paper are listed in this section.

$\mathcal{U}_n$	The set of all connected unicyclic graphs of order n.
$\mathcal{B}_n$	The set of all connected bicyclic graphs of order n.
$C_{n,r}$	Unicyclic graph with cycle C_n along with a path of length r whose pendent vertex is identified to some vertex of C_n.
$\mathcal{U}_n \vert \{G_1, \ldots, G_k\}$	The set of all connected unicyclic graphs of order n, except for the graphs $G_1, \ldots, G_k$.
G_2^0	Unicyclic graph of order n(even) with cycle C_{n-2} and two pendent edges attached at different vertices of C_{n-2}, separated at distance of $\dfrac{n-2}{2}$.

G_3^0	Unicyclic graph of order n(even) with a cycle C_{n-2} along with two pendent edges attached to different vertices of C_{n-2}, separated at distance of $\frac{n-4}{2}$.
G_3^1	Unicyclic graph of order n(odd) with a cycle C_{n-2} along with two pendent edges attached to different vertices of C_{n-2}, separated at distance of $\frac{n-3}{2}$.
$\Theta_{a,b,c}$	Bicyclic graph with two vertices u, v connected by three different paths of lengths a, b, c, respectively [26].
H_1^1	Bicyclic graph with two vertices u and v connected by three different paths of lengths $2, 2$ and $n-4$, respectively, along with a pendent edge attached to a vertex w such that the distance $d(u,w) = \frac{n-7}{2}$ or $d(v,w) = \frac{n-7}{2}$.
H_2^1	Bicyclic graph with vertices u and v connected by three different paths of lengths $1, 2$ and $n-3$, respectively, along with a pendent edge attached to a vertex w, such that the distance $d(u,w) = \frac{n-4}{2}$ or $d(v,w) = \frac{n-4}{2}$.
H_2^2	Bicyclic graph with vertices u and v connected by three different paths of lengths $1, 2$ and $n-3$, respectively, along with a pendent edge attached to a vertex w, such that the distance $d(u,w) = \frac{n-6}{2}$ or $d(v,w) = \frac{n-6}{2}$.
H_2^3	Bicyclic graph with vertices u and v connected by three different paths of lengths $1, 2$ and $n-3$, respectively, along with a pendent edge attached to a vertex w, such that the distance $d(u,w) = \frac{n-8}{2}$ or $d(v,w) = \frac{n-8}{2}$.

Table 1: List of Notations and Symbols.

3. Main Results

This section settles the inverse edge Mostar index problem for unicyclic and bicyclic graphs. In order to solve the inverse edge Mostar index problem for unicyclic graphs, one must obtain the second and third smallest values of the edge Mostar index for unicyclic graphs.

Proposition 3.1. *For* $n \geq 4$,

(a.) $Mo_e(C_{n-1,1}) = \begin{cases} 2n-2, & \text{if } n \text{ is odd.} \\ 2n-3, & \text{if } n \text{ is even.} \end{cases}$

(b.) $Mo_e(G_2^0) = 2n-2$, *where* n *is even.*

(c.) $Mo_e(G_3^1) = 2n$, *where* n *is odd.*

Proof. For each pendent edge, the contribution is $n-1$. Now in $C_{n-1,1}$, when n is odd, $n-1$ edges of the cycle contribute 1 each, and when n is even, $n-2$ edges of the cycle contribute 1 each. Therefore, $Mo_e(C_{n-1,1}) = 2n-2$ if n is odd and $Mo_e(C_{n-1,1}) = 2n-3$ if n is even. In G_2^0, all the edges of the cycle C_{n-2} contribute zero and each pendent edge contributes $n-1$. Therefore, $Mo_e(G_2^0) = 2n-2$.

Now in G_3^1, when n is odd, $Mo_e(G_3^1) = 2n$, since two pendent edges contribute $n-1$ each, and two edges e and e' incident to the pendent edges, contribute 1 each. All other edges in the cycle contribute zero. □

Corollary 3.2. *If G is a graph with the minimum edge Mostar index among all graphs in $\mathcal{U}_n|\{C_n\}$ of order $n \geq 4$, then the edge Mostar index $Mo_e(G) \leq 2n-2$.*

Theorem 3.3. *Let $n \geq 4$. Then $C_{n-1,1}$ is the unique graph with smallest value of edge Mostar index in $\mathcal{U}_n|\{C_n\}$.*

Proof. Let G be a graph which attains the minimum edge Mostar index in $\mathcal{U}_n|\{C_n\}$, $n \geq 4$. Then G must have the following properties.

Claim I: G has exactly one pendent edge.

If G has no pendent edge then $G \cong C_n$, impossible. Suppose that G has three or more pendent edges, then $Mo_e(G) \geq 3(n-1) > 2n-2$ since $n \geq 4$, impossible. Thus G has one or two pendent edges. Now consider the case that G has exactly two pendent edges. If at least one pendent edge is incident to a bridge e, then the bridge e contribute at least 1. Hence, $Mo_e(G) \geq 2(n-1)+1 > 2n-2$, impossible. If both the pendent edges incident to the same vertex on the cycle, then edges on the cycle adjacent to the pendent edges contribute at least 2, hence $Mo_e(G) \geq 2(n-1)+2 > 2n-2$, impossible. Thus both the pendent edges e and e' must be incident to different vertices of the cycle. If the distance $d(e,e') < \lfloor \frac{n-2}{2} \rfloor$, then either there exist two edges in the cycle adjacent with pendent edges which contribute at least one or there exists one edge in the cycle adjacent to one of the pendent edge which contribute at least 2. Therefore, $Mo_e(G) \geq 2(n-1)+2 > 2n-2$, impossible. Thus if G has two pendent edges, then G should be a graph with cycle C_{n-2} with two pendent edges attached at different vertices of C_{n-2} separated by a distance $\lfloor \dfrac{n-2}{2} \rfloor$. When n is even, then $G \cong G_2^0$ and $Mo_e(G_2^0) = 2n-2 > 2n-3$, impossible. When n is odd, there is no such graph since distance between pendent edges is always less than $\dfrac{n-2}{2}$. Now the only remaining case is that G has exactly one pendent edge, then G is of the form $C_{r,p}$ where $r+p=n, r \geq 3$.

Claim II: $p = 1$**.** Suppose that $p \geq 2$. If n and p are of the same parity, then $n-p$ edges of the cycle contribute p and $p-2$ edges of the path contribute at least 1 and the pendent edge contribute $n-1$. Thus, $Mo_e(G) \geq n-1+p(n-p)+p-2 \geq n-1+2(n-p)+p-2 = 3n-p-3$. Now, $3n-p-3 \leq 2n-2$ implies $n-p \leq 1$ implies $n \leq p+1$, impossible. If n and p are of different parity, then $n-p-1$ edges of the cycle contribute p and $p-1$ edges of the path contribute at least 1 and the pendent edge contribute $n-1$. Thus, $Mo_e(G) \geq n-1+p(n-p-1)+p-1 \geq n-1+2(n-p-1)+p-1 = 3n-p-4$. Now, $3n-p-4 \leq 2n-2$ implies $n-p \leq 2$ implies $n \leq p+2$, impossible. Thus $p=1$ and hence $G \cong C_{n-1,1}$. □

Similarly, the third smallest value of the edge Mostar index of unicyclic graphs is obtained in the following theorem.

Corollary 3.4. *If G is a graph with the minimum edge Mostar index among all graphs in $\mathcal{U}_n|\{C_n, C_{n-1,1}\}$ of order $n \geq 6$, then the edge Mostar index $Mo_e(G) \leq 2n$.*

Theorem 3.5. *Let $n \geq 6$.*

(a.) *If n is odd, then G_3^1 is the unique graph with smallest value of edge Mostar index in $\mathcal{U}_n|\{C_n, C_{n-1,1}\}$.*

(b.) *If n is even, then G_2^0 is the unique graph with smallest value of edge Mostar index in $\mathcal{U}_n|\{C_n, C_{n-1,1}\}$.*

Proof. Let G be the graph attaining the third smallest value of edge Mostar index in $\mathcal{U}_n$, $n \geq 6$. We proceed by establishing the following claims on G.

Claim I: G has exactly two pendent edges.

Suppose that G has three or more pendent edges, then $Mo_e(G) \geq 3(n-1) > 2n$ since $n \geq 6$, impossible. If G has no pendent edge, then $G \cong C_n$, impossible. If G has exactly one pendent edge, then G is of the form $C_{r,p}, r+p=n, p \geq 2$. Since $p \geq 2$, the pendent edge and the bridge incident of the pendent edge contributes $n-1$ and $n-3$, respectively. Now for the edges in the cycle, using the arguments in Theorem 3.3, $Mo_e(G) \geq n-1+n-3+p(n-p) \geq 2n-4+2(n-p) = 4n-2p-4$ if $r = n-p$ is even. Now, $4n-2p-4 \leq 2n$ implies $n \leq p+2$, impossible (since $n \geq p+4$). If r is odd, using the arguments in Theorem 3.3, $Mo_e(G) \geq n-1+n-3+p(n-p-1) \geq 2n-4+2(n-p-1) = 4n-2p-6$. Now, $4n-2p-6 \leq 2n$ implies $n \leq p+3$. If $n = p+3$, then $G = C_{3,n-3}$ and $Mo_e(G) \geq 2(n-3)+n-1+n-3 = 4n-10$. Now $4n-10 \leq 2n$ implies $n \leq 5$, impossible. Thus G cannot have exactly one pendent edge. Thus G has exactly two pendent edges.

Claim II : G cannot have any non-pendent bridges

Suppose at least one of the pendent edges is incident to a non- pendent bridge e, then $Mo_e(G) \geq 2(n-1)+n-3 = 3n-3$, now $3n-3 \leq 2n$ implies $n \leq 5$, impossible. Thus both the pendent edges of G are incident to the cycle.

Claim III : Both pendent edges cannot be incident to the same vertex of the cycle

Suppose both pendent edges are incident to the same vertex of the cycle. Then G is of the form of a cycle C_{n-2} with two pendent edges attached at some vertex of the cycle. Then at least $n-3$ edges of the cycle contribute 2. Thus $Mo_e(G) \geq 2(n-1)+2(n-3) = 4n-8$, now $4n-8 \leq 2n$ implies $n \leq 4$, impossible. Thus G is of the form C_{n-2} with pendent edges attached at different vertices of the cycle.

Let t be distance between the two pendent edges in G, $t \leq \lfloor \frac{n-2}{2} \rfloor$. When n is odd and $t < \frac{n-3}{2}$, then $2t-1$ edges in the cycle contribute zero and among the remaining $n-2-2t+1$ edges, 2 edges contribute 1 and rest of the edges contribute 2. Thus $Mo_e(G) \geq 2n-2+2+2(n-3-2t) = 4n-4t-6 > 2n$ whenever $t < \frac{n-3}{2}$, thus $t = \dfrac{n-3}{2}$, i.e., $G = G_3^1$. When n even and $t < \frac{n-2}{2}$,

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then $2t$ edges in the cycle contribute zero and the remaining $n-2-2t$ edges contribute 2. Thus, $Mo_e(G) \geq 2n-2+2(n-2-2t) = 4n-4t-6 > 2n$ whenever $t < \frac{n-2}{2}$, thus $t = \dfrac{n-2}{2}$, i.e., $G = G_2^0$. $\square$

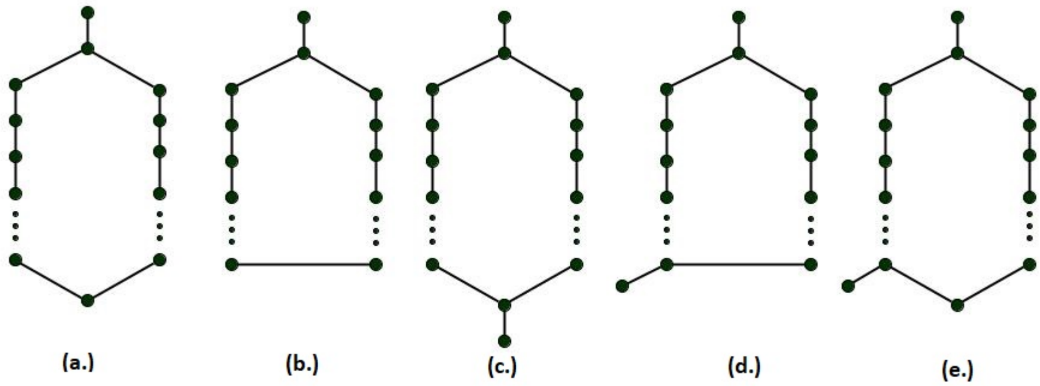

FIGURE 1. Graphs mentioned in Theorem 3.5 and its proof: (a.) $C_{n-1,1}$, n is odd (b.) $C_{n-1,1}$, n is even (c.) G_2^0 (d.) G_3^1 (e.) G_3^0.

Now, the inverse edge Mostar index problem on unicyclic molecular graphs is solved by the following theorem.

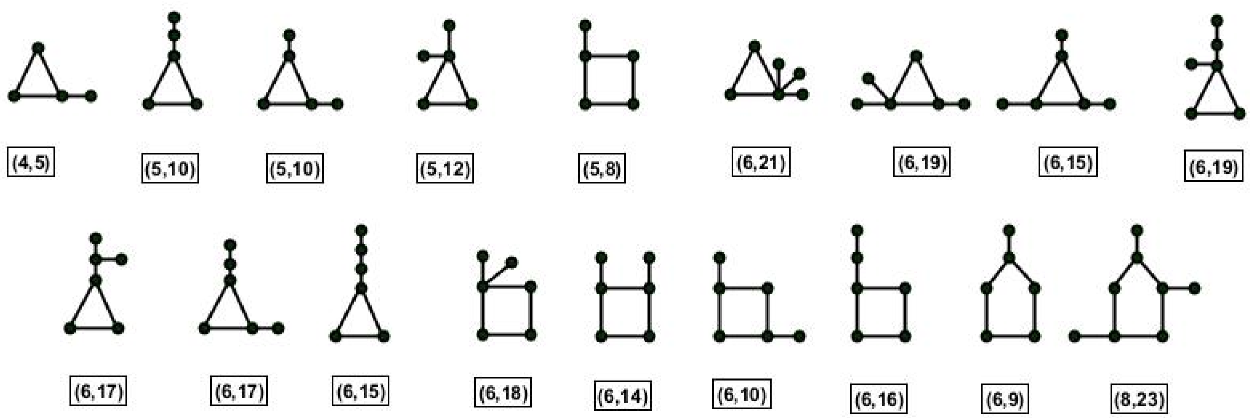

FIGURE 2. Unicyclic graphs of order 4,5,6 and their Mostar indices. The subscripts indicate order and edge Mostar index, respectively.

Theorem 3.6. *For every positive integer* $p \neq 1, 2, 3, 4, 6, 7, 11$, *there exists a unicyclic molecular graph* G *with* $Mo_e(G) = p$.

Proof. $Mo_e(C_r) = 0$ and for every unicyclic graph $G \ncong C_r$, $Mo_e(G) > 0$. Now, consider the unicyclic graphs which are not cycles. Let's divide the integers into four different cases.

Case I: $4k$**,** $k \geq 2$**:** Consider the graph $C_{n-1,1}$ with $n = 2k+1, k \geq 2$. $Mo_e(C_{n-1,1}) = 2n-2$, thus

$$Mo_e(G) = 2n-2 = 2(2k+1)-2 = 4k$$

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Case II: $4k+1$, $k \geq 1$**:** Consider the graph $C_{n-1,1}$ with $n = 2k+2, k \geq 1$. $Mo_e(C_{n-1,1}) = 2n-3$, thus

$$Mo_e(G) = 2n - 3 = 2(2k + 2) - 3 = 4k + 1$$

Case III: $4k+2, k \geq 2$**:** Consider the graph G_2^0 with $n = 2k+2, k \geq 2$. $Mo_e(G_2^0) = 2n-2$, thus

$$Mo_e(G_2^0) = 2n - 2 = 2(2k + 2) - 2 = 4k + 2$$

Case IV: $4k+3$, $k \geq 4$**:** We divide this into two subcases, $t = 8k+3, k \geq 2$ and $t = 8k+7, k \geq 2$. For $t = 8k+3, k \geq 2$, construct graph G with cycle $C_{n-3} = v_1 v_2 \cdots v_{n-3}$ with two pendent edges attached at v_1 and one pendent edge attached at $v_{\frac{n-2}{2}}$, where $n = 2k+2$. Now each pendent edge contributes $n-1$ and one edge in the cycle contributes 2, all other edges contribute 1 each. Thus,

$$Mo_e(G) = 3(n-1) + 2 + (n-4) = 4n - 5 = 4(2k+2) - 5 = 8k + 3$$

Now for $t = 8k+7, k \geq 3$, construct the graph G with cycle $C_{n-3} = v_1 v_2 \cdots v_{n-3}$ with two pendent edges attached at v_1 and one pendent edge attached at $v_{\frac{n-4}{2}}$, where $n = 2k+2, k \geq 3$. Now each pendent edge contribute $n-1$ and one edge in the cycle contribute 2. Among the rest of the edges, two edges incident to the pendent edges contribute 3 and all other edges contribute 1 each. Thus,

$$Mo_e(G) = 3(n-1) + 8 + (n-6) = 4n - 1 = 4(2k+2) - 1 = 8k + 7$$

Therefore, every positive integer other than 1,2,3,4,6,7,11,15,23 can be the edge Mostar index of some unicyclic molecular graph. Now from Figure 2, there exists unicyclic molecular graph with edge Mostar index 15 and 23. Now it is enough to check for the numbers 1,2,3,4,6,7,11. By Theorem 3.3, for any unicyclic graph G other than C_n, $Mo_e(G) \geq 5$ (since $n \geq 4$). Thus $1, 2, 3, 4$ cannot be edge Mostar index of any unicyclic graph. When $n \geq 7$, by Theorem 3.3, $Mo_e(G) \geq 12$, thus 6,7 and 11 cannot be the edge Mostar index of any unicyclic graph of order $n \geq 7$. All other possible graphs of order 4,5,6 and their edge Mostar index are plotted in Figure 2, thus there is no unicyclic molecular graphs with edge Mostar index $6, 7, 11$. □

Corollary 3.7. *For every positive integer* $p \neq 1, 2, 3, 4, 6, 7, 11$*, there exist a unicyclic graphs* G *with* $Mo_e(G) = p$.

Proof. Using Theorem 3.6, there does exist a unicyclic molecular graphs with edge Mostar index n where $p \neq 1, 2, 3, 4, 6, 7, 11$. Now, when the order $n \geq 7$, by Theorem 3.3 the edge Mostar index $Mo_e(G) \geq 12$. Therefore, there does not exist a unicyclic graph of order greater than 7 with any of these given numbers as its edge Mostar index. All other graphs of order 4,5,6 along with their edge Mostar indices are plotted in Figure 2, therefore the result follows. □

Now, let's settle the inverse edge Mostar index problem for bicyclic graphs.

Theorem 3.8. [2] *For* $n \geq 5$, $Mo_e(\Theta_{n-3,2,2}) = 2n - 4$.

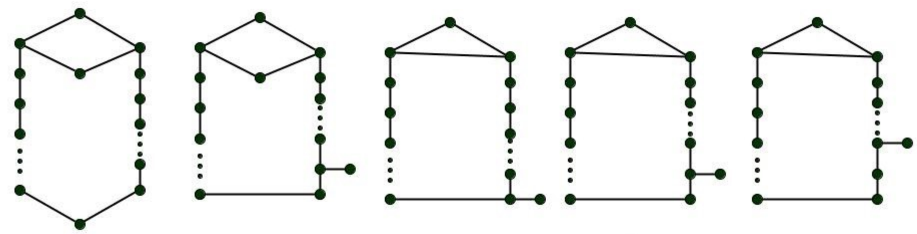

FIGURE 3. Graphs mentioned in Theorems 3.8, 3.9, 3.10, and their proofs: (a.) $\Theta_{n-3,2,2}$ (b.) H_1^1 (c.) H_2^1 (d.) H_2^2 (e.) H_2^3.

Theorem 3.9. [2] *Let $n \geq 9$. Then $\Theta_{n-3,2,2}$ is the unique bicyclic graph with minimum edge Mostar index.*

Theorem 3.10. *For odd integers $n \geq 7$, $Mo_e(H_1^1) = 2n + 3$.*

Proof. Let w be a vertex in H_1^1, such that the distance $d(u, w) = \dfrac{n-7}{2}$. Every pendent edge contribute n to Mo_e. For the two edges in one of the paths of length 2, the edge incident to v contribute 0 and the edge incident to u contribute 2. Also, the third edge incident to u contribute 2 and one edge incident to w contribute 3 to Mo_e. The rest of the $n-6$ edges contribute 1 each. Therefore, $Mo_e(H_1^1) = n + 9 + n - 3 = 2n + 3$. □

Theorem 3.11. *For even integers n,*

(a.) *$Mo_e(H_2^1) = 3n - 3$, where $n \geq 6$.*
(b.) *$Mo_e(H_2^2) = 3n + 1$, where $n \geq 6$.*
(c.) *$Mo_e(H_2^3) = 3n + 5$, where $n \geq 8$.*

Proof. (a.) Let w be a vertex in H_1^2, such that $d(u, w) = \dfrac{n-4}{2}$. Every pendent edge contribute n to Mo_e. The two edges in the path of length 2 contribute $\dfrac{n-4}{2} + 1$ and $\dfrac{n-4}{2} + 2$, respectively. The rest of the $n-2$ edges contribute 1 each. Therefore, $Mo_e(H_1^1) = n + \dfrac{n-4}{2} + 1 + \dfrac{n-4}{2} + 2 + n - 2 = 3n - 3$.

(b.) Let w be a vertex in H_2^2, such that $d(u, w) = \dfrac{n-6}{2}$. Every pendent edge contribute n to Mo_e. The two edges in the path of length 2 contribute $\dfrac{n-4}{2} + 1$ and $\dfrac{n-4}{2} + 2$, respectively. One edge incident to v and w, respectively, in the longest path contribute 3 each. The rest of the edges contribute 1 each. Therefore, $Mo_e(H_2^2) = n + \dfrac{n-4}{2} + 1 + \dfrac{n-4}{2} + 2 + 6 + n - 4 = 3n + 1$.

(c.) Let w be a vertex in H_2^2 such that $d(u, w) = \dfrac{n-8}{2}$. Two more edges on the longest path contribute 3 instead of 1 and all other edges contribute the same value as in the previous case. Therefore, $Mo_e(H_3^2) = n + \dfrac{n-4}{2} + 1 + \dfrac{n-4}{2} + 2 + 12 + n - 6 = 3n + 5$.

□

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Theorem 3.12. *For every positive integer $p \neq 1, 2, 3, 5, 7, 11, 13$, there exists a bicyclic molecular graph G with $Mo_e(G) = p$.*

Proof. We divide the integers into four different cases.
Case I: $2k$, $k \geq 2$: Clearly $Mo_e(\Theta_{2,2,1}) = 4$. Now for all other even positive integers, consider the graph $\Theta_{n-3,2,2}$, where $n = k + 2 \geq 5$ by Theorem 3.8, $Mo_e(\Theta_{n-3,2,2}) = 2n - 4 = 2k, k \geq 3$.
Case II: $6k + 3, k \geq 2$: Consider the graph H_2^1 with $n = 2k + 2, k \geq 2$. $Mo_e(H_2^2) = 3n - 3$, thus

$$Mo_e(H_2^1) = 3n - 3 = 3(2k + 2) - 3 = 6k + 3$$

Case III: $6k + 1$, $k \geq 3$: Consider the graph H_2^2 with $n = 2k, k \geq 3$. $Mo_e(H_2^2) = 3n + 1$, thus

$$Mo_e(H_2^1) = 3n + 1 = 3(2k) + 1 = 6k + 1$$

Case IV: $6k + 5$, $k \geq 4$: Consider the graph H_2^3 with $n = 2k, k \geq 4$. $Mo_e(H_2^3) = 3n + 5$, thus

$$Mo_e(H_2^3) = 3n + 5 = 3(2k) + 5 = 6k + 5$$

Thus every positive integer, other than 1,2,3,5,7,9,11,13,17 and 23 can be the edge Mostar index of some bicyclic molecular graph. Now, from Figure 4, there exists a bicyclic molecular graph with edge Mostar index 9,17 and 23. Now it is enough to check for the numbers 1,2,3,5,7,11,13. When $n \geq 9$, by Theorem 3.9, $Mo_e(G) \geq 14$, thus 1,2,3,5,7,11 and 13 cannot be the edge Mostar indices of any bicyclic graph of order $n \geq 9$. When $n \geq 7$, if G has at least two pendent edges, then 1,2,3,5, 7,11 and 13 cannot be the edge Mostar index of G, since $Mo_e(G) \geq 2n \geq 14$. Also, when $n \geq 7$, if a path of length at least two is attached at some vertex of the cycle in G, then G must have at least one edge in the cycle which contribute 2. Therefore, $Mo_e(G) \geq 2n \geq 14$. When $n = 6$, if G has two pendent edges, then there exist at least two edges in the cycle which contribute at least 1 each. Therefore, $Mo_e(G) \geq 2n + 2 \geq 14$. When $n \geq 6$ and G has two cycles C_a and C_b which do not share a common edge, where $a, b \geq 3$. If G does not have any pendent edge, then there exist at least two edges with the contribution at least 3 each and two edges with contribution at least 4 each. Therefore, $Mo_e(G) \geq 14$. If G has exactly one pendent edge, then along with contribution of the pendent edge, there exist two edges with contribution at least 4. Therefore, $Mo_e(G) \geq n + 8 > 14$. If G has two or more pendent edges, then $Mo_e(G) \geq 14$. Therefore, we only have to check for bicyclic graphs in which the cycles do not share a common edge and that have at most one pendent edge for orders 6,7,8. All other possible graphs of order 4,5,6,7,8 and their edge Mostar index are plotted in Figure 4, thus there is no bicyclic graph with edge Mostar index $1, 2, 3, 7, 11, 13$. □

Note that all integers of the form $4k + 1$, $k \geq 4$, can be attained using the graph H_1^1 with $n = 2k - 1, k \geq 4$. Now, the inverse edge Mostar index problem for bicyclic graphs can be established using this theorem.

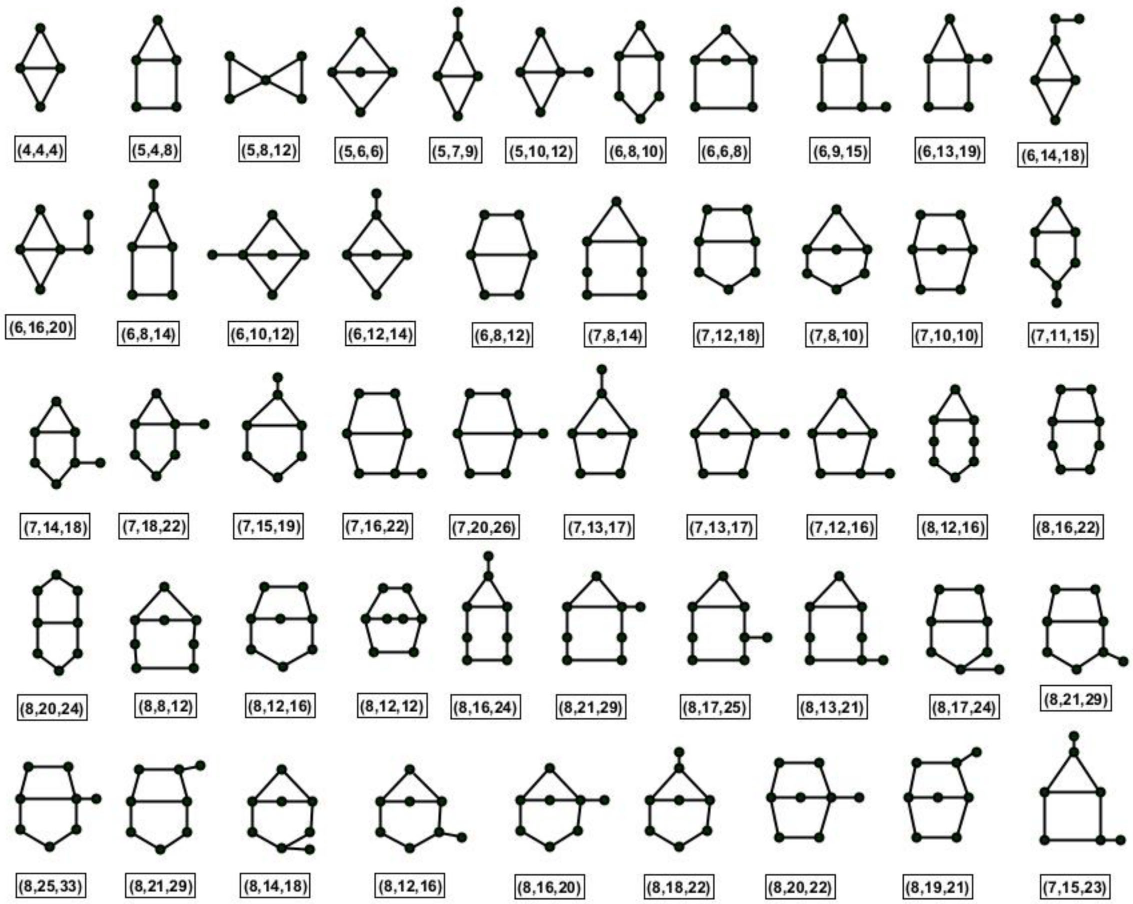

Figure 4. Bicyclic graphs of order 4,5,6,7,8, and their Mostar indices. The subscripts indicate order, Mostar index, and edge Mostar index, respectively.

Corollary 3.13. *For every positive integer* $p \neq 1, 2, 3, 5, 7, 11, 13$*, there exists a bicyclic graph* G *with* $Mo_e(G) = p$.

Now, let's solve the inverse Mostar index problem for bicyclic molecular graphs.

Proposition 3.14. [26] *If* n *is odd, then* $Mo(\Theta_{n-3,2,2}) = n + 1$. *Otherwise* $Mo(\Theta_{n-3,2,2}) = n$.

Theorem 3.15. [26] *Let* $n \geq 8$. *Then* $\Theta_{n-3,2,2}$ *is the unique bicyclic graph with minimum value of the Mostar index.*

Theorem 3.16. *For odd integers* $n \geq 7$, $Mo(H_1^1) = n + 6$.

Proof. Let u be a vertex of H_1^1, such that $d(u, w) = \dfrac{n-7}{2}$. Every pendent edge contribute $n - 2$ to Mo. For two edges in the path of length 2, the edge incident to v contribute 0, whereas the two edges incident to u contribute 2. Also, the third edge incident to v contributes 1 and one edge incident to w contribute 2 to Mo. Also, the edge which is at a distance $\dfrac{n-5}{2}$ from u contribute 1. The rest of the $n - 6$ edges contribute 0. Therefore, $Mo(H_1^1) = n - 2 + 8 = n + 6$. □

Theorem 3.17. *For every positive integer $p \neq 1, 2, 3, 5$, there exists a bicyclic molecular graph G with $Mo(G) = p$.*

Proof. We divide the integers into two different cases.
Case I: $2k$, $k \geq 2$: Clearly $Mo(\Theta_{2,2,1}) = 4$. Now for all other even positive integers, consider the graph $\Theta_{n-3,2,2}$, by Theorem 3.8 $Mo(\Theta_{n-3,2,2}) = n + 1$ with $n \geq 5$, n is odd.
Case II: $2k + 1$, $k \geq 6$: Consider the graph H_1^1 with $n = 2k - 5, k \geq 6$. $Mo_e(H_1^1) = n + 6$, thus

$$Mo(H_1^1) = n + 6 = (2k - 5) + 6 = 2k + 1$$

Thus every integer other than 1,2,3,5,7,9 and 11 can be the Mostar index of some bicyclic molecular graph. Now from Figure 4, there exist bicyclic graphs with Mostar index 7,9 and 11. Now it is enough to check for the numbers 1,2,3,5. By Theorem 3.15, for any bicyclic graph G of order $n \geq 8$, $Mo(G) \geq 8$. Therefore, $1, 2, 3, 5$ cannot be the Mostar index of any bicyclic graph of order $n \geq 8$. When $n \geq 6$, if G contains two or more pendent edges, then $Mo(G) \geq 2n - 4 \geq 8$. Also, if G contains a path of length 2 attached at some vertex of one of the cycles, then $Mo(G) \geq 2n - 6 \geq 6$. Therefore, we only have to check for bicyclic graph with at most 1 pendent vertex. When $n \geq 6$, if G has two distinct cycles C_a and C_b with no common edge between the cycles, $a, b \geq 3$, then there exist at least four edges with contribution at least 2 each. Therefore, $Mo(G) \geq 8$. Thus we only have to check for bicyclic graphs with cycles which do not share common edge and having at most one pendent edge for orders 4,5,6,7. All the possible graphs of order 4,5,6,7 and their Mostar index are plotted in Figure 4, thus there is no bicyclic molecular graph with Mostar index $1, 2, 3, 5$. □

From this result, we can also solve the inverse Mostar index problem for bicyclic graphs.

Corollary 3.18. *For every positive integer $p \neq 1, 2, 3, 5$, there exists a bicyclic graph G with $Mo(G) = p$.*

Theorem 3.19. [3] *For every positive integer k, there exists a chemical tree T with $Mo(T) = 2k$.*

Now, using these results one can partially solve the inverse Mostar index problem and inverse edge Mostar index problem for connected graphs.

Theorem 3.20. *For every non-negative integer $p \neq 1, 3, 5$, there exists a connected graph G such that $Mo(G) = p$.*

Theorem 3.21. *For every non-negative integer $p \neq 1, 3, 7, 11$, there exists a connected graph G such that $Mo_e(G) = p$.*

4. Concluding remarks

This paper resolves the inverse Mostar index problem for various classes of graphs. In connection with this, we propose the following conjectures.

Conjecture 4.1. *For any fixed $c \geq 3$, there exists a c-cyclic graph with Mostar index $Mo(G) = p$, where $p \in \mathbb{N} \backslash \{A\}$, A is a finite set.*

Conjecture 4.2. *For any fixed $c \geq 3$, there exists a c-cyclic graph with edge Mostar index $Mo_e(G) = p$, where $p \in \mathbb{N} \backslash \{B\}$, B is a finite set.*

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