

# INVERSE PROBLEM FOR MOSTAR INDEX OF CHEMICAL TREES AND UNICYCLIC GRAPHS

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**Abstract:** The Mostar index is a recently introduced topological index for graphs. By its very definition, the Mostar index of a graph is a positive integer. While the Mostar index has been computed and its bounds have been established for several classes of graphs, the inverse problem—that is, determining which positive integers can be the Mostar index of graphs has been less explored. In this paper, we study the inverse Mostar index problem for chemical trees and unicyclic graphs. We establish that the Mostar index of every tree is even, and that every even number can be attained by a chemical tree. We also settle the inverse problem for unicyclic graphs by proving that every integer greater than 13 can be the Mostar index of some unicyclic graph. Additionally, we compute the second and third lower bounds of the Mostar index for unicyclic graphs.

## 1 Introduction

Topological indices are numerical quantities which are independent of a vertex labelling and invariant under graph isomorphism. A bond additive index is an index whose value is the sum of contributions over edges. Through the past years, several bond additive indices were proposed and studied [6, 7, 13, 21]. One of such recently proposed indices is the Mostar index, defined in 2018 by Tomislav Došlić *et al.* [5]. For every edge  $e = xy$  in a graph  $G = (V, E)$ , let  $n_x(e|G)$  denote the number of vertices closer to the vertex  $x$  than to  $y$ . Then the Mostar index of  $G$ , denoted by  $Mo(G)$  is defined as

$$Mo(G) = \sum_{e=xy \in E} \phi(e)$$

where  $\phi(e) = |n_x(e|G) - n_y(e|G)|$  is the contribution of the individual edge  $e = xy$  to the Mostar index. For a detailed literature on Mostar index, see [1, 5, 10, 11, 12]

An inverse problem for a topological index analyzes the existence of a graph with a given integer as its topological index. Ivan Gutman *et al.* proposed the first version of this problem in 1994. They settled the inverse Wiener index problem for connected graphs and posed a conjecture on the inverse Wiener index problem for trees [9]. Mirko Lepović and Ivan Gutman studied this problem for trees upto integers 1206 and found the numbers which cannot be the Wiener index of a tree [15]. In 2004, Yih-En Andrew Ban *et al.* conducted an extensive search for inverse Wiener index problem on trees and proved that all integers between  $10^3$  and  $10^8$  can be the Wiener index of some caterpillar tree [2]. In 2006 this conjecture was independently settled by Hua Wang *et al.* and Stephan G Wagner. Wagner [26] proved that all integers greater than 470 can be the Wiener index of some tree. Hua Wang and Guang Yu [27] established that all but 49 integers can be the Wiener index of some trees. Several studies on inverse problems for other

topological indices have been carried out. In [20], Xueliang Li studied the inverse problem on the  $Z$ -index and  $\sigma$ -index for connected graphs. Wagner [25] settled the inverse Wiener index problem for unicyclic graphs in 2010. The inverse problem for the sigma index was solved by Ivan Gutman in [8]. Aysun Yurtas *et al.* studied the inverse Zagreb index problem for connected graphs and established that except for 4 and 8, all other even numbers can be the Zagreb index of some connected graph [28]. In [14], Joseph Varghese Kureethra *et al.* settled the inverse problem for the Forgotten index and Hyper Zagreb index of trees. In 2022, Güneş Yurttaş *et al.* proved that all even numbers except 4 are the Albertson index of some unicyclic graphs [29]. The inverse irregularity index problem on trees and  $c$ -cyclic graphs were studied in [4] by Darko Dimitrov *et al.*.

Let  $G$  be a graph of order  $n$ . Then a pendant edge contributes a value of  $(n - 2)$  to the Mostar index. Consequently the deficit of an edge  $e = xy$  is defined as the value  $n - 2 - \phi(e)$ . The sum of the deficit over all the edges is the deficit of the graph  $G$ , denoted by  $D(G)$  [24]. The distance between edges  $e, f$  in a graph  $G$  is the shortest distance between the end vertices of  $e, f$ . A chemical tree is a tree in which the degree of every vertex is less than or equal to 4. All the graphs considered in this paper are simple, finite, undirected and connected. In our work, we analyze the inverse Mostar index problem for chemical trees and unicyclic graphs. We also establish the second and third lower bounds of the Mostar index of unicyclic graphs.

## 2 Main Results

In this section, we discuss the inverse Mostar index problem for trees, unicyclic graphs. We also establish some basic properties of the Mostar index of some classes of graphs.

**Theorem 2.1.** *For a tree  $T$ , the Mostar index  $Mo(T)$  is even.*

*Proof.* Let  $T$  be a tree of order  $n$ . Since trees are bipartite graphs, for every edge  $e = uv \in T$ ,  $n_u(e|T) + n_v(e|T) = n$ . For convenience, let  $n_u(e|T) \geq n_v(e|T)$  where  $e = uv \in T$ . Then  $n_u(e|T) = n - n_v(e|T)$  and  $\phi(e) = |n_u(e|T) - n_v(e|T)| = n - 2n_v(e|T)$ . Now,

$$\begin{aligned} Mo(T) &= \sum_{e=uv \in E(T)} |n_u(e|T) - n_v(e|T)| = \sum_{e=uv \in E(T)} (n - 2n_v(e|T)) \\ &= (n - 1)n - \left( 2 \sum_{e=uv \in E(T)} n_v(e|T) \right) = \text{even} \end{aligned}$$

since  $n(n - 1)$  is even for every  $n$  and the rest is always even. □

**Theorem 2.2.** *Let  $G$  be a bipartite graph with order  $n$  and size  $m$ . Then*

- (a.) *If  $m$  or  $n$  is even, then  $Mo(G)$  is even.*
- (b.) *If  $m$  and  $n$  are odd, then  $Mo(G)$  is odd.*

*Proof.* For every edge  $e = uv$  of a bipartite graph,  $n_u(e|G) + n_v(e|G) = n$ . For convenience, let  $n_u(e|G) \geq n_v(e|G)$  where  $e = uv \in G$ . Then  $n_u(e|G) = n - n_v(e|G)$  and  $\phi(e) = |n_u(e|G) - n_v(e|G)| = n - 2n_v(e|G)$ . Now,

$$\begin{aligned} Mo(G) &= \sum_{e=uv \in E(G)} |n_u(e|G) - n_v(e|G)| = \sum_{e=uv \in E(G)} (n - 2n_v(e|G)) \\ &= mn - \left( 2 \sum_{e=uv \in E(G)} n_v(e|G) \right) \end{aligned}$$

Now  $mn$  is even if either  $m$  or  $n$  is even,  $mn$  is odd if both  $m, n$  are odd and consequently the conclusions hold. □

Now we establish the inverse Mostar index problem for chemical trees.

**Theorem 2.3.** [5] Let  $P_n$  be the path of  $n$  vertices, then  $Mo(P_n) = \begin{cases} \frac{(n-1)^2}{2}, & \text{if } n \text{ is odd} \\ \frac{n(n-2)}{2}, & \text{if } n \text{ is even} \end{cases}$

**Theorem 2.4.** For every positive even integer  $l$ , there exist a chemical tree  $T$  with  $Mo(T) = l$ .

*Proof.* By Theorem 2.1, Mostar index of every tree is even. Now, let  $l = 2t, t \geq 1$ .

When  $n = 2k + 1$ ,  $Mo(P_n) = 2k^2$  and when  $n = 2k + 2$ ,  $Mo(P_n) = 2k^2 + 2k$ .

Now let  $T_1 = P_{2k+1} = v_1v_2 \dots v_{2k+1}$ . Then  $T_1$  can be considered as the graph obtained from the path  $P_{2k}$  with a pendant edge at  $v_{2k}$ . Let  $T_2$  be the tree obtained from  $T_1$  by deleting the vertex  $v_{2k+1}$  and adding a pendant edge  $v_{2k-1}u$  at  $v_{2k-1}$ . We refer this operation as the transfer of the pendant edge from  $v_{2k}$  to  $v_{2k-1}$ . Then  $T_1$  has 2 edges each with contribution  $\phi(e) = 2k + 1 - 2j$  for  $j = 1, 2, \dots, k$  and  $T_2$  has three edges with  $\phi(e) = 2k - 1$  one edge with  $\phi(e) = 2k - 3$  and 2 edges each with  $\phi(e) = 2k + 1 - 2j, j = 3, 4, \dots, k$ . Thus

$$Mo(T_2) - Mo(T_1) = 3(2k - 1) - 2(2k - 1) + (2k - 3) - 2(2k - 3) = 2$$

Consequently  $Mo(T_2) = Mo(T_1) + 2$

Let  $T_i$  be a tree with path  $P_{2k} = v_1v_2 \dots v_{2k}$  along with a pendant edge at the vertex  $v_{2k+1-i}, i = 1, 2, 3, \dots, k - 1$ . Let  $T_{i+1}$  be the graph obtained by transferring the pendant edge from the vertex  $v_{2k+1-i}$  to  $v_{2k-i}$ . Then except for the edge  $v_{2k+1-i}v_{2k-i}$ , all the other edges of graph  $T_i$  has the same contribution as in the tree  $T_{i+1}$ . In the case of  $v_{2k+1-i}v_{2k-i}$ , in  $T_i$  the contribution is  $(2k + 1 - 2(i + 1))$  and in  $T_{i+1}$  the contribution is  $(2k + 1 - 2(i))$ . Thus,

$$Mo(T_{i+1}) - Mo(T_i) = (2k + 1 - 2(i)) - (2k + 1 - 2(i + 1)) = 2$$

Thus,  $Mo(T_1) = 2k^2$  and  $Mo(T_i) = 2k^2 + 2(i - 1), i = 2, 3, \dots, k$ . Thus for every even number  $l, 2k^2 \leq l < 2k^2 + 2k, k \geq 1$  there exist a tree  $T$  with  $Mo(T) = l$ .

Similarly, when  $n = 2k + 2, k \geq 1, Mo(P_n) = 2k^2 + 2k$  and when  $n = 2k + 3$ , then  $Mo(P_n) = 2k^2 + 4k + 2$ . There are  $k$  even numbers in between  $2k^2 + 4k + 2$  and  $2k^2 + 2k$ .

Now let  $T_1 = P_{2k+2} = v_1v_2 \dots v_{2k+2}$ . Then  $T_1$  can be considered as the graph obtained from the path  $P_{2k+1}$  with a pendant edge at  $v_{2k+1}$ . Let  $T_2$  be the graph obtained by transferring the pendant edge from  $v_{2k+1}$  to  $v_{2k}$ . Then  $T_1$  has 2 edges each with contribution  $\phi(e) = 2k + 2 - 2j$  for  $j = 1, 2, \dots, k$  and one edge with contribution zero.  $T_2$  has three edges with  $\phi(e) = 2k$ , one edge with  $\phi(e) = 2k - 2$  and 2 edges each with  $\phi(e) = 2k + 2 - 2j$  for  $j = 3, 4, \dots, k$  and one edge with contribution  $\phi(e) = 0$ . Thus,

$$Mo(T_2) - Mo(T_1) = 3(2k) - 2(2k) + (2k - 2) - 2(2k - 2) = 2$$

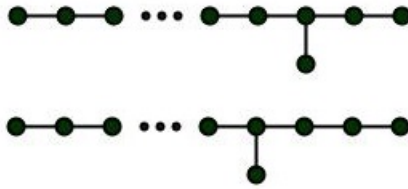
Consequently  $Mo(T_2) = Mo(T_1) + 2$

Now, let  $T_i$  be the graph with path  $P_{2k+1} = v_1v_2 \dots v_{2k+1}$  along with a pendant edge at  $v_{2k+2-i}, i = 1, 2, 3, \dots, k$  and  $T_{i+1}$  be the graph obtained by transferring the pendant edge from  $v_{2k+2-i}$  to  $v_{2k+1-i}$ . Then as in the previous case,  $T_i$  and  $T_{i+1}$  differs only in the contribution of the edge  $e = v_{2k+2-i}v_{2k+1-i}$ . In  $T_i, \phi(e) = 2k + 2 - 2(i + 1)$  and in  $T_{i+1}, \phi(e) = (2k + 2 - 2i)$ . Thus

$$Mo(T_{i+1}) - Mo(T_i) = (2k + 2 - 2(i)) - (2k + 2 - 2(i + 1)) = 2$$

Thus,  $Mo(T_1) = 2k^2 + 2k$  and  $Mo(T_i) = 2k^2 + 2k + 2(i - 1), i = 2, 3, \dots, k + 1$ . Thus for every even number  $l, 2k^2 + 2k \leq l < 2k^2 + 4k + 2, k \geq 1$  there exist a tree  $T$  with  $Mo(T) = l$ . Since degree of each vertex in these trees is less than or equal to 4, they all are chemical trees.  $\square$

Let  $\mathcal{U}_n$  denote the collection of all unicyclic graphs of order  $n$ . Let  $C_{n,r}$  denote the unicyclic graph with cycle  $C_n$  with a path of length  $r$  whose pendant vertex is identified with some vertex of  $C_n$ . Let  $U_{n,r}$  denote the unicyclic graph with the cycle  $v_1v_2 \dots v_nv_1$  with  $r$  pendant edges attached at the vertex  $v_1$  (or some other  $v_i$ ). Let  $\mathcal{U}_n \setminus \{G\}$  denote the collection of all unicyclic graphs of order  $n$  other than  $G$ . Let  $G_2^0$  denote the unicyclic graph of order  $n$ (even) with cycle  $C_{n-2}$  and two pendant edges attached at different vertices of  $C_{n-2}$  separated by a distance  $\frac{n-2}{2}$ .



**Figure 1.**  $T_i$  and  $T_{i+1}$  in Theorem 2.4.

$G_3^0$  denote a unicyclic graph of order  $n$ (even) with a cycle  $C_{n-2}$  along with two pendant edges attached at different vertices of  $C_{n-2}$  separated by a distance  $\frac{n-4}{2}$ .  $G_3^1$  denote a unicyclic graph of order  $n$ (odd) with a cycle  $C_{n-2}$  along with two pendant edges attached at different vertices of  $C_{n-2}$  separated by a distance  $\frac{n-3}{2}$ . In order to settle the inverse Mostar index problem for unicyclic graphs first we obtain the second smallest lower bound of the Mostar index for unicyclic graphs.

**Proposition 2.5.** For  $n \geq 4$ ,

$$(a.) Mo(C_{n-1,1}) = \begin{cases} 2n - 3, & \text{if } n \text{ is odd} \\ 2n - 4, & \text{if } n \text{ is even} \end{cases}$$

$$(b.) Mo(G_2^0) = 2n - 4, n \text{ is even.}$$

*Proof.* In  $C_{n-1,1}$ , when  $n$  is odd, the  $n - 1$  edges in the cycle  $C_{n-1}$  contribute 1 each and for the one remaining pendant edge the contribution is  $n - 2$ . When  $n$  is even, the  $n - 2$  edges in the cycle  $C_{n-1}$  contribute 1 each and the remaining one edge in the cycle contributes zero. Also, for the pendant edge, the contribution is  $n - 2$ . Now in  $G_2^0$ , two pendant edges contribute  $n - 2$  each and for every edge in the cycle  $C_{n-2}$ , the contribution is zero. Hence the result follows from the definition of Mostar index.  $\square$

**Corollary 2.6.** If  $G$  is a graph with the minimum Mostar index among all graphs in  $\mathcal{U}_n \setminus \{C_n\}$  of

$$\text{order } n \geq 4, \text{ then } Mo(G) \leq \begin{cases} 2n - 3, & \text{if } n \text{ is odd} \\ 2n - 4, & \text{if } n \text{ is even} \end{cases}$$

**Theorem 2.7.** Let  $n \geq 4$ .

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

(b.) If  $n$  is even then  $C_{n-1,1}$  and  $G_2^0$  are the only graphs with smallest value of Mostar index in  $\mathcal{U}_n \setminus \{C_n\}$ .

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

**Claim I:**  $G$  has either one or two pendant edges.

If  $G$  has no pendant edge then  $G \cong C_n$ , impossible. Suppose that  $G$  has three or more pendant edges, the  $Mo(G) > 3(n - 2) > 2n - 3$  since  $n \geq 4$ , impossible. Thus  $G$  has one or two pendant edges. Now consider the case that  $G$  has exactly two pendant edges. If at least one pendant edge is incident on a bridge  $e$  which is part of a tree  $T$ , then the bridge  $e$  contribute at least 1 and the edge on the cycle incident on  $T$  contribute at least 1 or the edge in the cycle incident on  $T$  contribute at least 2. Hence,  $Mo(G) > 2(n - 2) + 2 > 2n - 3$ , impossible. If both the pendant edges incident on the same vertex on cycle, then the edge on the cycle adjacent to the pendant edges contribute at least 2, hence  $Mo(G) > 2(n - 2) + 2 > 2n - 3$ , impossible. Thus both the pendant edges must be incident on the cycle. If both the pendant edges  $e$  and  $e'$  incident on different vertices of the cycle. If the distance  $d(e, e') < \frac{n-2}{2}$  then either there exist two edges in the cycle adjacent with pendant edges which contribute at least one or there exist one edge in the cycle adjacent to one of the pendant edge which contribute at least 2. Thus,

$Mo(G) > 2(n-2) + 2 > 2n-3$ , impossible. Thus if  $G$  has two pendant edges, then  $G$  should be a graph with cycle  $C_{n-2}$  with two pendant edges attached at different vertices of  $C_{n-2}$  separated by a distance  $\frac{n-2}{2}$ . When  $n$  is even, then  $Mo(G) = 2n-4$ , i.e.  $G \cong G_2^0$ . When  $n$

is odd, there is no such graph since distance between pendant edges is always less than  $\frac{n-2}{2}$ . Now the only remaining case is that  $G$  has exactly one pendant edge and consequently  $G$  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 pendant edge contribute  $n-2$ . Thus,  $Mo(G) \geq n-2+p(n-p)+p-2 \geq n-2+2(n-p)+p-2 = 3n-p-4$ . Now,  $3n-p-4 \leq 2n-3$  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 pendant edge contribute  $n-2$ . Thus  $Mo(G) \geq n-2+p(n-p-1)+p-1 \geq n-2+2(n-p-1)+p-1 = 3n-p-5$ . Now,  $3n-p-5 \leq 2n-3$  implies  $n-p \leq 2$  implies  $n \leq p+2$ , impossible. Thus  $p=1$  and hence  $G \cong C_{n-1,1}$ .  $\square$

**Proposition 2.8.** For  $n \geq 7$ ,

(a.)  $Mo(G_3^1) = 2n-2, n$  is odd.

(b.)  $Mo(G_3^0) = 2n, n$  is even.

*Proof.* When  $n$  is odd  $Mo(G_3^1) = 2n-2$ , since two pendant edges contribute  $n-2$  each and two edges  $e$  and  $e'$  incident on the pendant edges contribute 1 and all other edges in the cycle contribute zero. When  $n$  is even,  $Mo(G_3^0) = 2n$ , since pendant edges contribute  $n-2$  and two edges incident on the pendant edge on the cycle contribute 2 each and the rest of the edges does not contribute anything.  $\square$

Similarly we can obtain the third smallest value of Mostar index of unicyclic graphs

**Corollary 2.9.** If  $G$  is a graph with the minimum value of Mostar index among all graph in  $\mathcal{U}_n \setminus \{C_n, C_{n-1,1}, G_2^0\}$  of order  $n \geq 7$ , then the  $Mo(G) \leq \begin{cases} 2n-2, & \text{if } n \text{ is odd} \\ 2n, & \text{if } n \text{ is even} \end{cases}$ .

**Theorem 2.10.** Let  $n \geq 7$ .

(a.) If  $n$  is odd then  $G_3^1$  (See Figure 2) is the unique graph with smallest values of Mostar index in  $\mathcal{U}_n \setminus \{C_n, C_{n-1,1}\}$ .

(b.) If  $n$  is even then  $G_3^0$  (See Figure 2) is the unique graph with smallest values of Mostar index in  $\mathcal{U}_n \setminus \{C_n, C_{n-1,1}, G_2^0\}$ .

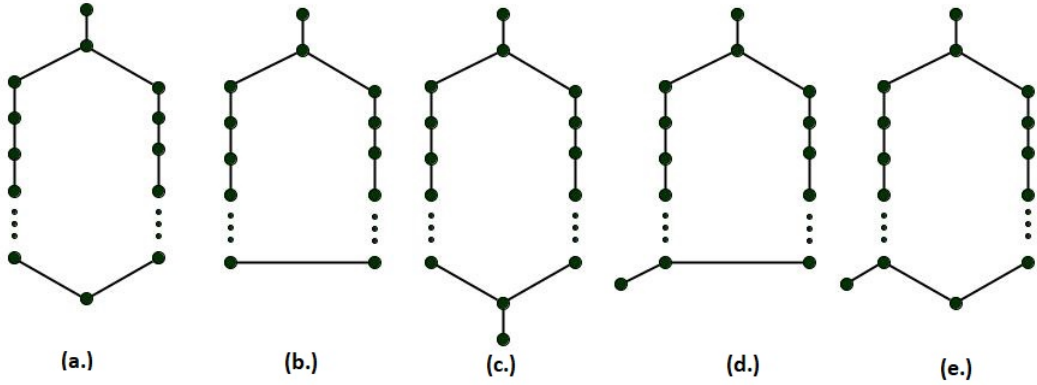
*Proof.* Let  $G$  be the graph which attains third minimum value of Mostar index in  $\mathcal{U}_n, n \geq 7$ . We proceed by establishing the following claims on  $G$ .

**Claim I:**  $G$  has exactly two pendant edges.

Suppose that  $G$  has three or more pendant edges, then  $Mo(G) > 3(n-2) > 2n$  since  $n \geq 7$ , impossible. If  $G$  has no pendant edge, then  $G \cong C_n$ , impossible. If  $G$  has exactly one pendant edge, then  $G$  is of the form  $C_{r,p}, r+p=n, p \geq 2$ . If  $r$  is even, then  $r=n-p \geq 4$  edges of the cycle contribute  $p$  and the pendant edge and the bridge incident on the pendant edge contribute  $n-2$  and  $n-4$  respectively. Thus,  $Mo(G) > n-2+n-4+p(n-p) \geq 2n-6+2(n-p) = 4n-2p-6$ . Now,  $4n-2p-6 \leq 2n$  implies  $n \leq p+3$ , impossible (since  $n \geq p+4$ ). If  $r$  is odd, then  $r-1=n-p-1 \geq 3$  edges of the cycle contribute  $p$  and the pendant edge and the bridge incident on the pendant edge contribute  $n-2$  and  $n-4$  respectively. Thus,  $Mo(G) > n-2+n-4+p(n-p-1) \geq 2n-6+2(n-p-1) = 4n-2p-8$ . Now,  $4n-2p-8 \leq 2n$  implies  $n < p+4$ , i.e.  $n \leq p+3$ , since  $r$  is odd. If  $n=p+3$ , then  $G=C_{3,n-3}$  and  $Mo(G) > 2(n-3)+n-2+n-4 > 4n-12$ . Now  $4n-12 \leq 2n$  implies  $n \leq 6$ , impossible. Thus  $G$  cannot have exactly one pendant edge. Thus  $G$  has exactly two pendant edges.

**Claim II :**  $G$  cannot have any non pendant bridges

Suppose at least one of the pendant edges is incident on a non- pendant bridge  $e$ . Then at least two edges on the cycle contribute at least one to the Mostar index. Thus,  $Mo(G) >$



**Figure 2.** (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.)  $G_3^0$

$2(n - 2) + n - 4 + 2 = 3n - 6$ . Now  $3n - 6 \leq 2n$  implies  $n \leq 6$ , impossible. Thus both the pendant edges of  $G$  are incident on the cycle.

**Claim III : Both pendant edges cannot be incident on the same vertex of the cycle**

Suppose both pendant edges are incident on the same vertex of the cycle. Then  $G$  is of the form of a cycle  $C_{n-2}$  with two pendant edges attached at some vertex of the cycle. Then at least  $n - 3$  edges of the cycle contribute 2. Thus  $Mo(G) \geq 2(n - 2) + 2(n - 3) = 4n - 10$ , now  $4n - 10 \leq 2n$  implies  $n \leq 5$ , impossible. Thus  $G$  is of the form  $C_{n-2}$  with pendant edges attached at different vertices of the cycle.

Let  $t$  be distance between the two pendant 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 edge contribute 1 and rest of the edges contribute 2. Thus  $Mo(G) > 2n - 4 + 2 + 2(n - 3 - 2t) = 4n - 4t - 8 > 2n - 2$  whenever  $t < \frac{n-3}{2}$ , thus  $t = \frac{n-3}{2}$ , i.e  $G = G_3^1$ . When  $n$  even and  $t < \frac{n-2}{2}$ , then  $2t$  edges in the cycle contribute zero and the remaining  $n - 2 - 2t$  edges contribute 2. Thus  $Mo(G) > 2n - 4 + 2(n - 2 - 2t) = 4n - 4t - 8 > 2n$  whenever  $t < \frac{n-4}{2}$ , thus  $t = \frac{n-4}{2}$ , i.e  $G = G_3^0$ . When  $t = \frac{n-2}{2}$ ,  $G = G_2^0$ , impossible, hence the result.  $\square$

Now we solve the inverse Mostar index problem on unicyclic graphs.

**Theorem 2.11.** For every positive integer  $n \neq 1, 2, 3, 5, 6, 9, 13$ , there exist a unicyclic graph  $G$  with  $Mo(G) = n$ .

*Proof.*  $Mo(C_n) = 0$  and for every unicyclic graph  $G \not\cong C_n$ ,  $Mo(G) > 0$ . Now we consider the unicyclic graphs which are not cycles. We divide the integers into into four different cases.

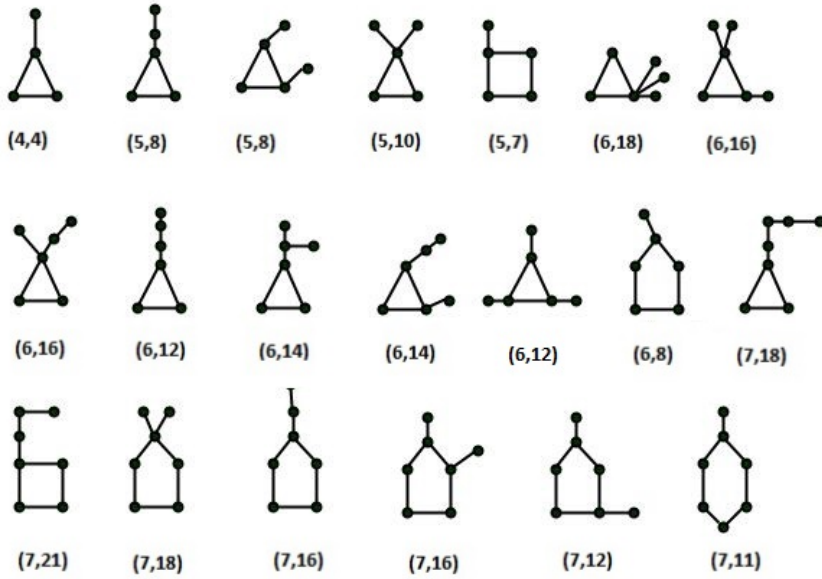
**Case I:**  $n = 4k, k \geq 1$ : When  $k = 1$ , the graph  $C_{3,1}$  has Mostar index 4. Therefore, let  $k \geq 2$ . Now construct the graph  $G$  with cycle  $C_{n-2}$  with pendant edges attached at the vertex  $v_1$  and  $v_{\frac{n-1}{2}}$  where  $n = 2k + 1, k \geq 2$ . Two edges in  $C_{n-2}$ ,  $e$  and  $e'$  incident at  $v_1$  and  $v_{\frac{n-1}{2}}$  contribute 1 and the rest of the edges in the cycle contribute zero. Each pendant edge contribute  $n - 2$ . Thus,

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

**Case II:**  $n = 4k + 1, k \geq 4$ : We divide this into two subcases,  $n = 8k + 1$  and  $n = 8k + 5$ . When  $n = 8k + 1$  construct a graph  $G$  of order  $n$  with cycle  $C_{n-3} = v_1v_2 \dots v_{n-3}v_1$ . Attach one pendant edge at  $v_1$  and identify the pendant vertex of a path of length 2 at  $v_{\frac{n-1}{2}}$  of the cycle, where  $n = 2k + 3, k \geq 2$ . The  $n - 3$  edges in  $C_{n-3}$  contribute 1 each and each pendant edge contribute  $n - 2$  and the one remaining bridge contribute  $n - 4$ . Thus

$$Mo(G) = 2(n - 2) + (n - 4) + n - 3 = 4n - 11 = 4(2k + 3) - 11 = 8k + 1$$

Now for  $n = 8k + 5$ , construct a graph  $G'$  with cycle  $C_{n-3} = v_1v_2 \dots v_{n-3}v_1$ . Attach one pendant edge at  $v_1$  and identify the pendant vertex of a path of length 2 at  $v_{\frac{n-3}{2}}$  where  $n = 2k + 3, k \geq 2$ .



**Figure 3.** Mostar index of some unicyclic graphs of orders 4,5,6,7. In  $(a, b)$ ,  $a$  indicate order of the graph and  $b$  indicate its Mostar index.

For two edges in  $C_{n-3}$ ,  $e$  and  $e'$  incident at  $v_1$  and  $v_{\frac{n-3}{2}}$  the contribution is 3 and for the remaining edges in  $C_{n-3}$  the contribution is 1. Each pendant edge contribute  $n - 2$  and for the remaining one bridge, the contribution is  $n - 4$ . Thus,

$$Mo(G') = 2(n - 2) + (n - 4) + n - 5 + 6 = 4n - 7 = 4(2k + 3) - 7 = 8k + 5$$

**Case III:**  $n = 4k + 2, k \geq 2$ : We divide this into two subcases,  $n = 8k + 2$  and  $n = 8k + 6$ . When  $n = 8k + 2$ , construct a graph  $G$  of order  $n$  with cycle  $C_{n-2} = v_1v_2 \dots v_{n-2}v_1$ . Attach two pendant edges at  $v_1$  where  $n = 2k + 3, k \geq 1$ . The  $n - 3$  edges in  $C_{n-2}$  contribute 2 each and each pendant edge contribute  $n - 2$ . Thus

$$Mo(G) = 2(n - 2) + 2(n - 3) = 4n - 10 = 4(2k + 3) - 10 = 8k + 2$$

Now for  $n = 8k + 6$ , construct a graph  $G'$  with cycle  $C_{n-2} = v_1v_2 \dots v_{n-2}v_1$ . Attach the pendant vertex of a path of length 2 at  $v_1$ , where  $n = 2k + 4, k \geq 1$ . The  $n - 2$  edges in  $C_{n-2}$  contribute 2 and the pendant edge and the remaining bridge contribute  $(n - 2)$  and  $(n - 4)$  respectively. Thus,

$$Mo(G') = 2(n - 2) + (n - 4) + n - 2 = 4n - 10 = 4(2k + 4) - 10 = 8k + 6$$

**Case IV:**  $n = 4k + 3, k \geq 1$ : Construct the graph  $C_{n-1,1}$  with  $n = 2k + 3, k \geq 1$ . Now for  $C_{n-1,1}$ , for  $n - 1$  edges in the cycle  $C_{n-1}$  the contribution is 1 and for the remaining one pendant edge the contribution is  $n - 2$ . Thus,

$$Mo(C_{n-1,1}) = n - 2 + n - 1 = 2n - 3 = 2(2k + 3) - 3 = 4k + 3$$

Thus every integer other than 1,2,3,5,6,9,13 can be the Mostar index of some unicyclic graph. Now by Theorem 2.7, for any unicyclic graph  $G$  other than  $C_n$ ,  $Mo(G) \geq 4$ . Thus 1, 2, 3 cannot be Mostar index of any unicyclic graph. When  $n \geq 5$ , by Theorem 2.7,  $Mo(G) \geq 7$  and there is no unicyclic graph of order less than or equal to 4 which has Mostar index 5 or 6 (See Figure 3). Thus 5,6 are not Mostar index of any unicyclic graph. When  $n \geq 9$ ,  $Mo(G) \geq 15$ , thus 9 and 13 cannot be the Mostar index of any unicyclic graph of order  $n \geq 9$ . When  $n = 8$ , first two non zero lower bounds for Mostar index are 12, 16 (by Theorem 2.7, Theorem 2.10), thus 9,13 cannot be the Mostar index of unicyclic graph of order 8. When  $n = 7$ , we cannot consider a

graph with two or more pendant edges and a bridge or with three or more pendant edges, since then  $Mo(G) > 5 + 5 + 3 + 1 > 13$ . All other possible graphs and their Mostar index are plotted in Figure 3, thus there is no unicyclic graph of order 7 which has the Mostar index 9,13. When  $n = 6$ , no bipartite graph of order 6 can have Mostar index 9,13, since by Theorem 2.2 it must be even. Thus the graph cannot have even cycle when order is even. When  $n = 5$  or 6 all other possible unicyclic graphs and their Mostar index are plotted in Figure 3. Thus there does not exist a unicyclic graph with Mostar index 9, 13.  $\square$

### 3 Conclusion

In this paper, we have resolved the inverse Mostar index problem for trees and unicyclic graphs. There are still lots of inverse topological index problems for several bond additive indices which still need further research.

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