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Maximum values of the edge Mostar index in tricyclic graphs

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Abstract. For a graph G, the edge Mostar index of G is the sum of $|m_u(e|G) - m_v(e|G)|$ over all edges $e = uv$ of G, where $m_u(e|G)$ denotes the number of edges of G that have a smaller distance in G to u than to v, and analogously for $m_v(e|G)$. This paper mainly studies the problem of determining the graphs that maximize the edge Mostar index among tricyclic graphs. To be specific, we determine a sharp upper bound for the edge Mostar index on tricyclic graphs and identify the graphs that attain the bound.

1. Introduction

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The order and size of G are the cardinality of $V(G)$ and $E(G)$, respectively. The distance between u and v in G is the least length of the path connecting u and v denoted by $d_G(u, v)$. For a vertex x and edge $e = uv$ of a graph G, the distance between x and e, denoted by $d_G(x, e)$, is defined as $d_G(x, e) = min\{d_G(x, u), d_G(x, v)\}$.

A single number that can be used to describe some properties of a graph is called a topological index, or graph invariant. Topological index is a graph theoretic property that is preserved by isomorphism, which is widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications.

Došlić et al. [7] introduced a bond-additive structural invariant as a quantitative refinement of the distance non-balancedness and also a measure of peripherality in graphs, named the Mostar index. For a graph G, the Mostar index is defined as

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

where $n_u(e|G)$ is the number of vertices of G closer to u than to v and $n_v(e|G)$ is the number of vertices closer to v than to u.

The problem of determining which graphs uniquely maximize (resp. minimize) the Mostar index in some classes of graphs has received much attention. For example, Doslić et al. [7] studied the Mostar index

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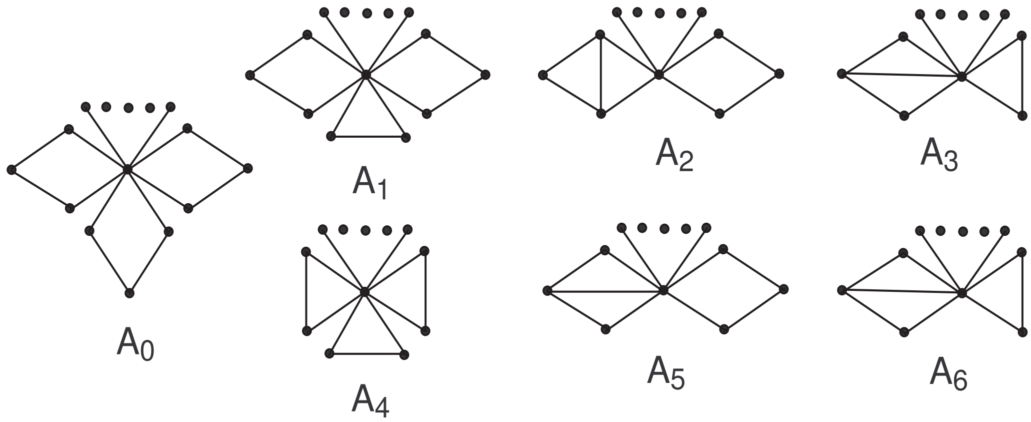

Figure 1: The Graphs A_i $(i = 0, 1, ..., 6)$ of size m in Theorem 1.1.

of trees and unicyclic graphs, and showed that path and star are, respectively, the unique tree having the minimum and maximum Mostar index among all trees with n vertices. Upper or lower bounds of the Mostar index for some special classes of graphs in terms of some fixed parameters were also presented, such as trees [3–5, 11, 15], unicyclic graphs [18], bicyclic graphs [21], cacti [14], tricyclic graphs [12], bipartite and split graphs [20]. For more studies about the Mostar index see [1, 6, 16, 22, 23].

Arockiaraj et al. [2], introduced the edge version of the Mostar index as a quantitative refinement of the distance non-balancedness, also it can measure the peripherality of every edge and consider the contributions of all edges into a global measure of peripherality for a given chemical graph. The edge Mostar index of G is defined as

$$Mo_e(G) = \sum_{e=uv \in E(G)} \psi_G(uv),$$

where $\psi_G(uv) = |m_u(e|G) - m_v(e|G)|$, and $m_u(e|G)$ denotes the number of edges of G that have a smaller distance in G to u than to v, and analogously for $m_v(e|G)$.

Up to now, a number of results were obtained on the edge Mostar index of a graph. In [17], the edge Mostar index of chemical structures and nanostructures was obtained. The extremal values of the edge Mostar index over trees and unicyclic graphs and the maximum and the second maximum value of the edge Mostar index among cactus graphs with a given number of vertices were obtained in [19]. In [8], the minimum values of the edge Mostar index of bicyclic graphs with a fixed size was determined. The edge Mostar index for several classes of cycle-containing graphs was computed in [10]. The Mostar and edge Mostar index of polymers was computed in [9]. Recently, Hayat et al. [13] determined the sharp upper bound for the edge Mostar index on bicyclic graphs with a fixed number of edges, and the graphs that achieve the bound are completely characterized.

To have a full understanding of the relationship between the edge Mostar index and the structural properties of graphs, in this paper, we consider the edge Mostar index over tricyclic graphs, and more precisely, we obtain the sharp upper bound for the edge Mostar index on tricyclic graphs with a fixed number of edges, and identify the graphs that attain the bound.

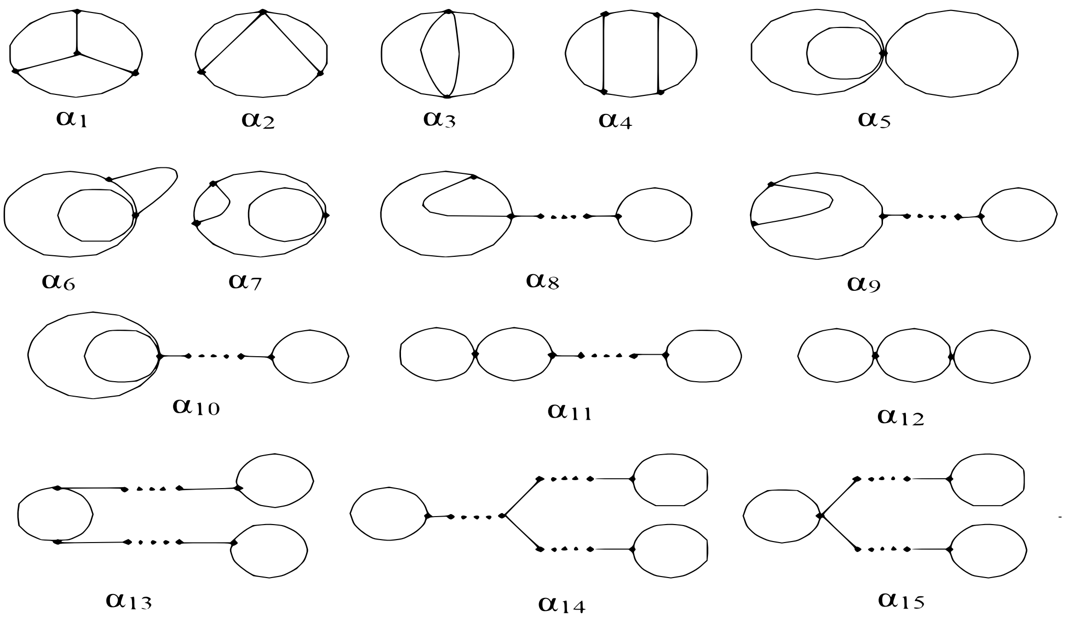

Figure 2: The braces in $\mathcal{G}_m$.

Theorem 1.1. *Let G be a tricyclic graph of size m. Then*

$$Mo_e(G) \leq \begin{cases} 12, & \text{if } m = 7, \text{ and equality holds iff } G \cong F_1, H_1; \\ 23, & \text{if } m = 8, \text{ and equality holds iff } G \cong A_3, F_1, H_1; \\ 36, & \text{if } m = 9, \text{ and equality holds iff } G \cong F_1, H_1, A_i (i = 2, ..., 6); \\ 53, & \text{if } m = 10, \text{ and equality holds iff } G \cong A_2; \\ 72, & \text{if } m = 11, \text{ and equality holds iff } G \cong A_1, A_2; \\ m^2 - m - 36, & \text{if } m \geq 12, \text{ and equality holds iff } G \cong A_0. \end{cases}$$

(Where A_i $(i = 0, 1, ..., 6)$ are depicted in Fig. 1.1, F_1, H_1 are depicted and Fig. 6 and Fig. 7, respectively).

In section 2, we give some definitions and preliminary results. Theorem 1.1 is proved in section 3.

2. Preliminaries

In this section, some basic notations and elementary results are listed, which will be useful in the proof of main results.

For $v \in V(G)$, let $N_G(v)$ be the set of vertices that are adjacent to v in G. The degree of $v \in V(G)$, denoted by $d_G(v)$, is the cardinality of $N_G(v)$. A vertex with degree one is called a pendent vertex and an edge incident to a pendent vertex is called a pendent edge. A graph G with n vertices is a tricyclic graph if $|E(G)| = n + 2$. As usual, by S_n, P_n and C_n we denote the star, path and cycle on n vertices, respectively.

Let $G_1 \cdot G_2$ be the graph obtained from G_1 and G_2 by identifying one vertex, say u of the two graphs. If G_1 contains a cycle and u belongs to some cycle, and G_2 is a tree, then we call G_2 a pendent tree in $G_1 \cdot G_2$ associated with u. For each $e \in E(G_1)$, every path from e to some edges of G_2 passes through u. Therefore, the contribution of G_2 to $\sum_{e \in E(G_1)} \psi(e)$ totally depends on the size of G_2, that is, changing the structure of G_2 cannot alter the value $\sum_{e \in E(G_1)} \psi(e)$. If a graph H is gotten by removing repeatedly all pendents (If any) of G. Then we say H is the brace of G. That is to say, H does not contain any pendent vertex. Obviously, for all connected tricyclic graphs, their braces are shown in Fig. 2. Let $\mathcal{G}_m^i$ be the collection whose element includes α_i as its brace for $i = 1, \ldots, 15$. For convenience, let $\mathcal{A} = \cup_{i=5}^{15} \mathcal{G}_m^i$.

In the following, Hayat et al. [13] determined a sharp upper bound for the edge Mostar index on bicyclic graphs with a fixed number of edges

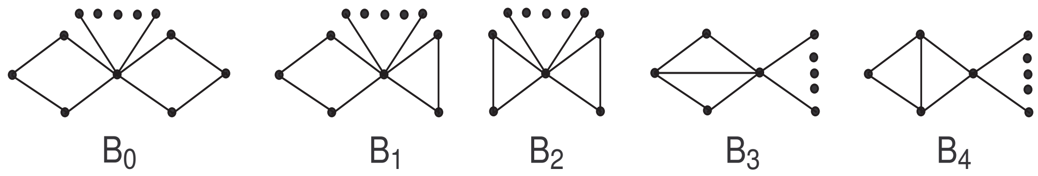

Figure 3: The Graphs B_i ($i = 0, 1, ..., 4$) of size m in Theorem 2.1.

Theorem 2.1. *Let G be a bicyclic graph of size m. Then*

$$Mo_e(G) \leq \begin{cases} 4, & \text{if } m = 5, \text{ and equality holds iff } G \cong B_3, B_4; \\ m^2 - 3m - 6, & \text{if } 6 \leq m \leq 8, \text{ and equality holds iff } G \cong B_1, B_3; \\ 48, & \text{if } m = 9, \text{ and equality holds iff } G \cong B_0, B_1, B_2, B_3, B_4; \\ m^2 - m - 24, & \text{if } m \geq 10, \text{ and equality holds iff } G \cong B_0. \end{cases}$$

(Where B_0, B_1, B_2, B_3, B_4 are depicted in Fig. 3).

Let $S_{m,r} \cong S_{m-r} \cdot C_r$, where the common vertex of S_{m-r} and C_r is the center of S_{m-r}.

Lemma 2.2. *[13] Let G_1 be a connected graph of size m_1 and G_2 be a unicyclic graph of size m_2. Then*
$Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,3})$ *for* $m_1 + m_2 \leq 8$;
$Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,3}) = Mo_e(G_1 \cdot S_{m_2,4})$ *for* $m_1 + m_2 = 9$;
$Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,4})$ *for* $m_1 + m_2 \geq 10$;
where the fusing vertex of $G_1 \cdot S_{m_2,3}$ (resp. $G_1 \cdot S_{m_2,4}$) is the center of $S_{m_2,3}$ (resp. $S_{m_2,4}$).

By means of Theorem 2.1 and the above result, the following conclusions are obtained.

Lemma 2.3. *Let $G = G_1 \cdot G_2$ be a tricyclic graph, where G_1 is a bicyclic graph of size m_1 and G_2 is a unicyclic graph of size m_2. Then*
$Mo_e(G) \leq Mo_e(B_3 \cdot S_{m_2,3})$ *for* $m_1 + m_2 = 8$;
$Mo_e(G) \leq Mo_e(B_2 \cdot S_{m_2,3}) = Mo_e(B_3 \cdot S_{m_2,3}) = Mo_e(B_3 \cdot S_{m_2,4}) = Mo_e(B_4 \cdot S_{m_2,3}) = Mo_e(B_4 \cdot S_{m_2,4})$ *for* $m_1 + m_2 = 9$;
$Mo_e(G) \leq Mo_e(B_0 \cdot S_{m_2,4})$ *for* $m_1 + m_2 \geq 12$;
where the fusing vertex of any of the above two graphs is the center of $S_{m_2,3}$ or $S_{m_2,4}$.

3. Proof of Theorem 1.1

For the proof of Theorem 1.1, we first develop several lemmas.
First, we obtain a sharp upper bound for $Mo_e(G)$ on $\mathcal{A} = \cup_{i=5}^{15} \mathcal{G}_m^i$.

Lemma 3.1. *Let $G \in \mathcal{A}$ of size m. Then*

$$Mo_e(G) \leq \begin{cases} 23, & \text{if } m = 8, \text{ and equality holds iff } G \cong A_3; \\ 36, & \text{if } m = 9, \text{ and equality holds iff } G \cong A_i (i = 2, ..., 6); \\ 53, & \text{if } m = 10, \text{ and equality holds iff } G \cong A_2; \\ 72, & \text{if } m = 11, \text{ and equality holds iff } G \cong A_1, A_2; \\ m^2 - m - 36, & \text{if } m \geq 12, \text{ and equality holds iff } G \cong A_0; \end{cases}$$

Proof. Suppose $G \in \mathcal{A}$, then G contains $\alpha_i (i = 5, 6, ..., 15)$ as its brace. Let G_1 be a bicyclic graph of size m_1 and G_2 be a unicyclic graph of size m_2 such that $G = G_1 \cdot G_2$. Then, in view of Lemmas 2.2 and 2.3, if $m = 8$, we get

$$\begin{aligned} Mo_e(G) &= Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,3}) \\ &\leq Mo_e(B_3 \cdot S_{m_2,3}) = Mo_e(A_3); \end{aligned}$$

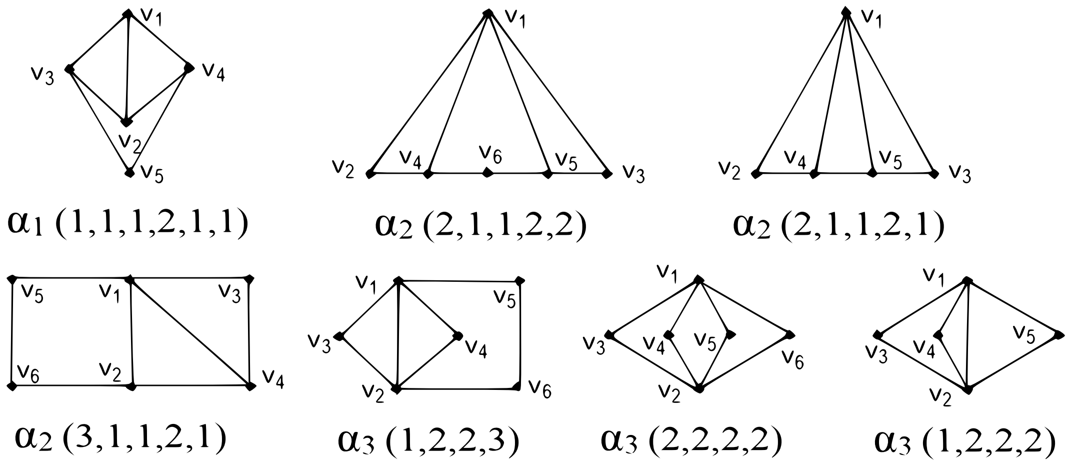

Figure 4: The Graphs for Lemmas 3.2, 3.4, 3.5, 3.6, 3.8, 3.9 and 3.10.

if $m = 9$, we get

$$\begin{aligned} Mo_e(G) &= Mo_e(G_1 \cdot G_2) \le Mo_e(B_2 \cdot S_{m_2,3}) = Mo_e(B_3 \cdot S_{m_2,3}) \\ &= Mo_e(B_3 \cdot S_{m_2,4}) = Mo_e(B_4 \cdot S_{m_2,3}) = Mo_e(B_4 \cdot S_{m_2,4}) \\ &= Mo_e(A_i)(i = 2, ..., 6); \end{aligned}$$

if $m \ge 12$, we have

$$\begin{aligned} Mo_e(G) &= Mo_e(G_1 \cdot G_2) \le Mo_e(G_1 \cdot S_{m_2,4}) \\ &\le Mo_e(B_0 \cdot S_{m_2,4}) = Mo_e(A_0). \end{aligned}$$

By simple calculation, it is easy to check that, $Mo_e(A_0) = m^2 - m - 36$, $Mo_e(A_1) = Mo_e(A_2) = m^2 - 2m - 27$, $Mo_e(A_3) = Mo_e(A_4) = m^2 - 4m - 9$, $Mo_e(A_5) = Mo_e(A_6) = Mo_e(A_7) = m^2 - 3m - 18$.

Clearly, $Mo_e(A_0) = m^2 - m - 36 > Mo_e(A_i)(i = 3, ..., 7)$, for $m \ge 10$, but A_0 contains at least 12 edges. Therefore, if $m = 11$, then $Mo_e(A_1) = Mo_e(A_2) > Mo_e(A_i)(i = 3, ..., 7)$; if $m = 10$, then $Mo_e(A_2) > A_i(i = 3, ..., 7)$. □

In what follows, we determine a sharp upper bound for $Mo_e(G)$ on $\cup_{i=1}^{4} \mathcal{G}_m^i$.

For $i = 1, ..., 4$, $\alpha_i(a_1, a_2, \dots)$ represents the number of edges in each portion of the brace α_i.

Lemma 3.2. *Let $G \in \mathcal{G}_m^1$ with brace $\alpha_1(1, 1, 1, 2, 1, 1)$. Then*

$$Mo_e(G) < \begin{cases} Mo_e(D_1) = m^2 - 3m - 24, & \text{if } 7 \le m \le 10; \\ Mo_e(D_1) = Mo_e(D_2) = 64, & \text{if } m = 11; \\ Mo_e(D_2) = m^2 - 2m - 35, & \text{if } m \ge 12. \end{cases}$$

Proof. Suppose that v_i $(i = 1, ..., 5)$ be the vertices in α_1 of G, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i $(i = 1, ..., 5)$. Suppose that $a_1 + a_3 \ge a_2 + a_4 \ge 1$. Let G_1 be the graph obtained from G by

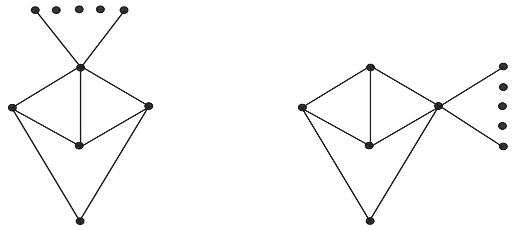

Figure 5: The Graphs D_1, D_2 of size m in Lemma 3.2.

shifting a_2 (resp. a_4) pendent edges from v_2 (resp. v_4) to v_1 (resp. v_3). We deduce that

$$
\begin{aligned}
& Mo_e(G_1) - Mo_e(G) = \\
& (a_1 + a_2 - a_3 - a_4 - a_5) - (a_1 + a_4 - a_3 - a_5) + (a_3 + a_4 + a_5 + 2 - 3) \\
- \ & (a_2 + a_4 + 3 - a_3 - a_5 - 2) + (a_3 + a_4 + a_5 + 2 - 3) - (a_2 + a_4 + 3 - a_3 - a_5 - 2) \\
+ \ & (a_1 + a_2 + a_3 + a_4 - a_5) - (a_1 + a_3 - a_4 - a_5) + (a_3 + a_4 + 3 - a_5 - 2) \\
- \ & (a_2 + a_3 + 3 - a_4 - a_5 - 2) + (a_3 + a_4 + 3 - a_5 - 2) - (a_2 + a_3 + 3 - a_4 - a_5 - 2) \\
+ \ & (a_1 + a_2) - (a_1 - a_2) + (a_1 + a_2 + a_3 + a_4 + 3 - a_5 - 1) - (a_1 + a_2 + a_3 + 3 - a_4 - a_5 - 1) \\
+ \ & (a_1 + a_2 + 3 - a_3 - a_4 - a_5 - 1) - (a_1 + a_2 + a_4 + 3 - a_3 - a_5 - 1) \\
= \ & 2(a_2 + a_3 + a_4 + a_5) - 2 > 0.
\end{aligned}
$$

For $a_5 > 0$, let G_2 be the graph obtained from G_1 by shifting a_5 pendent edges from v_5 to v_3. We obtain

$$
\begin{aligned}
& Mo_e(G_2) - Mo_e(G_1) = \\
& (a_1 + a_3 + a_5) - (a_1 + a_3 - a_5) + (a_3 + a_5 + 3 - 2) - (a_3 + 3 - a_5 - 2) \\
+ \ & (a_1 + a_3 + a_5 + 3 - 1) - (a_1 + a_3 + 3 - a_5 - 1) \\
= \ & 6a_5 > 0.
\end{aligned}
$$

Let G_3 be the graph obtained from G_2 by shifting a_1 pendent edges from v_1 to v_3. We obtain

$$
\begin{aligned}
& Mo_e(G_3) - Mo_e(G_2) = \\
& (a_1 + a_3) - (a_3 - a_1) + (a_1 + a_3 + 2 - 3) - (a_3 + 2 - 3) + (a_1 + a_3 + 3 - 2) - (a_3 + 3 - 2) \\
+ \ & 0 - a_1 + (a_1 + a_3 + 1 - 3) - (a_3 + 1 - a_1 - 3) \\
= \ & 5a_1 > 0.
\end{aligned}
$$

Clearly, $G_3 \cong D_2$, and $G_2 \cong D_1$ for $a_3 = 0$. Observe that $Mo_e(D_1) = m^2 - 3m - 24$, and $Mo_e(D_2) = m^2 - 2m - 35$. □

Lemma 3.3. *Let $G \in \mathcal{G}_m^1$ of size m. Then $Mo_e(G) < m^2 - m - 36$.*

Proof. Suppose that $G \in \mathcal{G}_m^1$, then G has a brace $\alpha_1(a_1, a_2, a_3, a_4, a_5, a_6)$ as shown in Fig. 8. We consider the following three possible cases.
Case 1. α_1 have at least three paths with length at least two.
Subcase 1.1. The three paths inclose a cycle.

Assume that the three paths are $P(a_1), P(a_2)$ and $P(a_6)$ by the symmetry of α_1. We choose nine edges, two edges in the path $P(a_1)$ such that each one is incident to x or u, two edges in the path $P(a_2)$ such that each one is incident to y or u, two edges in the path $P(a_6)$ such that each one is incident to y or z, one edge in the path $P(a_3)$ incident to z, one edge in the path $P(a_4)$ incident to z and one edge in the path $P(a_5)$ incident to z. Let e be one of the nine edges. Then $\psi(e) \leq m-7$. This fact is also true for the remaining eight edges. Thus,

$$Mo_e(G) \leq 9(m-7) + (m-9)(m-1) < m^2 - m - 36.$$

Subcase 1.2. The three paths composed a new path.

Assume that the three paths are $P(a_1), P(a_2)$ and $P(a_4)$ by the symmetry of α_1. We choose nine edges, two edges in the path $P(a_1)$ such that each one is incident to x or u, two edges in the path $P(a_2)$ such that each one is incident to y or u, two edges in the path $P(a_4)$ such that each one is incident to y or z, one edge in the path $P(a_3)$ incident to z, one edge in the path $P(a_5)$ incident to z and one edge in the path $P(a_6)$ incident to x. Thus,

$$Mo_e(G) \leq 2(m-6) + 4(m-7) + 2(m-8) + (m-9) + (m-9)(m-1) < m^2 - m - 36.$$

Subcase 1.3. The three paths share a common vertex.

Assume that the three paths are $P(a_1), P(a_2)$ and $P(a_3)$ by the symmetry of α_1. We choose nine edges, two edges in the path $P(a_1)$ such that each one is incident to x or u, two edges in the path $P(a_2)$ such that each one is incident to y or u, two edges in the path $P(a_3)$ such that each one is incident to u or z, one edge in the path $P(a_4)$ incident to y, one edge in the path $P(a_5)$ incident to z and one edge in the path $P(a_6)$ incident to x. We have,

$$Mo_e(G) \leq 3(m-7) + 3(m-8) + 3(m-9) + (m-9)(m-1) < m^2 - m - 36.$$

Case 2. α_1 have just two paths with length at least two.
Subcase 2.1. The two paths belong to the same cycle at α_1.

Assume that the two paths are $P(a_1)$ and $P(a_2)$ by the symmetry of α_1. We choose eight edges, two edges in the path $P(a_1)$ such that each one is incident to x or u, two edges in the path $P(a_2)$ such that each one is incident to y or u, one edge in the path $P(a_3)$ incident to u, one edge in the path $P(a_4)$ incident to y, one edge in the path $P(a_5)$ incident to x and one edge in the path $P(a_6)$ incident to x. We deduce that,

$$Mo_e(G) \leq 4(m-6) + 3(m-7) + (m-8) + (m-8)(m-1) < m^2 - m - 36.$$

Subcase 2.2. The two paths belong to the two different cycles at α_1.

We choose eight edges in a similar way, as in Subcase 2.1. We obtain

$$Mo_e(G) \leq 4(m-5) + 4(m-8) + (m-8)(m-1) < m^2 - m - 36.$$

Case 3. α_1 has exactly one path with length at least two.

Assume that the path is $P(a_4)$ with $a_4 \geq 2$. If $a_4 = 2$, then by Lemma 3.2, $Mo_e(G) < m^2 - m - 36$. If $a_4 \geq 3$, then similarly choose eight edges as in Subcase 2.1. We obtain

$$Mo_e(G) \leq 2(m-5) + 6(m-8) + (m-8)(m-1) < m^2 - m - 36.$$

□

Lemma 3.4. *Let $G \in \mathcal{G}_m^2$ with brace $\alpha_2(2,1,1,2,1)$. Then*

$$Mo_e(G) < \begin{cases} Mo_e(F_1) = m^2 - 4m - 9, & \text{if } 7 \leq m \leq 16; \\ Mo_e(F_1) = Mo_e(F_2) = 212, & \text{if } m = 17; \\ Mo_e(F_2) = m^2 - 3m - 26, & \text{if } m \geq 18. \end{cases}$$

Proof. Suppose that v_i $(i = 1, ..., 5)$ be the vertices in $\alpha_2(2,1,1,2,1)$ of G, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i $(i = 1, ..., 5)$. Suppose $a_2 + a_4 \geq a_3 + a_5 \geq 1$. For $a_1 < a_2 + 3a_3 + a_5 - 3$, let G_1

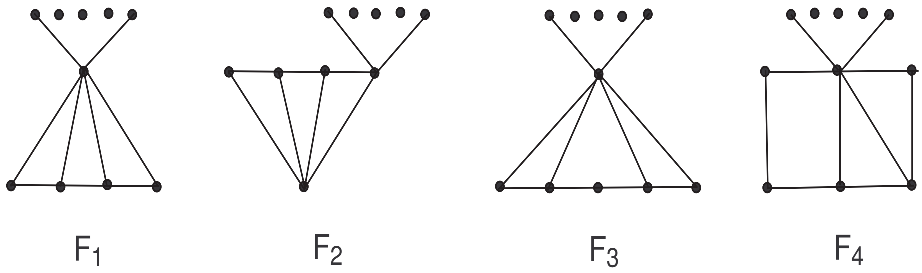

Figure 6: The Graphs F_1, F_2, F_3, F_4 of size m in Lemmas 3.4, 3.5 and 3.6.

be the graph obtained from G by shifting a_3 (resp. a_5) pendent edges from v_3 (resp. v_5) to v_2 (resp. v_4). We deduce that

$$\begin{aligned}
& Mo_e(G_1) - Mo_e(G) = \\
& (a_2 + a_3 + 1 - a_1 - 4) - (a_1 + a_3 + a_5 + 4 - a_2 - 1) + (1 + a_2 + a_3 - 3 - a_4 - a_5) \\
- \; & (a_2 + 1 - a_4 - a_5 - 3) + (a_1 + 3 - a_4 - a_5 - 2) - (a_1 + a_3 + 3 - a_4 - 2) \\
+ \; & (a_2 + a_3 + a_4 + a_5 + 3 - 3) - (a_2 + a_4 + 3 - a_5 - a_3 - 3) + (a_1 + a_2 + a_3 + a_4 + a_5 + 4 - 1) \\
- \; & (a_1 + a_2 + a_4 + 4 - a_3 - 1) + (a_4 + a_5 + 3 - 1) - (a_4 + a_5 + 3 - 1 - a_3) \\
+ \; & (a_1 + a_2 + a_3 + 3 - 2) - (a_1 + a_2 + a_3 - a_5 - 2) \\
= \; & 2a_2 + 6a_3 + 2a_5 - 2a_1 - 6 > 0.
\end{aligned}$$

Let G_2 be the graph obtained from G_1 by shifting a_4 pendent edges from v_4 to v_1. We obtain

$$\begin{aligned}
& Mo_e(G_2) - Mo_e(G_1) = \\
& (a_1 + a_4 + 4 - a_2 - 1) - (a_1 + 4 - a_2 - 1) + (a_1 + a_4 + 3 - 2) - (a_1 + 3 - a_4 - 2) \\
+ \; & (a_1 + a_2 + a_4 + 3 - 2) - (a_1 + a_2 + 3 - 2) + (a_2 + 1 - 3) - (a_2 + 1 - 3 - a_4) + (a_2 + 3 - 3) \\
- \; & (a_2 + a_4 + 3 - 3) + (3 - 1) - (a_4 + 3 - 1) \\
= \; & 3a_4 > 0.
\end{aligned}$$

Let G_3 be the graph obtained from G_2 by shifting a_2 pendent edges from v_2 to v_1. We obtain

$$\begin{aligned}
& Mo_e(G_3) - Mo_e(G_2) = \\
& (a_1 + a_2 + 4 - 1) - (a_1 + 4 - a_2 - 1) + (a_1 + a_2 + 3 - 2) - (a_1 + 3 - 2) + (1 - 3) \\
- \; & (a_2 + 1 - 3) + 0 - (a_2 + 3 - 3) \\
= \; & 2a_2 > 0.
\end{aligned}$$

For $a_1 > 6 - 2a_2$, let G_4 be the graph obtained from G_3 by shifting a_1 pendent edges from v_1 to v_2. We have

$$\begin{aligned}
& Mo_e(G_3) - Mo_e(G_2) = \\
& (a_1 + a_2 + 1 - 4) - (a_1 + 4 - a_2 - 1) + (3 - 2) - (a_1 + 3 - 2) + (a_1 + a_2 + 1 - 3) \\
- \; & (a_2 + 1 - 3) + (a_1 + a_2 + 3 - 3) - (a_2 + 3 - 3) \\
= \; & a_1 + 2a_2 - 6 > 0.
\end{aligned}$$

Clearly, $G_3 \cong F_1$ and $G_4 \cong F_2$. By simple calculation, we have $Mo_e(F_1) = m^2 - 4m - 9$, and $Mo_e(F_2) = m^2 - 3m - 26$. □

Lemma 3.5. *Let $G \in \mathcal{G}_m^2$ with brace $\alpha_2(2, 1, 1, 2, 2)$. Then $Mo_e(G) < Mo_e(F_3) = m^2 - 3m - 20$.*

Proof. Suppose that v_i ($i = 1, ..., 6$) be the vertices in $\alpha_2(2,1,1,2,2)$ of G, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i ($i = 1, ..., 6$). For $a_6 > 0$, let G_1 be the graph obtained from G by shifting a_6 pendent edges from v_6 to v_1. We obtain

$$\begin{aligned}
& Mo_e(G_1) - Mo_e(G) = \\
& (a_1 + a_3 + a_5 + a_6 + 5 - a_2 - 1) - (a_1 + a_3 + a_5 + 5 - a_2 - 1) \\
+ \quad & (a_1 + a_2 + a_4 + a_6 + 5 - a_3 - 1) - (a_1 + a_2 + a_4 + 5 - a_3 - 3) \\
+ \quad & (a_1 + a_3 + a_5 + a_6 + 4 - a_4 - 2) - (a_1 + a_3 + a_5 + 4 - a_4 - a_6 - 2) \\
+ \quad & (a_1 + a_2 + a_4 + a_6 + 4 - a_5 - 2) - (a_1 + a_2 + a_4 + 4 - a_5 - a_6 - 2) \\
+ \quad & (a_1 + a_2 + a_4 + a_6 + 4 - a_5 - 2) - (a_1 + a_2 + a_4 + 4 - a_5 - a_6 - 2) \\
+ \quad & (a_1 + a_3 + a_5 + 4 - a_4 - 2) - (a_1 + a_3 + a_5 + 4 - a_4 - a_6 - 2) \\
+ \quad & (a_2 + 1 - a_4 - 3) - (a_2 + 1 - a_4 - a_6 - 3) + (a_3 + 1 - a_5 - 3) - (a_3 + 1 - a_5 - a_6 - 3) \\
= \quad & 11a_6 > 0.
\end{aligned}$$

For $a_2 + a_3 > a_1$, let G_2 be the graph obtained from G_1 by shifting a_3 (resp. a_5) pendent edges from v_3 (resp. v_5) to v_2 (resp. v_4). We deduce that

$$\begin{aligned}
& Mo_e(G_2) - Mo_e(G_1) = \\
& (a_2 + a_3 + 1 - a_1 - 5) - (a_1 + a_3 + a_5 + 5 - a_2 - 1) + (a_1 + a_2 + a_3 + a_4 + a_5 + 5 - 1) \\
- \quad & (a_1 + a_2 + a_4 + 5 - a_3 - 1) + (a_1 + 4 - a_4 - a_5 - 2) - (a_1 + a_3 + a_5 + 4 - a_4 - 2) \\
+ \quad & (a_1 + a_2 + a_3 + a_4 + a_5 + 4 - 2) - (a_1 + a_2 + a_4 + 4 - a_5 - 2) + (a_2 + a_3 + 1 - a_4 - a_5 - 3) \\
- \quad & (a_2 + 1 - a_4 - 3) + (3 - 1) - (a_3 + 1 - a_5 - 3) + (a_1 + a_2 + a_3 + a_4 + a_5 - 2) \\
- \quad & (a_1 + a_2 + a_4 + 4 - a_5 - 2) + (a_1 + 4 - a_4 - a_5 - 2) - (a_1 + a_3 + a_5 + 4 - a_4 - 2) \\
= \quad & 2a_2 + 2a_3 - 2a_1 > 0.
\end{aligned}$$

For $a_2 + a_4 \geq 1$, let G_3 be the graph obtained from G_2 by shifting a_2 (resp. a_4) pendent edges from v_2 (resp. v_4) to v_1 (resp. v_4). We have

$$\begin{aligned}
& Mo_e(G_3) - Mo_e(G_2) = \\
& (a_1 + a_2 + a_4 + 5 - 1) - (a_1 + 5 - a_2 - 1) + (a_1 + a_2 + a_4 + 5 - 1) - (a_1 + 5 - a_2 - 1) \\
+ \quad & (a_1 + a_2 + a_4 + 4 - 2) - (a_1 + a_3 + a_5 + 4 - a_4 - 2) + (1 - 3) - (a_2 + 1 - a_4 - 3) \\
+ \quad & (a_1 + a_2 + a_4 + 4 - 2) - (a_1 + 4 - a_4 - 2) \\
= \quad & 5a_2 + 7a_4 > 0.
\end{aligned}$$

Clearly, $G_3 \cong F_3$, and $Mo_e(F_3) = m^2 - 3m - 20$. □

Lemma 3.6. *Let $G \in \mathcal{G}_m^2$ with brace $\alpha_2(3,1,1,2,1)$. Then $Mo_e(G) < Mo_e(F_4) = m^2 - 2m - 33$.*

Proof. Suppose that v_i ($i = 1, ..., 6$) be the vertices in $\alpha_2(3,1,1,2,1)$ of G, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i ($i = 1, ..., 6$). For $a_6 > 0$, let G_1 be the graph obtained from G by shifting a_5 (resp. a_6) pendent edges from v_5 (resp. v_6) to v_1. We obtain

$$\begin{aligned}
& Mo_e(G_1) - Mo_e(G) = \\
& (a_1 + a_3 + a_5 + a_6 + 3 - a_2 - 2) - (a_1 + a_3 + a_5 + 3 - a_2 - a_6 - 2) \\
+ \quad & (a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + 5 - 1) - (a_1 + a_2 + a_3 + a_4 + 5 - a_5 - a_6 - 1) \\
+ \quad & (a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + 5 - 1) - (a_1 + a_2 + a_3 + a_4 + 5 - a_5 - a_6 - 1) \\
+ \quad & (a_1 + a_3 + a_5 + a_6 + 3 - a_2 - 2) - (a_1 + a_3 + a_5 + 3 - a_2 - a_6 - 2) \\
+ \quad & (a_2 + a_4 + 3 - a_3 - 1) - (a_2 + a_4 + a_6 + 3 - a_3 - 1) + (a_3 + a_4 + 2 - a_2 - 3) \\
- \quad & (a_2 + a_6 + 3 - a_3 - a_4 - 2) + (a_1 + a_5 + a_6 + 4 - a_2 - 2) - (a_1 + a_5 + 4 - a_4 - 2) \\
= \quad & 2a_3 + 4a_5 + 7a_6 - 2a_2 - 2 > 0.
\end{aligned}$$

Let G_2 be the graph obtained from G_1 by shifting a_3 (resp. a_4) pendent edges from v_3 (resp. v_4) to v_1 (resp. v_2). We deduce that

$$\begin{aligned} & Mo_e(G_2) - Mo_e(G_1) = \\ & (a_1 + a_2 + a_3 + a_4 + 2 - 3) - (a_1 + a_3 + 3 - a_2 - 2) + (a_1 + a_2 + a_3 + a_4 + 2 - 3) \\ - \quad & (a_1 + a_3 + 3 - a_2 - 2) + (a_1 + a_2 + a_3 + a_4 + 5 - 1) - (a_1 + a_2 + 5 - a_3 - 1) \\ + \quad & (a_1 + a_2 + a_3 + a_4 + 3 - 1) - (a_2 + a_4 + 3 - a_3 - 1) + (a_1 + a_2 + a_3 + a_4 + 3 - 2) \\ - \quad & (a_2 + 3 - a_3 - a_4 - 2) \\ = \quad & a_1 + 3a_2 + 6a_3 + 5a_4 > 0. \end{aligned}$$

Let G_3 be the graph obtained from G_2 by shifting a_1 pendent edges from v_1 to v_2. We obtain

$$\begin{aligned} & Mo_e(G_3) - Mo_e(G_2) = \\ & (a_1 + a_2 + 2 - 3) - (a_1 + 3 - a_2 - 2) + (a_1 + a_2 + 2 - 3) - (a_2 + 2 - a_1 - 3) \\ + \quad & (a_1 + a_2 + 3 - 1) - (a_2 + 3 - 1) + (a_1 + a_2 + 3 - 2) - (a_2 + 3 - 2) + (4 - 2) - (a_1 + 4 - 2) \\ = \quad & 3a_1 + 2a_2 - 2 > 0. \end{aligned}$$

Thus, $Mo_e(G) < Mo_e(G_1) < Mo_e(G_2) < Mo_e(G_3)$. Clearly, $G_3 \cong F_4$, and $Mo_e(F_4) = m^2 - 2m - 33$. □

Lemma 3.7. *Let $G \in \mathcal{G}_m^2$ of size m. Then $Mo_e(G) < m^2 - m - 36$ for $m \geq 9$, and $Mo_e(G) \leq Mo_e(F_1)$ for $m \leq 9$.*

Proof. Suppose that $G \in \mathcal{G}_m^2$, then G has a brace $\alpha_2(a_1, a_2, a_3, a_4, a_5)$ as shown in Fig. 8. Assume that $a_4, a_5 \geq 2$. We consider the following three possible cases.

Case 1. $a_4, a_5 \geq 3$.

Subcase 1.1. $a_1 = a_2 = a_3 = 1$.

We choose nine edges, three edges in the path $P(a_4)$ such that two are incident to x or y and one is in the middle of $P(a_4)$, three edges in the path $P(a_5)$ such that two are incident to x or z and one is in the middle of $P(a_5)$, one edge in the path $P(a_2)$ incident to x, one edge in the path $P(a_3)$ incident to x and one edge in the path $P(a_1)$ incident to y. We have

$$Mo_e(G) \leq 4(m-4) + 4(m-7) + (m-9) + (m-9)(m-1) < m^2 - m - 36.$$

Subcase 1.2. At least one of a_1, a_2, a_3 is greater than 1.

If $a_2, a_3 \geq 2$, then we choose 10 edges, three edges in the path $P(a_4)$ such that two are incident to x or y and one is in the middle of $P(a_4)$, three edges in the path $P(a_5)$ such that two are incident to x or z and one is in the middle of $P(a_5)$, two edges in the path $P(a_2)$ incident to x or y, one edge in the path $P(a_3)$ incident to x and one edge in the path $P(a_1)$ incident to y. We have

$$Mo_e(G) \leq 2(m-4) + (m-5) + 2(m-6) + 2(m-8) + 3(m-9) + (m-10)(m-1) < m^2 - m - 36.$$

If $a_1 \geq 2$, then we choose 10 edges, three edges in the path $P(a_4)$ such that two are incident to x or y and one is in the middle of $P(a_4)$, three edges in the path $P(a_5)$ such that two are incident to x or z and one is in the middle of $P(a_5)$, two edges in the path $P(a_2)$ incident to x or y, one edge in the path $P(a_3)$ incident to x and two edges in the path $P(a_1)$ incident to y or z. We obtain

$$Mo_e(G) \leq 4(m-4) + 6(m-7) + (m-10)(m-1) < m^2 - m - 36.$$

Case 2. $a_4 \geq 3, a_5 = 2$.

Subcase 2.1.$a_4 \geq 4, a_5 = 2$, and $a_1 = a_2 = a_3 = 1$.

We choose nine edges, four edges in the path $P(a_4)$ such that two are incident to x or y and two are in the middle of $P(a_4)$, two edges in the path $P(a_5)$ such that one is incident to x and one is in the middle of $P(a_5)$, one edge in the path $P(a_2)$ incident to x, one edge in the path $P(a_3)$ incident to x and one edge in the path $P(a_1)$ incident to y. We have

$$Mo_e(G) \leq (m-4) + 2(m-5) + (m-6) + 2(m-7) + 3(m-8) + (m-9)(m-1) < m^2 - m - 36.$$

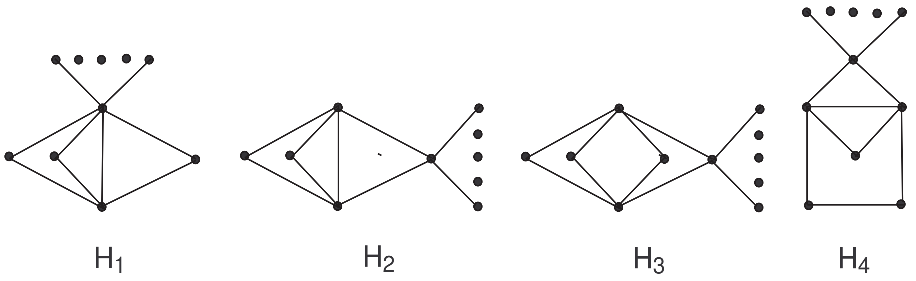

Figure 7: The Graphs H_1, H_2, H_3, H_4 of size m in Lemmas 3.8, 3.9 and 3.10.

Subcase 2.2.$a_4 = 3, a_5 = 2$, and $a_1 = a_2 = a_3 = 1$.

The Subcase follows from Lemma 3.6.

Subcase 2.3.$a_4 \geq 3, a_5 = 2$, and at least one of a_1, a_2, a_3 is greater than 1.

The proof is similar to the Subcase 2.1.

Case 3. $a_4 = a_5 = 2$.

Subcase 3.1. At least one of a_1, a_2, a_3 is greater than 1.

If $a_2, a_3 \geq 2$, then we choose eight edges, three edges in the path $P(a_4)$ such that two are incident to x or y and one is in the middle of $P(a_4)$, two edges in the path $P(a_5)$ such that one is incident to x and other is in the middle of $P(a_5)$, two edges in the path $P(a_2)$ incident to x or y, one edge in the path $P(a_3)$ incident to x and one edge in the path $P(a_1)$ incident to y. We have

$$Mo_e(G) \leq 4(m-5) + 4(m-7) + (m-8)(m-1) < m^2 - m - 36.$$

If $a_1 \geq 3$, then we choose nine edges, two edges in the path $P(a_4)$ such that one is incident to x and other is in the middle of $P(a_4)$, two edges in the path $P(a_5)$ such that one is incident to x and the other is in the middle of $P(a_5)$, one edge in the path $P(a_2)$ incident to x, one edge in the path $P(a_3)$ incident to x and three edges in the path $P(a_1)$ such that two are incident to y or z and one is in the middle of $P(a_1)$. We obtain

$$Mo_e(G) \leq 2(m-5) + 2(m-6) + 4(m-7) + (m-9) + (m-9)(m-1) < m^2 - m - 36.$$

If $a_1 = 2$, then by Lemma 3.5, $Mo_e(G) \leq m^2 - 3m - 20 < m^2 - m - 36$.

Subcase 3.2. $a_1 = a_2 = a_3 = 1$.

By Lemma 3.4, we have $Mo_e(G) < m^2 - m - 36$ for $m \geq 9$, and $Mo_e(G) \leq Mo_e(F_1)$ for $m \leq 9$. □

Lemma 3.8. *Let $G \in \mathcal{G}_m^3$ with brace $\alpha_3(1,2,2,2)$. Then*

$$Mo_e(G) < \begin{cases} Mo_e(H_1) = m^2 - 4m - 9, & \text{if } 7 \leq m \leq 10; \\ Mo_e(H_1) = Mo_e(H_2) = 68, & \text{if } m = 11; \\ Mo_e(H_2) = m^2 - 2m - 31, & \text{if } m \geq 12. \end{cases}$$

Proof. Suppose that v_i $(i = 1, ..., 5)$ be the vertices in $\alpha_3(1,2,2,2)$ of G with $d_G(v_1) = d_G(v_2) = 4$ and $d_G(v_3) = d_G(v_4) = d_G(v_5) = 2$, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i $(i = 1, ..., 5)$. Suppose that $a_3 \geq a_4 \geq a_5$. For $a_4 + a_5 > a_1 + a_2 + 8$, let G_1 be the graph obtained from G by shifting a_4 (resp. a_5) pendent edges from v_4 (resp. v_5) to v_3. We deduce that

$$\begin{aligned} & Mo_e(G_1) - Mo_e(G) = \\ & (a_3 + a_4 + a_5 + 1 - a_1 - 3) - (a_1 + a_4 + a_5 + 3 - a_3 - 1) + (a_3 + a_4 + a_5 + 1 - a_2 - 3) \\ - \; & (a_1 + a_4 + a_5 + 3 - a_3 - 1) + (a_1 + a_3 + a_4 + a_5 + 3 - 1) - (a_1 + a_3 + a_5 + 3 - a_4 - 1) \\ + \; & (a_2 + a_3 + a_4 + a_5 + 3 - 1) - (a_2 + a_3 + a_5 + 3 - a_4 - 1) + (a_1 + a_3 + a_4 + a_5 + 3 - 1) \\ - \; & (a_1 + a_3 + a_4 + 3 - a_5 - 1) + (a_1 + a_3 + a_4 + a_5 + 3 - 1) - (a_2 + a_3 + a_4 + 3 - a_5 - 1) \\ = \; & 4(a_3 + a_4 + a_5) - 2(a_1 + a_2) - 8 > 0. \end{aligned}$$

For $a_2 + a_3 > 1$, let G_2 be the graph obtained from G_1 by shifting a_2) pendent edges from v_2 to v_1. We have

$$\begin{aligned} & Mo_e(G_2) - Mo_e(G_1) = \\ & (a_1 + a_2 + 3 - a_3 - 1) - (a_1 + 3 - a_3 - 1) + (a_3 + 1 - 3) - (a_2 + 3 - a_3 - 1) \\ + \quad & (a_1 + a_2 + 3 - 3) - (a_1 + 3 - a_2 - 3) + (a_1 + a_2 + a_3 + 3 - 1) - (a_1 + a_3 + 3 - 1) \\ + \quad & (a_3 + 3 - 1) - (a_2 + a_3 + 3 - 1) + (a_1 + a_2 + a_3 + 3 - 1) - (a_1 + a_3 + 3 - 1) \\ + \quad & (a_3 + 3 - 1) - (a_2 + a_3 + 3 - 1) \\ = \quad & 2(a_2 + a_3) - 4 > 0. \end{aligned}$$

Clearly, $G_2 \cong H_2$ for $a_1 = 0, a_3 > 0$, and $G_2 \cong H_1$ for $a_3 = 0, a_1 > 0$. For $a_1 + a_3 > 2$, let G_3 be the graph obtained from G_2 by shifting a_1 pendent edges from v_1 to v_3. We have

$$\begin{aligned} & Mo_e(G_2) - Mo_e(G_1) = \\ & (a_1 + a_3 + 1 - 3) - (a_1 + 3 - a_3 - 1) + (a_1 + a_3 + 1 - 3) - (a_3 + 1 - 3) + (3 - 3) \\ - \quad & (a_1 + 3 - 3) + (a_1 + a_3 + 3 - 1) - (a_3 + 3 - 1) + (a_1 + a_3 + 3 - 1) - (a_3 + 3 - 1) \\ = \quad & 2(a_1 + a_3) - 4 > 0. \end{aligned}$$

Thus, $Mo_e(G) < Mo_e(G_1) < Mo_e(G_2) < Mo_e(G_3)$. Clearly, $G_3 \cong H_2$, and by simple calculation, we deduce that $Mo_e(H_2) = m^2 - 2m - 31$, $Mo_e(H_1) = m^2 - 4m - 9$. □

Lemma 3.9. *Let $G \in \mathcal{G}_m^3$ with brace $\alpha_3(2,2,2,2)$. Then $Mo_e(G) < Mo_e(H_3) = m^2 - m - 48$.*

Proof. Suppose that v_i ($i = 1, ..., 6$) be the six vertices in $\alpha_3(2,2,2,2)$ of G with $d_G(v_1) = d_G(v_2) = 4$ and $d_G(v_3) = d_G(v_4) = d_G(v_5) = d_G(v_6) = 2$, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i ($i = 1, ..., 6$). Suppose that $a_3 \geq a_4 \geq a_5 \geq a_6 > 0$. Let G_1 be the graph obtained from G by shifting a_i ($i \geq 4$) pendent edges from v_i ($i \geq 4$) to v_3. We obtain

$$\begin{aligned} & Mo_e(G_1) - Mo_e(G) = \\ & (a_2 + a_3 + a_4 + a_5 + a_6 + 1 - a_1 - 3) - (a_1 + a_4 + a_5 + a_6 + 3 - a_2 - a_3 - 1) \\ + \quad & (a_1 + a_3 + a_4 + a_5 + a_6 + 1 - a_2 - 3) - (a_2 + a_4 + a_5 + a_6 + 3 - a_1 - a_3 - 1) \\ + \quad & (a_1 + a_3 + a_4 + a_5 + a_6 + 3 - a_2 - 1) - (a_1 + a_3 + a_5 + a_6 + 3 - a_4 - a_2 - 1) \\ + \quad & (a_2 + a_3 + a_4 + a_5 + a_6 + 3 - a_1 - 1) - (a_2 + a_3 + a_5 + a_6 + 3 - a_1 - a_4 - 1) \\ + \quad & (a_1 + a_3 + a_4 + a_5 + a_6 + 3 - a_2 - 1) - (a_1 + a_3 + a_4 + a_6 + 3 - a_2 - a_5 - 1) \\ + \quad & (a_2 + a_3 + a_4 + a_5 + a_6 + 3 - a_1 - 1) - (a_2 + a_3 + a_4 + a_6 + 3 - a_1 - a_5 - 1) \\ + \quad & (a_1 + a_3 + a_4 + a_5 + a_6 + 3 - a_2 - 1) - (a_1 + a_3 + a_4 + a_5 + 3 - a_2 - a_6 - 1) \\ + \quad & (a_2 + a_3 + a_4 + a_5 + a_6 + 3 - a_1 - 1) - (a_2 + a_3 + a_4 + a_5 + 3 - a_1 - a_6 - 1) \\ = \quad & 4(a_3 + a_4 + a_5 + a_6) - 8 > 0. \end{aligned}$$

For $a_1 + a_2 > 0$, let G_2 be the graph obtained from G_1 by shifting a_1 (resp. a_2) pendent edges from v_1 (resp. v_2) to v_3. We have

$$\begin{aligned} & Mo_e(G_2) - Mo_e(G_1) = \\ & (a_1 + a_2 + a_3 + 1 - 3) - (a_2 + a_3 + 1 - a_1 - 1) + (a_1 + a_2 + a_3 + 1 - 3) \\ - \quad & (a_2 + 3 - a_1 - a_3 - 1) + (a_1 + a_2 + a_3 + 3 - 1) - (a_1 + a_3 + 3 - a_2 - 1) \\ + \quad & (a_1 + a_2 + a_3 + 3 - 1) - (a_2 + a_3 + 3 - a_1 - 1) + (a_1 + a_2 + a_3 + 3 - 1) \\ - \quad & (a_1 + a_3 + 3 - a_2 - 1) + (a_1 + a_2 + a_3 + 3 - 1) - (a_2 + a_3 + 3 - a_1 - 1) \\ + \quad & (a_1 + a_2 + a_3 + 3 - 1) - (a_1 + a_3 + 3 - a_2 - 1) + (a_1 + a_2 + a_3 + 3 - 1) \\ - \quad & (a_2 + a_3 + 3 - a_1 - 1) \\ = \quad & 10a_1 + 6a_2 + 2a_3 - 8 > 0. \end{aligned}$$

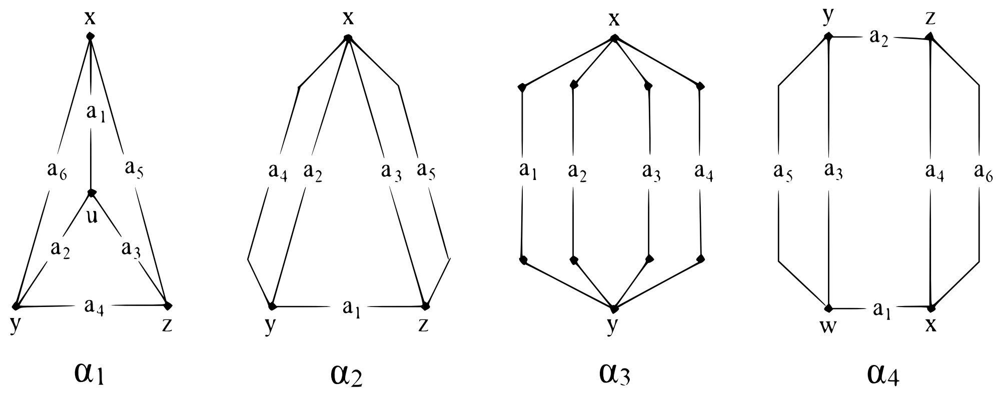

Figure 8: The Graphs for Lemmas 3.3, 3.7, 3.11 and 3.12.

Thus, $Mo_e(G) < Mo_e(G_1) < Mo_e(G_2)$. Clearly, $G_2 \cong H_3$, and by simple calculation, we obtain $Mo_e(H_3) = m^2 - m - 48$. □

Lemma 3.10. *Let $G \in \mathcal{G}_m^3$ with brace $\alpha_3(1,2,2,3)$. Then $Mo_e(G) < Mo_e(H_4) = m^2 - 3m - 24$.*

Proof. Suppose that v_i $(i = 1, ..., 6)$ be the six vertices in $\alpha_3(1,2,2,3)$ of G with $d_G(v_1) = d_G(v_2) = 4$ and $d_G(v_3) = d_G(v_4) = d_G(v_5) = d_G(v_6) = 2$, as shown in Fig. 4. Let a_i be the number of pendent edges of v_i $(i = 1, ..., 6)$. Assume that $a_3 \geq a_2$, and $a_4 + a_5 + a_6 > 1$. Let G_1 be the graph obtained from G by shifting a_i ($i \geq 4$) pendent edges from v_i ($i \geq 4$) to v_3. We get

$$
\begin{aligned}
& Mo_e(G_1) - Mo_e(G) = \\
& (a_1 + 4 - a_3 - a_4 - a_5 + -a_6 - 1) - (a_1 + a_4 + a_5 + 4 - a_3 - 1) \\
+ \quad & (a_3 + a_4 + a_5 + a_6 + 1 - a_2 - 4) - (a_2 + a_4 + a_6 + 4 - a_3 - 1) \\
+ \quad & (a_1 + a_3 + a_4 + a_5 + a_6 + 4 - 1) - (a_1 + a_3 + a_5 + 4 - a_4 - 1) \\
+ \quad & (a_2 + a_3 + a_4 + a_5 + a_6 + 4 - 1) - (a_2 + a_3 + a_6 + 4 - a_4 - 1) \\
+ \quad & (a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + 5 - 1) - (a_1 + a_2 + a_2 + a_4 + 5 - a_5 - a_6 - 1) \\
+ \quad & (a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + 5 - 1) - (a_1 + a_2 + a_2 + a_4 + 5 - a_5 - a_6 - 1) \\
+ \quad & (a_1 + 3 - a_2 - 3) - (a_1 + a_5 + 3 - a_2 - a_6 - 3) + (a_1 + 3 - a_2 - 3) \\
- \quad & (a_1 + a_5 + 3 - a_2 - a_6 - 3) \\
= \quad & 2(a_3 + a_4 + a_5) + 6a_6 - 2a_2 - 12 > 0.
\end{aligned}
$$

For $a_1 + a_2 > 0$, let G_2 be the graph obtained from G_1 by shifting a_1 (resp. a_2) pendent edges from v_1 (resp. v_2) to v_3. We have

$$
\begin{aligned}
& Mo_e(G_2) - Mo_e(G_1) = \\
& (a_1 + a_2 + a_3 + 1 - 4) - (a_3 + 1 - a_1 - 4) + (a_1 + a_2 + a_3 + 1 - 4) - (a_3 + 1 - a_2 - 4) \\
+ \quad & (a_1 + a_2 + a_3 + 4 - 1) - (a_1 + a_3 + 4 - 1) + (a_1 + a_2 + a_3 + 4 - 1) - (a_2 + a_3 + 4 - 1) \\
+ \quad & (3 - 3) - (a_1 + 3 - a_2 - 3) + (3 - 3) - (a_1 + 3 - a_2 - 3) \\
= \quad & 2a_1 + 6a_2 > 0.
\end{aligned}
$$

Thus, $Mo_e(G) < Mo_e(G_1) < Mo_e(G_2)$. Clearly, $G_2 \cong H_4$, and by simple calculation, we get $Mo_e(H_4) = m^2 - 3m - 248$. □

Lemma 3.11. *Let $G \in \mathcal{G}_m^3$ of size m. Then $Mo_e(G) < m^2 - m - 36$ for $m \geq 9$, and $Mo_e(G) \leq Mo_e(H_1)$ for $m \leq 9$.*

Proof. Suppose that $G \in \mathcal{G}_m^3$, then G has a brace $\alpha_2(a_1, a_2, a_3, a_4)$ as shown in Fig. 8. Assume that $1 \leq a_1 \leq a_2 \leq a_3 \leq a_4$. We proceed with the following three possible cases.
Case 1. $3 \leq a_1 \leq a_2 \leq a_3 \leq a_4$.

We choose twelve edges, eight edges in the paths $P(a_i)$ $(i = 1, 2, 3, 4)$ such that each one is incident to x or y, four edges in the middle of $P(a_i)$ $(i = 1, 2, 3, 4)$. We deduce that

$$Mo_e(G) \leq 8(m-8) + 4(m-12) + (m-12)(m-1) < m^2 - m - 36.$$

Case 2. $a_1 = 2$.
Subcase 2.1. $3 \leq a_2 \leq a_3 \leq a_4$.

We choose eleven edges, eight edges in the paths $P(a_i)$ $(i = 1, 2, 3, 4)$ such that each one is incident to x or y, three edges in the middle of $P(a_i)$ $(i = 2, 3, 4)$. We deduce that

$$Mo_e(G) \leq 6(m-7) + 2(m-9) + 3(m-11) + (m-11)(m-1) < m^2 - m - 36.$$

Subcase 2.2. $a_2 = a_3 = a_4 = 2$.

The Subcase follows from Lemma 3.9.
Case 3. $a_1 = 1$.
Subcase 3.1. $3 \leq a_2 \leq a_3 \leq a_4$.

We choose ten edges, six edges in the paths $P(a_i)$ $(i = 2, 3, 4)$ such that each one is incident to x or y, three edges in the middle of $P(a_i)$ $(i = 2, 3, 4)$, and one edge in $P(a_1)$ incident to x. It follows that

$$Mo_e(G) \leq 6(m-4) + 4(m-10) + (m-10)(m-1) < m^2 - m - 36.$$

Subcase 3.2. $a_2 = 2, 3 \leq a_3 \leq a_4$.

The proof is similar to the Subcase 3.1.
Subcase 3.3. $a_2 = a_3 = 2, 3 \leq a_4$.

If $a_4 = 3$, then it follows from Lemma 3.10. If $a_4 \geq 4$, then we choose nine edges, four edges in the path $P(a_4)$ such that two are incident to x or y and the other two are in the middle of $P(a_4)$, two edges in the path $P(a_3)$ (resp. $P(a_2)$) such that one is incident to x and the other is in the middle of $P(a_3)$ (resp. $P(a_2)$) and one edge in $P(a_1)$ incident to x. We have

$$Mo_e(G) \leq 2(m-5) + 2(m-7) + 4(m-6) + (m-9) + (m-9)(m-1) < m^2 - m - 36.$$

Subcase 3.4. $a_2 = a_3 = a_4 = 2$.

By Lemma 3.8, $Mo_e(G) < m^2 - m - 36$ for $m \geq 9$, and $Mo_e(G) \leq Mo_e(H_1)$ for $m \leq 9$. □

Lemma 3.12. *Let $G \in \mathcal{G}_m^4$ of size m. Then $Mo_e(G) < m^2 - m - 36$.*

Proof. Suppose that $G \in \mathcal{G}_m^4$, then G has a brace $\alpha_4(a_1, a_2, a_3, a_4, a_5, a_6)$ as shown in Fig. 8. We choose eight edges, two edges in the path $P(a_5)$ such that each is incident to w or y, two edges in the path $P(a_6)$ such that each is incident to z or x, the four edges yz, yw, wx, zx. We obtain

$$Mo_e(G) \leq 4(m-5) + 4(m-8) + (m-8)(m-1) < m^2 - m - 36.$$

□

The proof of Theorem 1.1 follows from Lemmas 3.1, 3.3, 3.7, 3.11 and 3.12.

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References

[1] A. Ali, T. Došlić, *Mostar index: results and perspectives*, Appl. Math. Comput. **404** (2021), 126245.
[2] M. Arockiaraj, J. Clement, N. Tratnik, *Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems*, Int. J. Quantum Chem. **119** (2019), e26043.
[3] K. Deng, S. Li, *On the extremal values for the Mostar index of trees with given degree sequence*, Appl. Math. Comput. **390** (2021), 125598.
[4] K. Deng, S. Li, *On the extremal Mostar indices of trees with a given segment sequence*, Bull. Malays. Math. Sci. Soc. **45** (2021), 593–612.
[5] K. Deng, S. Li, *Chemical trees with extremal Mostar index*, MATCH Commun. Math. Comput. Chem. **85** (2021), 161–180.
[6] K. Deng, S. Li, *Extremal catacondensed benzenoid with respect to the Mostar index*, J. Math. Chem. **58** (2020), 1437–1465.
[7] T. Došlić, I. Martinjak, R. Škrekovski, S. T. Spužević, I. Zubac, *Mostar index*, J. Math. Chem. **56** (2018), 2995–3013.
[8] A. Ghalvandi, A. R. Ashrafi, M. H. Nezhaad, *On Mostar and edge Mostar indices of graphs*, J. Math. (2021), 6651220.
[9] N. Ghanbari, S. Alikhani, *Mostar index and edge Mostar index of polymers*, Comput. Appl. Math. **40** (2021), 260.
[10] O. C. Havare, *Mostar index and edge Mostar index for some cycle related graphs*, Rom. J. Math. Comput. Sci. **10** (2020), 53–66.
[11] F. Hayat, S.-J. Xu, *Extremal results on the Mostar index of trees with parameters*, Discrete Math. Algor. Appl. (2024), DOI: 10.1142/S1793830924500253.
[12] F. Hayat, S.-J. Xu, *A lower bound on the Mostar index of tricyclic graphs*, Filomat **38** (2024), 6291–6297.
[13] F. Hayat, S.-J. Xu, B. Zhou, *Disproof of a conjecture on the edge Mostar index*, (2023), arXiv.2306.02761.
[14] F. Hayat, B. Zhou, *On cacti with large Mostar index*, Filomat **33** (2019), 4865–4873.
[15] F. Hayat, B. Zhou, *On Mostar index of trees with parameters*, Filomat **33** (2019), 6453–6458.
[16] S. Huang, S. Li, M. Zhang, *On the extremal Mostar indices of hexagonal chains*, MATCH Commun. Math. Comput. Chem. **84** (2020), 249–271.
[17] M. Imran, S. Akhter, Z. Iqbal, *Edge Mostar index of chemical structures and nanostructures using graph operations*, Int. J. Quan. Chem. **120** (2020), e26259.
[18] G. Liu, K. Deng, *The maximum Mostar indices of unicyclic graphs with given diameter*, Appl. Math. Comput. **439** (2023), 127636.
[19] H. Liu, L. Song, Q. Xiao, Z. Tang, *On edge Mostar index of graphs*, Iranian J. Math. Chem. **11** (2020), 95–106.
[20] Š. Miklavič, J. Pardey, D. Rautenbach, F. Werner, *Maximizing the Mostar index for bipartite graphs and split graphs*, Discrete Optim. **48** (2023), 100768.
[21] A. Tepeh, *Extremal bicyclic graphs with respect to Mostar index*, Appl. Math. Comput. **355** (2019), 319–324.
[22] Q. Xiao, M. Zeng, Z. Tang, *The hexagonal chains with the first three maximal Mostar indices*, Discrete Appl. Math. **288** (2020), 180–191.
[23] Q. Xiao, M. Zeng, Z. Tang, H. Deng, H. Hua, *Hexagonal chains with first three minimal Mostar indices*, MATCH Commun. Math. Comput. Chem. **85** (2021), 47–61.