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Disproof of a Conjecture on the Edge Mostar Index

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ABSTRACT

For a connected graph G, the edge Mostar index $Mo_e(G)$ is defined as $Mo_e(G) = \sum_{e=uv\in E(G)} |m_u(e|G) - m_v(e|G)|$, where $m_u(e|G)$ and $m_v(e|G)$ are respectively, the number of edges of G lying closer to vertex u than to vertex v and the number of edges of G lying closer to vertex v than to vertex u. We determine a sharp upper bound for the edge Mostar index on bicyclic graphs and identify the graphs that achieve the bound, which disproves a conjecture proposed by Liu et al. [Iranian J. Math. Chem. 11(2) (2020) 95–106].

Keywords: Mostar index, Edge Mostar index, Bicyclic graph, Distance-balanced graph

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1. Introduction

Let G 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, denoted by $d_G(u,v)$, is the shortest path connecting u and v in G. 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 molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule. A topological graph index, also called a molecular descriptor, is a mathematical formula that can be applied to any graph which models some molecular structure. From this index, it is possible to analyse mathematical values and further investigate some physic-

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ochemical properties of a molecule. Therefore, it is an efficient method in avoiding expensive and time-consuming laboratory experiments.

Došlić et al. [7] introduced the Mostar index, which is a measure of peripherality in graphs. It can also be considered as a bond-additive structural invariant as a quantitative refinement of the distance non-balancedness. 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.

Since its introduction in 2018, the Mostar index has already incited a lot of research, mostly concerning trees [1, 6, 5, 4, 8, 12, 14], unicyclic graphs [18], bicyclic graphs [20], tricyclic graphs [11], cacti [13] and chemical graphs [3, 16, 21, 22].

Arockiaraj et al. [2], introduced the edge Mostar index as a quantitative refinement of the distance non-balancedness, also 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 $\psi_G(uv) = |m_u(e|G) - m_v(e|G)|$, $m_u(e|G)$ and $m_v(e|G)$ are respectively, the number of edges of G lying closer to vertex u than to vertex v and the number of edges of G lying closer to vertex v than to vertex u. We use $\psi(uv) = |m_u(e) - m_v(e)|$ for short, if there is no ambiguity.

The problem of determining which graphs uniquely maximize (resp. minimize) the edge Mostar index in various classes of graphs has received much attention. For example, Imran et al. [17] studied the edge Mostar index of chemical structures and nanostructures using graph operations. Havare [10] computed the edge Mostar index for several classes of cycle-containing graphs. Hayat et al. [15] obtained a sharp upper bound for the edge Mostar index on tricyclic graphs and identified the graphs that attain the bound. Liu et al. [19] determined the extremal values of the edge Mostar index among trees, unicyclic graphs, cacti and posed two conjectures for the extremal edge Mostar index among bicyclic graphs. Ghalavand et al. [9] gave proof to a conjecture in [19], and obtained the graph that minimizes the edge Mostar index among bicyclic graphs.

Motivated directly by [19] and [9], we determine the unique graph that maximizes the edge Mostar index over all bicyclic graphs with fixed size, which disproves the following conjecture.

Conjecture 1.1. *[19] If the size m of bicyclic graphs is large enough, then the bicyclic graphs B_m (see Figure 1) and B^5_m (see Figure 2) have the maximum edge Mostar index.*

We disprove Conjecture 1.1, by presenting the following result.

Theorem 1.2. *Let G be a bicyclic graph of size $m \geq 5$. Then*

$$Mo_e(G) \leq \begin{cases} 4, & \text{if } m = 5, \text{ and equality holds iff } G \cong B^3_m, B^4_m; \\ m^2 - 3m - 6, & \text{if } 6 \leq m \leq 8, \text{ and equality holds iff } G \cong B^1_m, B^3_m; \\ 48, & \text{if } m = 9, \text{ and equality holds iff } G \cong B_m, B^1_m, B^2_m, B^3_m, B^4_m; \\ m^2 - m - 24, & \text{if } m \geq 10, \text{ and equality holds iff } G \cong B_m. \end{cases}$$

(Where B_m, B^1_m, B^2_m and B^3_m, B^4_m are depicted in Figure 1 and Figure 2, respectively).

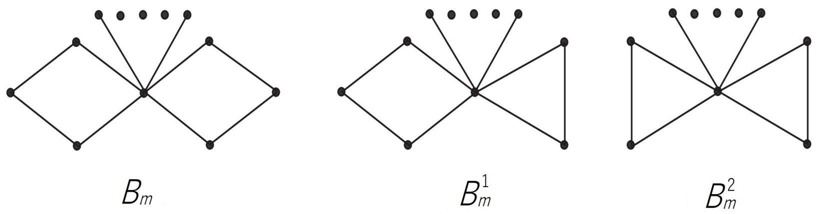

Fig. 1. The graphs B_m, B_m^1, and B_m^2, each of size m, have $m-8$, $m-7$, and $m-6$ pendent edges, respectively

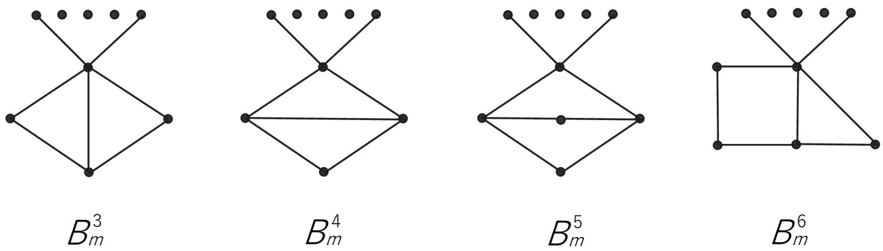

Fig. 2. The graphs B_m^3, B_m^4, B_m^5, and B_m^6 of size m, have $m-5$, $m-5$, $m-6$, and $m-6$ pendent edges, respectively

Based on the above Theorem, if the size m of bicyclic graphs is large, then B_m is the unique graph that maximizes the edge Mostar index. Therefore, Conjecture 1.1 is disproved.

In Section 2, we provide some definitions and preliminary results. The proof of Theorem 1.2 is presented in Section 3.

2. Preliminaries

In this section, we present some basic notations and elementary results, which will be useful in the proof of our main result.

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 bicyclic graph if $|E(G)| = n+1$. As usual by S_n, P_n, and C_n we denote the star, path, and cycle graph on n vertices, respectively.

The join of two graphs G_1 and G_2 is denoted by $G_1 \cdot G_2$, is obtained by identifying one vertex from G_1 and G_2. Let u be the identified vertex in both G_1 and G_2. If G_1 contains a cycle and u belongs to some cycle, while 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 in G_2 pass 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. In other words, changing the structure of G_2 does not affect the value of $\sum_{e\in E(G_1)} \psi(e)$.

Lemma 2.1. *[19] Let G be a graph of size m with a cut edge $e = uv$. Then $\psi(e) \leq m-1$ with equality if and only if $e = uv$ is a pendent edge.*

By Lemma 2.1, if e is a pendent edge, then $\psi(e)$ is maximum. Therefore, it is easy to verify the following result.

Lemma 2.2. *Let H be a graph of size m. Then*

$$Mo_e(H_1 \cdot H) \leq Mo_e(H_1 \cdot S_m),$$

where the common vertex of H_1 and S_m is the center of S_m, while the common vertex of H_1 and H can be chosen arbitrarily.

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

Lemma 2.3. *[19] Let G be a unicyclic graph of size $m \geq 3$. Then*

$$Mo_e(G) \leq \begin{cases} m^2 - 2m - 3, & \text{if } 3 \leq m \leq 8, \text{ and equality holds iff } G \cong S_{m,3}; \\ 60, & \text{if } m = 9, \text{ and equality holds iff } G \cong S_{m,3}, S_{m,4}; \\ m^2 - m - 12, & \text{if } m \geq 10, \text{ and equality holds iff } G \cong S_{m,4}. \end{cases}$$

Lemma 2.4. *Let G_1 be a connected graph of size m_1 and G_2 be a unicyclic graph of size m_2. Then*

$$Mo_e(G_1 \cdot G_2) \leq \begin{cases} Mo_e(G_1 \cdot S_{m_2,3}) & \text{for } m_1 + m_2 \leq 8; \\ Mo_e(G_1 \cdot S_{m_2,3}) = Mo_e(G_1 \cdot S_{m_2,4}) & \text{for } m_1 + m_2 = 9; \\ Mo_e(G_1 \cdot S_{m_2,4}) & \text{for } m_1 + m_2 \geq 10; \end{cases}$$

where the common vertex of G_1 and $S_{m_2,3}$ (resp. G_1 and $S_{m_2,4}$) is the center of $S_{m_2,3}$ (resp. $S_{m_2,4}$), while the common vertex of G_1 and G_2 can be chosen arbitrarily.

Proof. If $m_1 + m_2 \leq 8$, then by Lemma 2.3, we have

$$\begin{aligned} Mo_e(G_1 \cdot G_2) &= \sum_{e=uv \in E(G_1 \cdot G_2)} \psi_{G_1 \cdot G_2}(uv) \\ &= \sum_{e=uv \in E(G_1)} \psi_{G_1 \cdot G_2}(uv) + \sum_{e=uv \in E(G_2)} \psi_{G_1 \cdot G_2}(uv) \\ &= \sum_{e=uv \in E(G_1)} \psi_{G_1 \cdot G_2}(uv) + Mo_e(S_{m_1} \cdot G_2) - m_1(m-1) \\ &\leq \sum_{e=uv \in E(G_1)} \psi_{G_1 \cdot S_{m_2,3}}(uv) + Mo_e(S_{m_1} \cdot S_{m_2,3}) - m_1(m-1) \\ &= \sum_{e=uv \in E(G_1)} \psi_{G_1 \cdot S_{m_2,3}}(uv) + \sum_{e=uv \in E(S_{m_2,3})} \psi_{G_1 \cdot S_{m_2,3}}(uv) \\ &= Mo_e(G_1 \cdot S_{m_2,3}). \end{aligned}$$

Similarly, if $m_1 + m_2 = 9$, then $Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,3}) = Mo_e(G_1 \cdot S_{m_2,4})$; if $m_1 + m_2 \geq 10$, then $Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,4})$. □

3. Proof of Theorem 1.2

The Θ-graph is a graph that connects two fixed vertices with three internally disjoint paths. If the lengths of these paths are l_1, l_2, and l_3 where $l_1 \leq l_2 \leq l_3$, the graph is denoted as $\Theta(l_1, l_2, l_3)$.

Let $\mathcal{G}_m^1$ represent the set of bicyclic graphs of size m that contain exactly two edge-disjoint cycles. Let $\mathcal{G}_m^2$ denote the set of bicyclic graphs of size m that contain exactly three cycles. Moreover, if $G \in \mathcal{G}_m^2$, then G contains a Θ-graph as a subgraph, which is called as the brace of G.

For the proof of Theorem 1.2, we first develop several lemmas. In the first step, we establish a sharp upper bound for $Mo_e(G)$ on the set $\mathcal{G}_m^1$.

Lemma 3.1. *Let $G \in \mathcal{G}_m^1$. Then*

$$Mo_e(G) \leq \begin{cases} m^2-3m-6, & \text{if } 6 \leq m \leq 8, \text{ and equality holds iff } G \cong B_m^2; \\ 48, & \text{if } m = 9, \text{ and equality holds iff } G \cong B_m, B_m^1, B_m^2; \\ m^2-m-24, & \text{if } m \geq 10, \text{ and equality holds iff } G \cong B_m. \end{cases}$$

Proof. Let $G \in \mathcal{G}_m^1$. Then there are two unicyclic graphs G_1 and G_2 with size m_1 and m_2, respectively such that $G = G_1 \cdot G_2$. Then, in view of Lemma 2.4. If $6 \leq m \leq 8$, we get

$$\begin{aligned} Mo_e(G) &= Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,3}) \\ &\leq Mo_e(S_{m_1,3} \cdot S_{m_2,3}) = Mo_e(B_m^2); \end{aligned}$$

if $m = 9$, then

$$\begin{aligned} Mo_e(G) &= Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,3}) = Mo_e(G_1 \cdot S_{m_2,4}) \\ &\leq Mo_e(S_{m_1,3} \cdot S_{m_2,3}) = Mo_e(S_{m_1,3} \cdot S_{m_2,4}) = Mo_e(B_m^2) \\ &= Mo_e(S_{m_1,4} \cdot S_{m_2,4}) = Mo_e(B_m) = Mo_e(B_m^1) = Mo_e(B_m^2). \end{aligned}$$

If $m \geq 10$, we have

$$\begin{aligned} Mo_e(G) &= Mo_e(G_1 \cdot G_2) \leq Mo_e(G_1 \cdot S_{m_2,4}) \\ &\leq Mo_e(S_{m_1,4} \cdot S_{m_2,4}) = Mo_e(B_m). \end{aligned}$$

By simple calculation, we get $Mo_e(B_m) = m^2-m-24$, $Mo_e(B_m^1) = m^2-2m-15$, and $Mo_e(B_m^2) = m^2-3m-6$. If $m = 9$, then $Mo_e(B_m) = Mo_e(B_m^1) = Mo_e(B_m^2) = 48$. This completes the proof. □

In the following, we determine a sharp upper bound for $Mo_e(G)$ on the set $\mathcal{G}_m^2$.

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

$$Mo_e(G) \leq \begin{cases} 4, & \text{if } m = 5, \text{ and equality holds iff } G \cong B_m^3, B_m^4; \\ m^2-3m-6, & \text{if } 6 \leq m \leq 8, \text{ and equality holds iff } G \cong B_m^3; \\ 48, & \text{if } m = 9, \text{ and equality holds iff } G \cong B_m^3, B_m^4; \\ m^2-2m-15, & \text{if } m \geq 10, \text{ and equality holds iff } G \cong B_m^4. \end{cases}$$

Proof. Let $G \in \mathcal{G}_m^2$ with brace $\Theta(1,2,2)$. Suppose that v_1, v_2, v_3, v_4 be the vertices in $\Theta(1,2,2)$ of G with $d_G(v_1) = d_G(v_2) = 3$, and $d_G(v_3) = d_G(v_4) = 2$. Let a_i be the number of pendent edges of v_i $(i = 1,2,3,4)$. Suppose that $a_1 \geq a_2$ and $a_3 \geq a_4$. Let G_1 be the graph obtained from G by shifting a_2 pendent edges from v_2 to v_1. We have

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

Hence, $Mo_e(G_1) \geq Mo_e(G)$ and equality holds if and only if $a_2 = 0$, i.e., $G \cong G_1$.

Let G_2 be the graph obtained from G_1 by shifting a_4 pendent edges from v_4 to v_3. We have

$$\begin{aligned} Mo_e(G_2) - Mo_e(G_1) =& (a_1 + 2 - 2) - (a_1 + 2 - 2) + (a_3 + a_4 + 1 - a_1 - 2) \\ & - (a_3 + 1 - a_1 - a_4 - 2) + (a_1 + a_3 + a_4 + 2 - 1) \\ & - (a_1 + a_3 + 2 - a_4 - 1) + (a_3 + a_4 + 1 - 2) \\ & - (a_3 + 1 - a_4 - 2) + (a_3 + a_4 + 2 - 1) - (a_3 + 2 - a_4 - 1) \\ =& 8a_4 \geq 0. \end{aligned}$$

Hence, $Mo_e(G_2) \geq Mo_e(G_1)$ and equality holds if and only if $a_4 = 0$, i.e., $G_2 \cong G_1$.

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

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

Hence, $Mo_e(G_3) \geq Mo_e(G_2)$ and equality holds if and only if $a_1 = 0$, i.e., $G_3 \cong G_2$. Clearly, $G_2 \cong B^3_m$ with $a_3 = 0$, and $G_3 \cong B^4_m$. Also, by simple calculation, we have $Mo_e(B^3_m) = m^2 - 3m - 6$, $Mo_e(B^4_m) = m^2 - 2m - 15$. □

Lemma 3.3. *Let $G \in \mathcal{G}^2_m$ with brace $\Theta(2, 2, 2)$. If $m \geq 6$, then $Mo_e(G) \leq m^2 - m - 28$ with equality if and only if $G \cong B^5_m$ (see Figure 2).*

Proof. Let $G \in \mathcal{G}^2_m$ with brace $\Theta(2, 2, 2)$. Let v_1, v_2, v_3, v_4, v_5 be vertices in $\Theta(2, 2, 2)$ of G with $d_G(v_1) = d_G(v_2) = 3$ and $d_G(v_3) = d_G(v_4) = d_G(v_5) = 2$. Let a_i be the number of pendent edges of v_i $(i = 1, 2, 3, 4, 5)$. Suppose that $a_1 \geq a_2$ and $a_3 \geq a_4 \geq a_5$. Let G_1 be the graph obtained from G by shifting a_2 pendent edges from v_2 to v_1. We have

$$\begin{aligned} Mo_e(G_1) - Mo_e(G) =& (a_1 + a_2 + a_4 + a_5 + 2 - a_3 - 1) - (a_1 + a_4 + a_5 + 2 - a_2 - a_3 - 1) \\ & + (a_1 + a_2 + a_3 + a_5 + 2 - a_4 - 1) - (a_1 + a_3 + a_5 + 2 - a_2 - a_4 - 1) \\ & + (a_1 + a_2 + a_3 + a_4 + 2 - a_5 - 1) - (a_1 + a_3 + a_4 + 2 - a_2 - a_5 - 1) \\ & + (a_1 + a_2 + a_3 + 1 - a_4 - a_5 - 2) - (a_1 + a_3 + 1 - a_2 - a_4 - a_5 - 2) \\ & + (a_1 + a_2 + a_4 + 1 - a_3 - a_5 - 2) - (a_1 + a_4 + 1 - a_2 - a_3 - a_5 - 2) \\ & + (a_1 + a_2 + a_5 + 1 - a_3 - a_4 - 2) - (a_1 + a_5 + 1 - a_2 - a_3 - a_4 - 2) \\ =& 12a_2 \geq 0. \end{aligned}$$

Hence, $Mo_e(G_1) \geq Mo_e(G)$ and equality holds if and only if $a_2 = 0$, i.e., $G \cong G_1$.

Let G_2 be the graph obtained from G_1 by shifting a_5 pendent edges from v_5 to v_3. We get

$$\begin{aligned} Mo_e(G_2) - Mo_e(G_1) =& (a_3 + a_5 + 1 - a_1 - a_4 - 2) - (a_3 + 1 - a_1 - a_4 - a_5 - 2) \\ & + (a_1 + a_3 + a_5 + 2 - a_4 - 1) - (a_1 + a_3 + a_5 + 2 - a_4 - 1) \\ & + (a_1 + a_3 + a_4 + a_5 + 2 - 1) - (a_1 + a_3 + a_4 + 2 - a_5 - 1) \\ & + (a_1 + a_3 + a_5 + 1 - a_4 - 2) - (a_1 + a_3 + 1 - a_4 - a_5 - 2) \\ & + (a_3 + a_5 + 2 - a_1 - a_4 - 1) - (a_3 + a_5 + 2 - a_1 - a_4 - 1) \\ & + (a_3 + a_4 + a_5 + 2 - a_1 - 1) - (a_3 + a_4 + 2 - a_1 - a_5 - 1) \\ =& 8a_5 \geq 0. \end{aligned}$$

Hence, $Mo_e(G_2) \geq Mo_e(G_1)$ and equality holds if and only if $a_5 = 0$, i.e., $G_2 \cong G_1$.

Let G_3 be the graph obtained from G_2 by shifting a_4 pendent edges from v_4 to v_3. By symmetry, $Mo_e(G_3) \geq Mo_e(G_2)$, and equality holds if and only if $G_3 \cong G_2$. Let G_4 be the graph obtained from G_3 by shifting a_1 pendent edges from v_1 to v_3. We get

$$\begin{aligned} Mo_e(G_4) - Mo_e(G_3) =& (a_1 + a_3 + 1 - 2) - (a_3 + 1 - a_1 - 2) + (a_1 + a_3 + 2 - 1) \\ & - (a_1 + a_3 + 2 - 1) + (a_1 + a_3 + 2 - 1) - (a_1 + a_3 + 2 - 1) \\ & + (a_1 + a_3 + 1 - 2) - (a_1 + a_3 + 1 - 2) + (a_1 + a_3 + 2 - 1) \\ & - (a_3 + 2 - a_1 - 1) + (a_1 + a_3 + 2 - 1) - (a_3 + 2 - a_1 - 1) \\ =& 6a_1 \geq 0. \end{aligned}$$

Hence, $Mo_e(G_4) \geq Mo_e(G_3)$ and equality holds if and only if $a_1 = 0$, i.e., $G_4 \cong G_3$. Note that $G_4 \cong B_m^5$. Clearly, $Mo_e(B_m^5) = m^2 - m - 28$. □

Lemma 3.4. *Let $G \in \mathcal{G}_m^2$ with brace $\Theta(1,2,3)$. If $m \geq 6$, then $Mo_e(G) \leq m^2 - 2m - 16$ with equality if and only if $G \cong B_m^6$ (see Figure 2).*

Proof. Let $G \in \mathcal{G}_m^2$ with brace $\Theta(1,2,3)$. Let v_1, v_2, v_3, v_4, v_5 be vertices in $\Theta(1,2,3)$ of G with $d_G(v_1) = d_G(v_2) = 3$ and $d_G(v_3) = d_G(v_4) = d_G(v_5) = 2$. Let a_i be the number of pendent edges of v_i $(i = 1,2,3,4,5)$. Suppose that $a_1 + a_4 \geq a_2 + a_5$. Let G_1 be the graph obtained from G by shifting a_2 (resp. a_5) pendent edges from v_2 (resp. v_5) to v_1 (resp. v_4). We deduce that

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

Hence, $Mo_e(G_1) \geq Mo_e(G)$ and equality holds if and only if $a_2 = a_5 = 0$, i.e., $G \cong G_1$.

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

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

Hence, $Mo_e(G_2) \geq Mo_e(G_1)$ and equality holds if and only if $a_4 = 0, a_1 = a_3$, i.e., $G_2 \cong G_1$.
Let G_3 be the graph obtained from G_2 by shifting a_3 pendent edges from v_3 to v_1. We have

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

Hence, $Mo_e(G_3) \geq Mo_e(G_2)$ and equality holds if and only if $a_3 = 0$, i.e., $G_3 \cong G_2$. Note that $G_3 \cong B_m^6$. Clearly, $Mo_e(B_m^6) = m^2 - 2m - 16$. □

Lemma 3.5. *Let $G \in \mathcal{G}_m^2$ with brace $\Theta(a, b, c)$. Then*

$$Mo_e(G) \leq \begin{cases} 4, & \text{if } m = 5, \text{ and equality holds iff } G \cong B_m^3, B_m^4;\\ m^2 - 3m - 6, & \text{if } 6 \leq m \leq 8, \text{ and equality holds iff } G \cong B_m^3;\\ 48, & \text{if } m = 9, \text{ and equality holds iff } G \cong B_m^3, B_m^4;\\ m^2 - 2m - 15, & \text{if } 10 \leq m \leq 12, \text{ and equality holds iff } G \cong B_m^4;\\ 128, & \text{if } m = 13, \text{ and equality holds iff } G \cong B_m^4, B_m^5;\\ m^2 - m - 28, & \text{if } m \geq 14, \text{ and equality holds iff } G \cong B_m^5.\end{cases}$$

Proof. Suppose that x and y are the vertices with degree 3 in $\Theta(a, b, c)$ of G. Let $P_{a+1}, P_{b+1}, P_{c+1}$ be the three disjoint paths connecting x and y. We now proceed by considering the following three possible cases.

Case 1. $c \geq b \geq a \geq 3$.

Subcase 1.1. $c = b = a \geq 3$.

We choose six edges such that each one is incident to x or y in $\Theta(a, b, c)$. Let e be one of these six edges. Then $\psi(e) \leq m - 7$. This property holds for the remaining five edges as well. Therefore,

$$Mo_e(G) \leq 6(m - 7) + (m - 6)(m - 1) < m^2 - m - 28.$$

Subcase 1.2. $c \geq b \geq 4, a = 3$.

Let e_1 be one of the four edges incident to x or y in the paths P_{b+1} and P_{c+1}, and e_2 be one of the two edges incident to x or y in the path P_{a+1}. Then $\psi(e_1) \leq m - 8$, and $\psi(e_2) \leq m - 9$. Hence,

$$Mo_e(G) \leq 4(m - 8) + 2(m - 9) + (m - 6)(m - 1) < m^2 - m - 28.$$

Case 2. $c \geq b \geq a = 2$.

Subcase 2.1. $c = b = a = 2$.

The Subcase follows from Lemma 3.3.

Subcase 2.2. $c \geq 3, b = a = 2$.

Let e_1 be one of the four edges in the paths P_{a+1} and P_{b+1}, and e_2 be one of the two edges incident to x or y in the path P_{c+1}. Then $\psi(e_1) \leq m-7$, and $\psi(e_2) \leq m-6$. Hence,

$$Mo_e(G) \leq 4(m-7) + 2(m-6) + (m-6)(m-1) < m^2 - m - 28.$$

Subcase 2.3. $c \geq b \geq 3, a = 2$.

Let e_1 be one of the four edges incident to x or y in the paths P_{b+1} and P_{c+1}, and e_2 is an edge in the path P_{a+1}. Then $\psi(e_1) \leq m-6$, and $\psi(e_2) \leq m-9$. Hence,

$$Mo_e(G) \leq 4(m-6) + 2(m-9) + (m-6)(m-1) < m^2 - m - 28.$$

Case 3. $c \geq b \geq 2 \geq a = 1$.

Subcase 3.1. $c = b = 3, a = 1$.

By Lemma 3.2 and simple calculation, we have if $m \geq 14$, then $Mo_e(B_m^5) > Mo_e(B_m^4)$; if $m = 13$, then $Mo_e(B_m^3) = Mo_e(B_m^4) > Mo_e(B_m^5)$; if $10 \leq m \leq 12$, then $Mo_e(B_m^4) > Mo_e(B_m^5)$; if $m = 9$, then $Mo_e(B_m^3) = Mo_e(B_m^4) > Mo_e(B_m^5)$; if $6 \leq m \leq 8$, $Mo_e(B_m^3) > Mo_e(B_m^4) > Mo_e(B_m^5)$; if $m = 5$, then $Mo_e(B_m^3) = Mo_e(B_m^4)$.

Subcase 3.2. $c = 3, b = 2, a = 1$.

This Subcase follows from Lemma 3.4.

Subcase 3.3. $c \geq 4, b = 2, a = 1$.

Let $e_1 = xy$, e_2 be one of the four edges in the paths P_{b+1} and P_{c+1} that are incident to x or y, and e_3 be one of the two edges in the middle of the path P_{c+1}. Then $\psi(e_1) = 0$, $\psi(e_2) \leq m-5$, and $\psi(e_3) \leq m-6$. Thus,

$$Mo_e(G) \leq 4(m-5) + 2(m-6) + (m-7)(m-1) < m^2 - m - 28.$$

Subcase 3.4. $c \geq 4, b = 3, a = 1$.

Let $e_1 = xy$, e_2 be one of the two edges in the path P_{b+1} that are incident to x or y, e_3 be one of the two edges in the path P_{c+1} that are incident to x or y, and e_4 be one of the two edges in the middle of the path P_{c+1}. Then $\psi(e_1) = 0$, $\psi(e_2) \leq m-4$, $\psi(e_2) \leq m-5$, and $\psi(e_4) \leq m-6$. Hence,

$$Mo_e(G) \leq 2(m-4) + 2(m-5) + 2(m-6) + (m-7)(m-1) < m^2 - m - 28.$$

□

The proof of Theorem 1.2 directly follows from Lemmas 3.1 and 3.5.

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Declarations

The authors declare no conflict of interest.

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