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Research article

On the maximal additively weighted Mostar index of cacti

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Abstract: Let G be a simple, undirected, and connected graph. The additively weighted Mostar index of G is defined as $w^+Mo(G) = \sum_{e=uv\in E(G)}(d_G(u) + d_G(v))|n_u(e) - n_v(e)|$, where $d_G(u)$ denotes the degree of vertex u in G, $n_u(e)$ represents the number of vertices in G which are closer to u than to v, and $d_G(v), n_v(e)$ are defined analogously. In this paper, we determine the maximum value of the additively weighted Mostar index over all n-vertex cacti with exactly p pendant vertices and identify the unique extremal cactus attaining the maximum. Moreover, for the family of n-vertex cacti with precisely b cut edges, we establish both the largest and the second largest values of the additively weighted Mostar index and fully characterize the corresponding extremal graphs for each value.

Keywords: distance; topological indices; Mostar index; additively weighted Mostar index; cactus
Mathematics Subject Classification: 05C09, 05C12, 05C92

1. Introduction

All graphs considered in this paper are finite, simple, and undirected. Let $G = (V(G), E(G))$ be a connected graph of order n. For a vertex $u \in V(G)$, its degree, denoted by $d_G(u)$, is the number of vertices adjacent to u in G. If $d_G(u) = 1$, then u is called a pendant vertex, and the unique edge incident to u is called a pendant edge. A cycle C in G is an end-block of G if exactly one vertex in $V(C)$ has degree greater than 2 in G. An edge $e \in E(G)$ is a cut edge (or bridge) if $G - e$ is disconnected. The distance between two vertices u and v in G, denoted by $d_G(u, v)$, is the length of a shortest path connecting them in G. The diameter of G is defined as $d(G) = \max\{d_G(u, v) \mid u, v \in V(G), u \neq v\}$. For a subset $D \subseteq E(G)$, let $G - D$ denote the spanning subgraph of G with edge set $E(G) \setminus D$. Let G^c denote the complement of G, i.e., the simple graph on vertex set $V(G)$ such that for all distinct $x, y \in V(G)$, $xy \in E(G^c)$ if and only if $xy \notin E(G)$. If $D \subseteq E(G^c)$, let $G + D$ denote the graph on vertex set $V(G)$ with edge set $E(G) \cup D$. Let C_n, P_n, and S_n denote the cycle, path, and star of order n, respectively.

For an edge $e = uv \in E(G)$, we define the following three disjoint subsets of $V(G)$:

$$N_u(e) = \{w \in V(G) \mid d_G(w,u) < d_G(w,v)\},$$

$$N_v(e) = \{w \in V(G) \mid d_G(w,v) < d_G(w,u)\},$$

$$N_0(e) = \{w \in V(G) \mid d_G(w,u) = d_G(w,v)\}.$$

Let $n_u(e), n_v(e)$, and $n_0(e)$ denote the cardinalities of $N_u(e), N_v(e)$, and $N_0(e)$, respectively. Then $n = n_u(e) + n_v(e) + n_0(e)$. For all other terminology not explicitly defined here, we refer the reader to [1].

In chemical graph theory, a molecule is represented as a molecular graph, where atoms and chemical bonds correspond to vertices and edges, respectively. Topological descriptors, also known as topological indices, are numerical invariants derived exclusively from the topology of such graphs. These indices can serve as essential numerical measures that capture structural features of molecules [2, 3] and are mainly grouped into distance-based, degree-based, and spectrum-based families. Owing to their computational efficiency and structural sensitivity, topological indices have been proven very important in QSPR/QSAR (quantitative structure-property/quantitative structure-activity relationship) modeling. When integrated into machine learning and statistical models, they enable accurate and robust prediction of key physicochemical properties including melting points, boiling points, solubility, heat capacity, and molecular stability. In addition, topological indices support predictive modeling of drug-likeness and molecular interactions, thereby enhancing the efficiency and rationality of early-stage drug discovery and molecular design.

The Wiener index, introduced by H. Wiener in 1947 in his study of alkane boiling points [4], is among the earliest and most extensively studied topological indices in mathematical chemistry. Formally, the Wiener index of a connected graph G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v).$$

Wiener showed that among alkane isomers with the same number of carbon atoms, molecules with more branches exhibit lower boiling points and smaller values of the Wiener index. He also derived a more efficient formula for trees: $W(G) = \sum_{e=uv \in E} n_u(e) \cdot n_v(e)$. To extend this concept to general connected graphs-including those containing cycles, Gutman introduced the Szeged index in 1994 [5]. Its definition is given by

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

For acyclic molecules, the Szeged index coincides with the Wiener index. Several studies have employed the Szeged index to develop predictive and effective models for some key physicochemical properties of compounds [6, 7].

In 2018, Došlić et al. [8] proposed the Mostar index, which is a Szeged-like topological index defined as

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

They pointed out that the Mostar index quantitatively refines the distance-non-balancedness of G and can serve as a measure of graph peripherality. Furthermore, they established its extremal values over the family of trees and unicyclic graphs, and fully characterized the corresponding extremal

graphs. Since then, the Mostar index has received substantial attention in both mathematics and chemistry. For example, Tepeh [9] determined the extremal bicyclic graphs for Mostar index; Hayat and Zhou [10] identified all cacti of order n containing exactly k cycles that maximize the Mostar index, and subsequently characterized all cacti of order n attaining the maximum value. The potential biological and chemical applications of the Mostar index were presented in [11]. In addition, the correlations between the Mostar index and some key physicochemical properties of octane isomers and benzenoid hydrocarbons were revealed in [12]. Further extremal results and chemical applications of the Mostar index can be found in [13–17].

By taking into account the vertex degrees, Arockiaraj et al. [11] introduced several degree-weighted variants of the Mostar index. The additively weighted Mostar index, denoted by $w^+Mo(G)$, is one such invariant defined as

$$w^+Mo(G) = \sum_{e=uv\in E(G)} (d_G(u) + d_G(v))\,|n_u(e) - n_v(e)|.$$

Since its introduction, the additively weighted Mostar index has been extensively investigated. Closed-form expressions for this index have been derived via the cut method for several chemically significant graphs [11, 18]. Ali and Došlić [19] determined the extremal values of $w^+Mo(G)$ over the family of trees of order n and characterized the corresponding extremal trees. Asmat et al. [20] established a sharp upper bound for $w^+Mo(G)$ among n-vertex trees with diameter $d \geq 6$, and identified the extremal trees achieving this bound. He and Liu [21] characterized the extremal bicyclic graphs for $w^+Mo(G)$. Explicit formulae for $w^+Mo(G)$ were computed for conical graphs and generalized gear graphs [22]. Furthermore, the relationships between the additively weighted Mostar index and some chemical properties were examined for octane isomers and benzenoid hydrocarbons [23].

A cactus is a connected graph G in which every block is either a cycle or an edge. Recently, Liu and Zhen [24] identified the n-vertex cacti with exactly k cycles that attain the maximum and second maximum values of the additively weighted Mostar index $w^+Mo(G)$, respectively. Building upon this work, it is both natural and scientifically meaningful to explore the extremal behavior of $w^+Mo(G)$ with respect to other graph parameters of cacti, particularly the number of pendant vertices and the number of cut edges. In this paper, we establish the sharp upper bounds for $w^+Mo(G)$ among n-vertex cacti with a prescribed number of pendant vertices/cut edges. Moreover, we determine not only the maximum but also the second largest value of $w^+Mo(G)$ under a fixed number of cut edges. In Section 2, we introduce a series of graph transformations, each of which strictly increases $w^+Mo(G)$ whenever applicable. Applying these transformations, in Section 3, we determine the maximum value of $w^+Mo(G)$ over all n-vertex cacti with exactly p pendant vertices. We also identify the unique extremal cactus attaining the maximum. In Section 4, we establish both the largest and the second largest possible values of $w^+Mo(G)$ for n-vertex cacti with a prescribed number of cut edges. For each extremal value, we completely characterize the corresponding extremal cacti.

2. Preliminaries

In this section, we introduce some graph transformations that strictly increase the additively weighted Mostar index of a graph. For brevity, we define the contribution of each edge $e = uv \in E(G)$ to the Mostar index and the additively weighted Mostar index of a graph G as $\phi_G(e) = |n_u(e) - n_v(e)|$ and $\Phi_G(e) = (d_G(u) + d_G(v))\,|n_u(e) - n_v(e)|$, respectively. Then $w^+Mo(G) = \sum_{uv\in E(G)} \Phi_G(e) = \sum_{uv\in E(G)} (d_G(u) +$

$d_G(v))\phi_G(e)$.

Lemma 2.1. *[21] Let G be a connected graph, and let $e = uv \in E(G)$ be a cut edge that is not pendant. Denote by G^* the graph obtained from G by contracting the edge $e = uv$ to the vertex u and then attaching a new pendant edge to u (see Figure 1). Then $w^+Mo(G) < w^+Mo(G^*)$.*

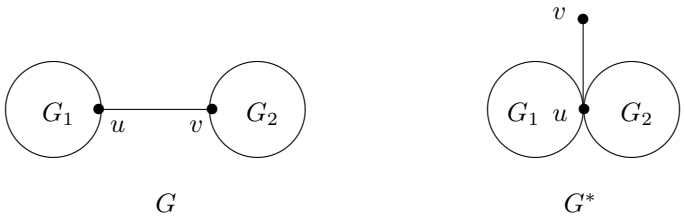


Figure 1. Graphs G and G^* in Lemma 2.1.

Lemma 2.2. *[24] If G is a cactus of order n with maximum additively weighted Mostar index, then all cycles in G are end-blocks.*

Based on the proof of Lemma 2.2, the following structural observation holds for cacti.

Remark 2.1. *Let G be a cactus with a cycle $C = v_1v_2\cdots v_mv_1$, and for each $k = 1, 2, \ldots, m$, let G_k denote the connected component of $G - E(C)$ containing v_k. Define G' as the graph obtained from G by moving all G_k ($k = 2, \ldots, m$) to v_1; specifically, for each $k = 2, \ldots, m$ and each vertex $w \in N_{G_k}(v_k)$, delete the edge v_kw and add the edge v_1w. Then $w^+Mo(G) \le w^+Mo(G')$, with equality if and only if C is an end-block of G.*

Lemma 2.3. *Let G be either a cycle C_k or a graph containing an end-block $C_k = u_1u_2\cdots u_ku_1$, where $k \ge 5$ and u_1 is the unique vertex of C_k with $d_G(u_1) = \max\{d_G(u_i) \mid i = 1, \ldots, k\}$. Define $G^* = (G - u_3u_4) + \{u_1u_3, u_1u_4\}$. Then $w^+Mo(G) < w^+Mo(G^*)$.*

Proof. For brevity, denote $d_G(u_1)$ by d_{u_1}. Obviously, $G-\{u_2, u_3, \cdots, u_k\} \cong G^*-\{u_2, u_3, \cdots, u_k\}$. Denote it by H. Then $\Phi_G(e) = \Phi_{G^*}(e)$ for each edge $e \in E(H)$ not incident to u_1, while $\Phi_{G^*}(e) \ge \Phi_G(e)$ for each edge $e \in E(H)$ incident to u_1. Therefore,

$$w^+Mo(G^*) - w^+Mo(G) \ge \sum_{e\in E(G^*)\setminus E(H)} \Phi_{G^*}(e) - \sum_{e\in E(G)\setminus E(H)} \Phi_G(e).$$

Case 1. k is odd.

Then $\phi_G(u_{\frac{k+1}{2}}u_{\frac{k+3}{2}}) = 0$ and $\phi_G(e) = n - k$ for all other edges $e \in E(C_k)$. Consequently, $\Phi_G(u_{\frac{k+1}{2}}u_{\frac{k+3}{2}}) = 0$, $\Phi_G(u_1u_2) = \Phi_G(u_ku_1) = (d_{u_1} + 2)(n - k)$, and $\Phi_G(e) = 4(n - k)$ for each edge $e \in E(C_k)\setminus\{u_{\frac{k+1}{2}}u_{\frac{k+3}{2}}, u_1u_2, u_ku_1\}$. Thus, $\sum_{e\in E(G)\setminus E(H)} \Phi_G(e) = \sum_{e\in E(C_k)} \Phi_G(e) = 2(d_{u_1}+2)(n-k)+4(k-3)(n-k)$.

In G^*, we have $\phi_{G^*}(u_2u_3) = \phi_{G^*}(u_{\frac{k+3}{2}}u_{\frac{k+5}{2}}) = 0$, $\phi_{G^*}(u_1u_2) = \phi_{G^*}(u_1u_3) = n - 3$, and $\phi_{G^*}(e) = n - k + 2$ for all edges $e \in E(G^*) \setminus (E(H) \cup \{u_1u_2, u_1u_3, u_2u_3, u_{\frac{k+3}{2}}u_{\frac{k+5}{2}}\})$. Since $d_{G^*}(u_1) = d_{u_1} + 2$, it follows that $\Phi_{G^*}(u_2u_3) = \Phi_{G^*}(u_{\frac{k+3}{2}}u_{\frac{k+5}{2}}) = 0$, $\Phi_{G^*}(u_1u_2) = \Phi_{G^*}(u_1u_3) = (d_{u_1} + 4)(n - 3)$, $\Phi_{G^*}(u_1u_4) = \Phi_{G^*}(u_1u_k) = (d_{u_1} + 4)(n - k + 2)$, and $\Phi_{G^*}(e) = 4(n - k + 2)$ for all remaining edges $e \in E(G^*) \setminus E(H)$. Therefore,

$\sum_{e\in E(G^*)\setminus E(H)} \Phi_{G^*}(e) = 2(d_{u_1}+4)(n-k+2) + 4(k-5)(n-k+2) + 2(d_{u_1}+4)(n-3)$. Then

$$\begin{aligned}
&\sum_{e\in E(G^*)\setminus E(H)} \Phi_{G^*}(e) - \sum_{e\in E(G)\setminus E(H)} \Phi_G(e)\\
&= [2(d_{u_1}+4)(n-k+2) + 4(k-5)(n-k+2) + 2(d_{u_1}+4)(n-3)]\\
&\quad - [2(d_{u_1}+2)(n-k) + 4(k-3)(n-k)]\\
&= 2(n-1)d_{u_1} + 4n + 12(k-4) > 0.
\end{aligned}$$

Case 2. k is even.

A parallel computation gives

$$\begin{aligned}
&\sum_{e\in E(G^*)\setminus E(H)} \Phi_{G^*}(e) - \sum_{e\in E(G)\setminus E(H)} \Phi_G(e)\\
&= [2(d_{u_1}+4)(n-k+2) + 4(k-4)(n-k+2) + 2(d_{u_1}+4)(n-3)]\\
&\quad - [2(d_{u_1}+2)(n-k) + 4(k-2)(n-k)]\\
&= 2(n-1)d_{u_1} + 4n + 12(k-4) + 8 > 0.
\end{aligned}$$

Hence, $w^+Mo(G^*) - w^+Mo(G) > 0$. □

Lemma 2.4. *Let G be a graph containing two end-blocks $C_1 = uu_1u_2u_3u$ and $C_2 = uv_1v_2v_3u$ that share the common vertex u. Define $G' = (G - \{u_1u_2, v_1v_2\}) + \{uu_2, uv_2, u_1v_1\}$. Then $w^+Mo(G) < w^+Mo(G')$.*

Proof. Obviously, $G - \{u_1, u_2, u_3, v_1, v_2, v_3\} \cong G' - \{u_1, u_2, u_3, v_1, v_2, v_3\}$. Denote it by H. Then $\Phi_G(e) = \Phi_{G'}(e)$ for each edge $e \in E(H)$ not incident to u, while $\Phi_{G'}(e) \geq \Phi_G(e)$ for each edge $e \in E(H)$ incident to u. Consequently,

$$\begin{aligned}
&w^+Mo(G') - w^+Mo(G)\\
&\geq 6\Phi_{G'}(uu_3) - [4\Phi_G(uu_1) + 4\Phi_G(u_1u_2)]\\
&= [6(d_G(u)+4)(n-3)] - [4(d_G(u)+2)(n-4) + 16(n-4)]\\
&= 2(n-1)d_G(u) + 24 > 0.
\end{aligned}$$

□

Lemma 2.5. *Let G be a graph containing two adjacent cut edges $e_1 = u_1u_2$ and $e_2 = u_2u_3$. For $i = 1, 2, 3$, let G_i denote the connected component of $G - \{e_1, e_2\}$ that contains u_i. Let G' be the graph obtained from G by first moving G_2 and G_3 to u_1, and then adding a new edge $e_3 = u_1u_3$ (see Figure 2). If $\min\{d_G(u_1), d_G(u_3)\} \geq 2$, then $w^+Mo(G) < w^+Mo(G')$.*

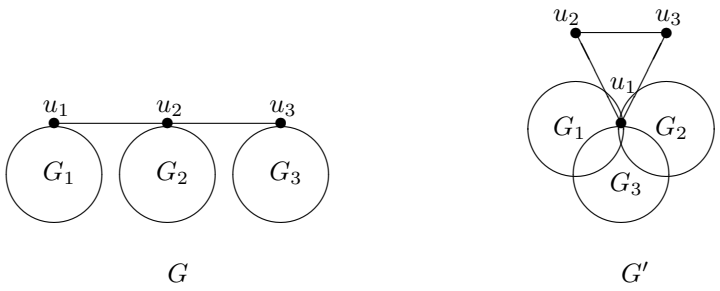


Figure 2. Graphs G and G' in Lemma 2.5.

Proof. For $i = 1, 2, 3$, let $|V(G_i)| = n_i + 1$, and denote $d_{G_1}(u_1) = a$, $d_{G_2}(u_2) = b$, and $d_{G_3}(u_3) = c$, where $a, c \geq 1$. Obviously, for each $i \in \{1, 2, 3\}$, $\Phi_G(e) = \Phi_{G'}(e)$ holds for every edge $e \in E(G_i)$ that is not incident to u_i. Furthermore, $\Phi_G(e) \leq \Phi_{G'}(e)$ holds for every edge $e \in E(G_i)$ incident to u_i. Therefore,

$$\begin{aligned}
&w^+Mo(G') - w^+Mo(G)\\
&\geq \Phi_{G'}(u_1u_2) + \Phi_{G'}(u_1u_3) - \Phi_G(u_1u_2) - \Phi_G(u_2u_3)\\
&= 2(a+b+c+4)(n-3) - (a+b+3)|n_2+n_3+1-n_1| - (b+c+3)|n_1+n_2+1-n_3|\\
&> 2(a+b+c+4)(n-3) - (a+b+3)(n-3) - (b+c+3)(n-3) > 0.
\end{aligned}$$

□

Each of the above graph transformations strictly increases the additively weighted Mostar index whenever applicable. Critically, every transformation preserves both the number of vertices and the prescribed number of pendant vertices or cut edges. By iteratively applying these transformations, any extremal cactus can be progressively reduced to a restricted configuration consisting mainly of short end-blocks and pendant edges clustered around particular vertices. Such reduction is not merely technical but is foundational to the extremal characterizations established in Sections 3 and 4.

3. Maximum additively weighted Mostar index of cacti with a fixed number of pendant vertices

Let C_n^p denote the set of all cacti of order n with exactly p pendant vertices. In this section, we determine the maximum value of the additively weighted Mostar index over C_n^p. Let $G_n^p(l_1, l_2, \ldots, l_k) \in C_n^p$ be a cactus with exactly k end-blocks of lengths $l_1, l_2, \ldots, l_k$ sharing one common vertex that is adjacent to each of the p pendant vertices, where $k \geq 1$, $3 \leq l_1 \leq l_2 \leq \cdots \leq l_k$ and $\sum_{i=1}^{k} l_i = n + k - p - 1$. Denote by $DS_n(a, b)$ the tree obtained from two stars S_{a+1} and S_{b+1} by adding the edge uv, where $a \geq b$, $a + b = n - 2$ and u, v are the centers of S_{a+1} and S_{b+1}, respectively.

Theorem 3.1. *Let $G \in C_n^p$ be a graph attaining the maximum additively weighted Mostar index, where $n \geq 7$ and $0 \leq p \leq n - 2$.*

(1) If $p = n - 2$, then $w^+Mo(G) = n^3 - 5n^2 + 10n - 12$ and $G \cong DS_n(n-3, 1)$;

(2) If $0 \leq p \leq n-3$ and $n - p$ is odd, then $w^+Mo(G) = n^3 - 3n^2 - n + 3p + 3$ and $G \cong G_n^p(\underbrace{3, 3, \ldots, 3}_{\frac{n-p-1}{2}})$

(see Figure 3);

(3) If $0 \leq p \leq n-4$ *and* $n-p$ *is even, then* $w^+Mo(G) = n^3 - 5n^2 + 12n + 2p - 32$ *and* $G \cong G_n^p(\underbrace{3,3,\ldots,3}_{\frac{n-p-4}{2}},4)$ *(see Figure 3).*



Figure 3. Extremal graphs among C_n^p when $p \leq n-3$.

Proof. If $p = n-2$, then $G \cong DS_n(a,b)$ for some integers a and b, where $a \geq b \geq 1$ and $a+b = n-2$. Suppose $a \neq n-3$. Observe that $w^+Mo(G) = a(a+2)(n-2) + b(b+2)(n-2) + n(a-b)$ and $w^+Mo(DS_n(a+1,b-1)) = (a+1)(a+3)(n-2) + (b-1)(b+1)(n-2) + n(a-b+2)$. Hence, $w^+Mo(DS_n(a+1,b-1)) - w^+Mo(G) = 2(a-b+1)(n-2) + 2n > 0$, a contradiction to the definition of G. Therefore, $a = n-3$, i.e., $G \cong DS_n(n-3,1)$, and consequently, $w^+Mo(G) = n^3 - 5n^2 + 10n - 12$.

Now consider the case $0 \leq p \leq n-3$. Suppose to the contrary that G is acyclic, i.e., G is a tree. Since $p \leq n-3$, the diameter $d(G)$ satisfies $d(G) \geq 4$. Let $P = v_0v_1\cdots v_{d(G)}$ be a path of length $d(G)$ in G, and for $i = 1,2,3$, let G_i denote the connected component of $G - \{v_1v_2, v_2v_3\}$ containing v_i. Construct G' from G by first moving G_2 and G_3 to v_1, and then adding a new edge v_1v_3. Then $G' \in C_n^p$, and by Lemma 2.5, $w^+Mo(G) < w^+Mo(G')$, a contradiction. Hence, the following claim holds.

Claim 1. G contains at least one cycle.

By Remark 2.1 and Lemma 2.3, every cycle in G is an end-block and has length either 3 or 4. Consequently, at most one cut edge is non-pendant in G by Lemma 2.5. Furthermore, by Lemma 2.4, no two end-blocks of length 4 share a common vertex.

It is straightforward to verify that $w^+Mo(G_n^p(\underbrace{3,3,\ldots,3}_{\frac{n-p-1}{2}})) = n^3 - 3n^2 - n + 3p + 3$ if $n-p$ is odd, and $w^+Mo(G_n^p(\underbrace{3,3,\ldots,3}_{\frac{n-p-4}{2}},4) = n^3 - 5n^2 + 12n + 2p - 32$ if $n-p$ is even. To complete the proof, it suffices to show that every cut edge in G is pendant. Suppose not. Then, by Lemma 2.5, exactly one cut edge in G is non-pendant. Denote it by $e = uv$. Let p_1, t_1, and q_1 (respectively, p_2, t_2, and q_2) be the numbers of pendant edges, triangles, and quadrangles attached at u (respectively, at v). Then $(2t_1 + 3q_1 + p_1) + (2t_2 + 3q_2 + p_2) = n-2$ and $p_1 + p_2 = p$. Moreover, by Lemma 2.4, $q_i \in \{0,1\}$ for $i = 1,2$. The resulting structure of G is depicted in Figure 4.

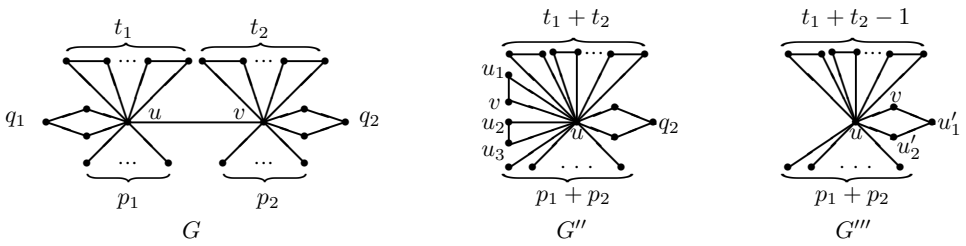


Figure 4. G, G'', and G''' in the proof of Theorem 3.1.

Suppose $q_1 = 1$. Let $C = uu_1u_2u_3u$ denote the quadrangle attached at u and G'' be the graph obtained from $G - u_1u_2$ by first moving all pendant edges, triangles, and quadrangles from v to u, and then adding the edges vu_1 and uu_2 (see Figure 4). Then $G'' \in C_n^p$ and $d_{G''}(u) = d_G(u) + d_G(v)$. Therefore,

$$\begin{aligned}
&w^+Mo(G'') - w^+Mo(G)\\
&> 4\Phi_{G''}(uu_1) + 2\Phi_{G''}(vu_1) - [2\Phi_G(uu_1) + 2\Phi_G(u_1u_2) + \Phi_G(uv)]\\
&= 4(d_{G''}(u)+2)(n-3) - 2(d_G(u)+6)(n-4) - (d_G(u)+d_G(v))|p_1 + 2t_1 + 3 - p_2 - 2t_2 - 3q_2|\\
&= 4(d_G(u)+d_G(v)+2)(n-3) - 2(d_G(u)+6)(n-4) - (d_G(u)+d_G(v))|p_1 + 2t_1 + 3 - p_2 - 2t_2 - 3q_2|\\
&> 4(d_G(u)+d_G(v)+2)(n-3) - 2(d_G(u)+6)(n-4) - (d_G(u)+d_G(v))(n-3)\\
&> 3(d_G(u)+4)(n-3) - 2(d_G(u)+6)(n-4) > 0,
\end{aligned}$$

a contradiction to the definition of G. Hence, $q_1 = 0$. By symmetry, $q_2 = 0$. Consequently, G has no quadrangles.

Suppose $t_1 > 0$. Then $d_G(u) \geq 3$. Let $C_3 = uu_1'u_2'u$ denote a triangle attached at u. Construct G''' from $G - uu_1'$ by first moving all pendant edges and triangles from v to u, and then adding the edge vu_1' (see Figure 4). Then $G''' \in C_n^p$ and $d_{G'''}(u) = d_G(u) + d_G(v) - 2$. A direct computation yields $w^+Mo(G) = p_1(d_G(u)+1)(n-2) + 2t_1(d_G(u)+2)(n-3) + p_2(d_G(v)+1)(n-2) + 2t_2(d_G(v)+2)(n-3) + (d_G(u)+d_G(v))|d_G(u) - d_G(v)|$ and $w^+Mo(G''') = (p_1+p_2)(d_G(u)+d_G(v)-1)(n-2) + 2(t_1+t_2-1)(d_G(u)+d_G(v))(n-3) + 2(d_G(u)+d_G(v))(n-4) + 8(n-4)$. Since $d_G(u)+d_G(v) = n$, it follows that

$$\begin{aligned}
&w^+Mo(G''') - w^+Mo(G)\\
&= p_1(n-2)(d_G(v)-2) + p_2(n-2)(d_G(u)-2) + 2t_1(n-3)(d_G(v)-2)\\
&\quad + 2t_2(n-3)(d_G(u)-2) + 6n - 32 - n|d_G(u) - d_G(v)|.
\end{aligned}$$

If $d_G(v) = 2$, then $p_2 = 1$ and $t_2 = 0$. As $n \geq 7$, we have $d_G(u) \geq 5$. Therefore,

$$\begin{aligned}
&w^+Mo(G''') - w^+Mo(G)\\
&= (n-2)(d_G(u)-2) + 6n - 32 - n|d_G(u) - d_G(v)|\\
&= (n-2)(d_G(u)-2) + 6n - 32 - n(n-4)\\
&= 4n - 24 > 0,
\end{aligned}$$

a contradiction.

If $d_G(v) > 2$, then

$$w^+Mo(G''') - w^+Mo(G)$$

$$
\begin{aligned}
&> p_1(n-2) + p_2(n-2) + 2t_1(n-3) + 2t_2(n-3) + 6n - 32 - n(n-4)\\
&> p_1(n-3) + p_2(n-3) + 2t_1(n-3) + 2t_2(n-3) + 6n - 32 - n(n-4)\\
&= (p_1 + p_2 + 2t_1 + 2t_2)(n-3) - n^2 + 10n - 32\\
&= (n-2)(n-3) - n^2 + 10n - 32 = 5n - 26 > 0,
\end{aligned}
$$

a contradiction. Therefore, $t_1 = 0$. By symmetry, $t_2 = 0$. This contradicts Claim 1. Hence, every cut edge in G is pendant. Then $G \cong G_n^p(l_1, l_2, \ldots, l_k)$, where $k \geq 1$, $3 \leq l_1 \leq l_2 \leq \cdots \leq l_k$, $\sum_{i=1}^{k} l_i = n+k-p-1$, and $l_i \in \{3, 4\}$ for $i = 1, \ldots, k$. By Lemma 2.4, $l_i = 3$ for $i = 1, \ldots, k-1$ if $k \geq 2$. It follows that $l_k = \sum_{i=1}^{k} l_i - 3(k-1) = n+k-p-1-3(k-1) = n-p-2(k-1)$. Thus, $l_k \equiv n-p \pmod 2$. Consequently, if $n-p$ is odd, then $l_k = 3$ and $G \cong G_n^p(\underbrace{3, 3, \ldots, 3}_{\frac{n-p-1}{2}})$; if $n-p$ is even, then $l_k = 4$ and $G \cong G_n^p(\underbrace{3, 3, \ldots, 3}_{\frac{n-p-4}{2}}, 4)$.

The theorem follows. □

4. The additively weighted Mostar index of cacti with a fixed number of cut edges

Let $C(n, b)$ denote the set of all cacti of order n containing exactly b cut edges, where $0 \leq b \leq n-3$. In this section, we determine the extremal graphs that achieve the maximum and second-maximum values of the additively weighted Mostar index among $C(n, b)$.

Theorem 4.1. *Let G be a graph with maximum additively weighted Mostar index among $C(n, b)$, where $0 \leq b \leq n-3$. Then $G \cong G_n^b(\underbrace{3, 3, \ldots, 3}_{\frac{n-b-1}{2}})$ with $w^+Mo(G) = n^3 - 3n^2 - n + 3b + 3$ if $n-b$ is odd, and $G \cong G_n^b(\underbrace{3, 3, \ldots, 3}_{\frac{n-b-4}{2}}, 4)$ with $w^+Mo(G) = n^3 - 5n^2 + 12n + 2b - 32$ if $n-b$ is even.*

Proof. Since $b \leq n-3$, G is not a tree. By Lemma 2.1 and Remark 2.1, each cut edge is pendant, and every cycle is an end-block in G. Therefore, $G \cong G_n^b(l_1, l_2, \ldots, l_k)$, where $k \geq 1$, $3 \leq l_1 \leq l_2 \leq \cdots \leq l_k$ and $\sum_{i=1}^{k} l_i = n + k - b - 1$. By Lemma 2.3, $l_i \in \{3, 4\}$ for $i = 1, \ldots, k$. Moreover, Lemma 2.4 implies that $l_i = 3$ for $i = 1, \ldots, k-1$ if $k \geq 2$. It follows that $l_k = \sum_{i=1}^{k} l_i - 3(k-1) = n+k-b-1-3(k-1) = n-b-2(k-1)$. Thus, $l_k \equiv n-b \pmod 2$. Consequently, $l_k = 3$ if $n-b$ is odd, and $l_k = 4$ if $n-b$ is even. Since $w^+Mo(G_n^b(\underbrace{3, 3, \ldots, 3}_{\frac{n-b-1}{2}})) = n^3 - 3n^2 - n + 3b + 3$ ($n-b$ is odd), and $w^+Mo(G_n^b(\underbrace{3, 3, \ldots, 3}_{\frac{n-b-4}{2}}, 4)) = n^3 - 5n^2 + 12n + 2b - 32$ ($n-b$ is even), the theorem follows. □

We now determine the graphs that achieve the second largest value of the additively weighted Mostar index among $C(n, b)$, where $0 \leq b \leq n-3$ and $n \geq 5$. Let $C^*(n, b) = C(n, b) \setminus \{G_n^b(\underbrace{3, 3, \ldots, 3, 3}_{\frac{n-b-1}{2}})\}$ if $n-b$ is odd, and $C^*(n, b) = C(n, b) \setminus \{G_n^b(\underbrace{3, 3, \ldots, 3}_{\frac{n-b-4}{2}}, 4)\}$ otherwise.

We define four subsets of $C^*(n, b)$ as follows:

- $\mathcal{F}_1(n,b)$: the family of cacti in $C^*(n,b)$ containing a cycle of length at least 5;
- $\mathcal{F}_2(n,b)$: the family of cacti in $C^*(n,b)$ containing two end-blocks of length 4 that share a common vertex;
- $\mathcal{F}_3(n,b)$: the family of cacti in $C^*(n,b)$ containing at least one cycle that is not an end-block;
- $\mathcal{F}_4(n,b)$: the family of cacti in $C^*(n,b)$ containing a cut edge that is not pendant.

It follows that $C^*(n,b) = \bigcup_{i=1}^{4} \mathcal{F}_i(n,b)$. Since the additively weighted Mostar index is maximized over $C^*(n,b)$, it suffices to compute the maximum value of this index over each family $\mathcal{F}_i(n,b)$ $(i = 1,2,3,4)$ separately and compare the resulting maxima. The corresponding maximal values are established in Lemmas 4.1–4.4, respectively.

Lemma 4.1. *Let G be a cactus in $\mathcal{F}_1(n,b)$, where $n-b \geq 5$.*

(1) If $n-b$ is odd, then $w^+Mo(G) \leq n^3 - 7n^2 + 19n + b - 45$, with equality if and only if $G \cong G_n^b(\underbrace{3,3,\ldots,3}_{\frac{n-b-5}{2}},5)$.

(2) If $n-b=6$, then $w^+Mo(G) \leq n^3 - 9n^2 + 36n - 108$, with equality if and only if $G \cong G_n^b(6)$.

(3) If $n-b$ is even and $n-b \geq 8$, then $w^+Mo(G) \leq n^3 - 9n^2 + 36n - 84$, with equality if and only if $G \cong G_n^b(\underbrace{3,3,\ldots,3}_{\frac{n-b-8}{2}},4,5)$.

Proof. Among the graphs in $\mathcal{F}_1(n,b)$, let H be a graph with the maximum additively weighted Mostar index. By Lemmas 2.1, 2.3 and Remark 2.1, every cut edge is pendant, every cycle is an end-block, and H contains exactly one end-block of length at least 5. Moreover, by Lemma 2.4, no two end-blocks of length 4 share a common vertex. Consequently, $H \cong G_n^b(l_1,l_2,\ldots,l_k)$ for some integer $k \geq 1$, where $l_i = 3$ for $i = 1,\ldots,k-2$ (if $k \geq 3$), $l_{k-1} \in \{3,4\}$ (if $k \geq 2$), $l_k \geq 5$, and $\sum_{i=1}^{k}(l_i - 1) = n-b-1$.

If $n-b=5$, then $k=1$ and $H \cong G_n^{n-5}(5)$. Since $w^+Mo(G_n^{n-5}(5)) = n^3 - 7n^2 + 20n - 50 = n^3 - 7n^2 + 19n + (n-5) - 45$, statement (1) holds for $n-b=5$. If $n-b=6$, then $k=1$ and $H \cong G_n^{n-6}(6)$. Since $w^+Mo(G_n^{n-6}(6)) = n^3 - 9n^2 + 36n - 108$, statement (2) holds.

Now assume $n-b \geq 7$. If $k=1$, then $H \cong G_n^b(n-b)$. However, by Lemma 2.3, there exists a graph $G_n^b(3,n-b-2)$ such that $w^+Mo(H) < w^+Mo(G_n^b(3,n-b-2))$, contradicting the maximality of H. Therefore, $k \geq 2$. Observe that $l_{k-1} + l_k = n-b-1+k-3(k-2) = n-b-2k+5$. It follows that $l_{k-1} + l_k \equiv n-b+1 \pmod 2$.

Case 1. $n-b$ is odd.

Then $l_{k-1}+l_k$ is even. If $l_{k-1}=3$, then $l_k = 5$ by Lemma 2.3. Thus, $k = \frac{n-b-3}{2}$ and $H \cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-5}{2}},5)$. Similarly, if $l_{k-1}=4$, then $l_k = 6$. Thus, $k = \frac{n-b-5}{2}$ and $H \cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-9}{2}},4,6)$. A direct computation yields that $w^+Mo(G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-5}{2}},5)) - w^+Mo(G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-9}{2}},4,6)) = (n^3 - 7n^2 + 19n + b - 45) - (n^3 - 11n^2 + 55n - b - 149) = 4n^2 - 36n + 2b + 104 > 0$ if $n-b \geq 9$. Hence, $H \cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-5}{2}},5)$, and statement (1) holds for all odd $n-b \geq 7$.

Case 2. $n-b$ is even.

Then $l_{k-1}+l_k$ is odd. If $l_{k-1}=4$, then $l_k=5$ and $k=\frac{n-b-4}{2}$, so $H\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-8}{2}},4,5)$. If $l_{k-1}=3$, then $l_k=6$ and $k=\frac{n-b-4}{2}$, so $H\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-6}{2}},6)$. Since $w^+Mo(G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-8}{2}},4,5))-w^+Mo(G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-6}{2}},6))=(n^3-9n^2+36n-84)-(n^3-9n^2+36n-108)=24>0$ if $n-b\geq 8$, we get $H\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-8}{2}},4,5)$, and statement (3) holds. □

Lemma 4.2. *Let G be a cactus in $\mathcal{F}_2(n,b)$, where $n-b\geq 7$ and $n-b\neq 8$.*

(1) If $n-b$ is odd, then $w^+Mo(G)\leq n^3-7n^2+27n+b-69$, with equality if and only if $G\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-7}{2}},4,4)$.

(2) If $n-b$ is even, then $w^+Mo(G)\leq n^3-9n^2+44n-108$, with equality if and only if $G\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-10}{2}},4,4,4)$.

Proof. Among all graphs in $\mathcal{F}_2(n,b)$, let H be a graph with the maximum additively weighted Mostar index. By Lemmas 2.1 and 2.3, together with Remark 2.1, $H\cong G_n^b(\underbrace{3,\ldots,3}_{t},\underbrace{4,\ldots,4}_{q})$ for some $t\geq 0$ and $q\geq 2$, where $2t+3q+b+1=n$. Equivalently, $n-b=2t+3q+1$. Since $t\geq 0$ and $q\geq 2$, it follows that $n-b\geq 7$ and $n-b\neq 8$.

If $n-b$ is odd, then q must be even. Suppose $q\geq 4$. Then, by Lemma 2.4, $w^+Mo(H)<w^+Mo(G_n^b(\underbrace{3,\ldots,3}_{t+3},\underbrace{4,\ldots,4}_{q-2}))$, a contradiction. Hence, $q=2$, which yields $t=\frac{n-b-7}{2}$, $H\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-7}{2}},4,4)$, and consequently, $w^+Mo(H)=n^3-7n^2+27n+b-69$. Similarly, if $n-b$ is even, then $q=3$, $t=\frac{n-b-10}{2}$, $H\cong G_n^b(\underbrace{3,\ldots,3}_{\frac{n-b-10}{2}},4,4,4)$, and $w^+Mo(H)=n^3-9n^2+44n-108$. Therefore, statements (1) and (2) hold. □

Lemma 4.3. *Let G be a cactus in $\mathcal{F}_3(n,b)$, where $n-b\geq 3$. Let H_1, H_2, G_1, G_2, and G_4 denote the graphs depicted in Figure 5. Then the upper bounds for $w^+Mo(G)$ and the corresponding extremal graphs are summarized in Table 1.*

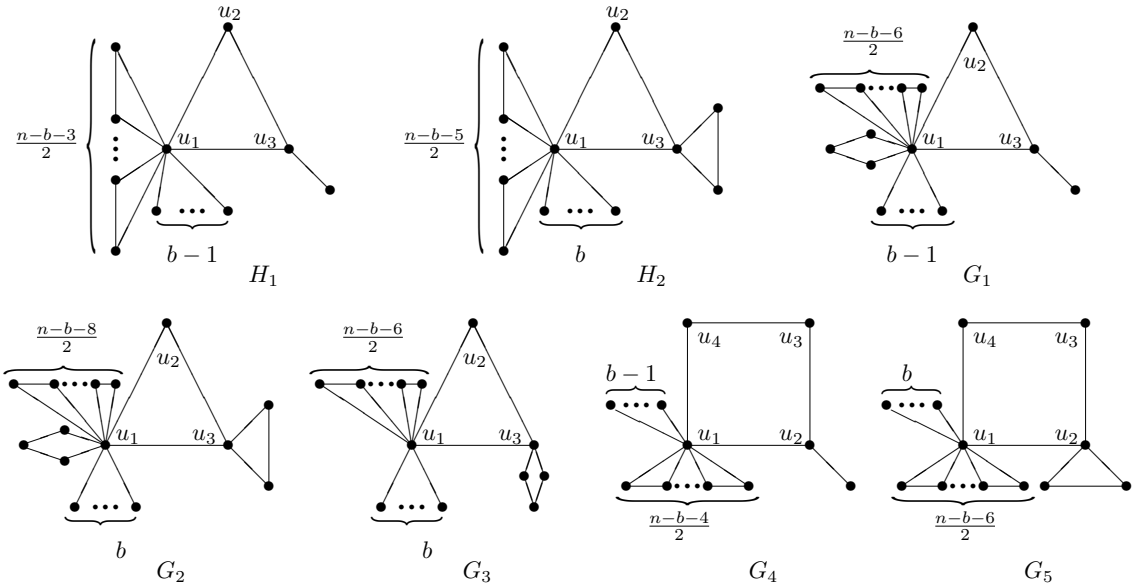


Figure 5. Graphs $H_1, H_2, G_1, G_2, G_3, G_4$, and G_5.

Table 1. The bounds of $w^+Mo(G)$ in Lemma 4.3.

Case	Parameter Conditions	Bound for $w^+Mo(G)$	Equality holds iff
$b \geq 1$	$n-b$ is odd, $n \geq 5$	$\leq n^3 - 5n^2 + 8n + 2b - 10$	$G \cong H_1$
	$n-b$ is even,(i) $n-b \geq 6, n \geq 10$, or(ii) $n-4 = b \geq 2$	$\leq n^3 - 7n^2 + 25n + b - 64$	$G \cong G_4$
	$n-b$ is even, $n-b \geq 6, n \leq 9$	$\leq n^3 - 7n^2 + 23n + b - 45$	$G \cong G_1$
$b = 0$	$n \geq 9$, n is odd	$< n^3 - 7n^2 + 27n - 69$	None
	$n \geq 9$, n is even	$< n^3 - 9n^2 + 44n - 108$	None
	$n = 8$	≤ 178	$G \cong G_2$
	$n = 7$	$= 120$	$G \cong H_2$

Proof. The case for $n = 7$ and $b = 0$ is trivial. In the following, we always assume $n \geq 8$ whenever $b = 0$. For integers n and b satisfying $n - b \geq 3$, let H denote a graph that achieves the maximum additively weighted Mostar index among all graphs in $\mathcal{F}_3(n, b)$. By Lemmas 2.1 and 2.3 together with Remark 2.1, the following structural properties hold for H: (i) H contains exactly one cycle that is not an end-block; (ii) all other cycles, if they exist, are of length 3 or 4; (iii) every cut edge in H is pendant, provided $b \geq 1$. Denote by l the length of the unique non-end-block cycle.

Suppose $l \geq 5$. Then $n - b \geq l$. Especially, $n \geq 9$ if $b = 0$.

First, suppose $n - b$ is odd. By Lemma 4.1, $w^+Mo(H) < n^3 - 7n^2 + 19n + b - 45$. Since $(n^3 - 7n^2 + 27n + b - 69) - (n^3 - 7n^2 + 19n + b - 45) = 8n - 24 > 0$ for $n \geq 9$, and $(n^3 - 5n^2 + 8n + 2b - 10) - (n^3 - 7n^2 + 19n + b - 45) = 2n^2 - 11n + b + 35 > 0$ for $n, b \geq 0$, it follows that $w^+Mo(H) < n^3 - 7n^2 + 27n + b - 69$ if $b = 0$, and $w^+Mo(H) < n^3 - 5n^2 + 8n + 2b - 10 = w^+Mo(H_1)$ if $b \geq 1$.

Next, suppose $n - b$ is even. Then Lemma 4.1 yields $w^+Mo(H) < n^3 - 9n^2 + 36n - 84$. Notice

that $(n^3 - 9n^2 + 44n - 108) - (n^3 - 9n^2 + 36n - 84) = 8n - 24 > 0$ for $n \geq 9$, and for $n, b \geq 0$, $(n^3 - 7n^2 + 25n + b - 64) - (n^3 - 9n^2 + 36n - 84) = 2n^2 - 11n + b + 20 > 0$ and $(n^3 - 7n^2 + 23n + b - 45) - (n^3 - 9n^2 + 36n - 84) = 2n^2 - 13n + b + 39 > 0$. It follows that $w^+Mo(H) < n^3 - 9n^2 + 44n - 108$ if $b = 0$, and $w^+Mo(H) < \min\{w^+Mo(G_4), w^+Mo(G_1)\} = \min\{n^3 - 7n^2 + 25n + b - 64, n^3 - 7n^2 + 23n + b - 45\}$ if $b \geq 1$. Therefore, the result holds whenever $l \geq 5$.

In what follows, we assume $l \in \{3, 4\}$. Let $C_l = u_1u_2 \cdots u_lu_1$ denote this cycle. For $i = 1, \ldots, l$, let t_i, q_i, and b_i denote, respectively, the number of triangles, quadrangles, and pendant edges attached at u_i in H. By Lemma 2.4, $q_i \in \{0, 1\}$. Define $n_i = b_i + 2t_i + 3q_i$ for $i = 1, \ldots, l$. For brevity, denote $d_H(u_i)$ by d_{u_i}. Then $d_{u_i} = b_i + 2t_i + 2q_i + 2$.

Case 1. $n - b$ is odd, $l = 4$.

Since $\sum_{i=1}^{4}(2t_i + 3q_i) = n - 4 - \sum_{i=1}^{4} b_i = n - 4 - b$, it follows that $3\sum_{i=1}^{4} q_i \equiv n - b \pmod 2$. Hence, $\sum_{i=1}^{4} q_i \in \{1, 3\}$. Combined with $l = 4$, this implies that H contains at least two quadrangles. Furthermore, $n - b \geq 7$. In particular, $n \geq 9$ when $b = 0$. By Remark 2.1 and Lemma 2.4, we obtain $w^+Mo(H) < w^+Mo(G_n^b(\underbrace{3, \ldots, 3}_{\frac{n-b-7}{2}}, 4, 4)) = n^3 - 7n^2 + 27n + b - 69$. Since $(n^3 - 5n^2 + 8n + 2b - 10) - (n^3 - 7n^2 + 27n + b - 69) = 2n^2 - 19n + b + 59 > 0$ for $n, b \geq 0$, we have $w^+Mo(H) < n^3 - 7n^2 + 27n + b - 69 < n^3 - 5n^2 + 8n + 2b - 10$ if $b \geq 1$ and $n - b \geq 7$. Therefore, the result holds in this case.

Case 2. $n - b$ is odd, $l = 3$.

Without loss of generality, assume $n_1 \geq n_3 \geq n_2$. If $b_3 \neq 0$ (respectively, $t_3 \neq 0$ or $q_3 \neq 0$), let G' (respectively, G'' or G''') denote the graph obtained from H by moving one cut edge (one triangle or one quadrangle) from u_3 to u_1, as illustrated in Figure 6. Then

$$\begin{aligned} w^+Mo(H) = {} & b_1(d_{u_1} + 1)(n - 2) + 2t_1(d_{u_1} + 2)(n - 3) + [2q_1(d_{u_1} + 2) + 8q_1](n - 4) \\ & + b_2(d_{u_2} + 1)(n - 2) + 2t_2(d_{u_2} + 2)(n - 3) + [2q_2(d_{u_2} + 2) + 8q_2](n - 4) \\ & + b_3(d_{u_3} + 1)(n - 2) + 2t_3(d_{u_3} + 2)(n - 3) + [2q_3(d_{u_3} + 2) + 8q_3](n - 4) \\ & + (d_{u_1} + d_{u_2})|n_1 - n_2| + (d_{u_2} + d_{u_3})|n_2 - n_3| + (d_{u_1} + d_{u_3})|n_1 - n_3|, \end{aligned}$$

$$\begin{aligned} w^+Mo(G') = {} & (b_1 + 1)(d_{u_1} + 2)(n - 2) + 2t_1(d_{u_1} + 3)(n - 3) + [2q_1(d_{u_1} + 3) + 8q_1](n - 4) \\ & + b_2(d_{u_2} + 1)(n - 2) + 2t_2(d_{u_2} + 2)(n - 3) + [2q_2(d_{u_2} + 2) + 8q_2](n - 4) \\ & + (b_3 - 1)d_{u_3}(n - 2) + 2t_3(d_{u_3} + 1)(n - 3) + [2q_3(d_{u_3} + 1) + 8q_3](n - 4) \\ & + (d_{u_1} + d_{u_2} + 1)|n_1 + 1 - n_2| + (d_{u_2} + d_{u_3} - 1)|n_2 - n_3 + 1| + (d_{u_1} + d_{u_3})|n_1 + 1 - n_3 + 1|, \end{aligned}$$

$$\begin{aligned} w^+Mo(G'') = {} & b_1(d_{u_1} + 3)(n - 2) + 2(t_1 + 1)(d_{u_1} + 4)(n - 3) + [2q_1(d_{u_1} + 4) + 8q_1](n - 4) \\ & + b_2(d_{u_2} + 1)(n - 2) + 2t_2(d_{u_2} + 2)(n - 3) + [2q_2(d_{u_2} + 2) + 8q_2](n - 4) \\ & + b_3(d_{u_3} - 1)(n - 2) + 2(t_3 - 1)d_{u_3}(n - 3) + (2q_3d_{u_3} + 8q_3)(n - 4) \\ & + (d_{u_1} + d_{u_2} + 2)|n_1 + 2 - n_2| + (d_{u_2} + d_{u_3} - 2)|n_2 - n_3 + 2| + (d_{u_1} + d_{u_3})|n_1 + 2 - n_3 + 2|, \end{aligned}$$

$$\begin{aligned} w^+Mo(G''') = {} & b_1(d_{u_1} + 3)(n - 2) + 2t_1(d_{u_1} + 4)(n - 3) + [2(q_1 + 1)(d_{u_1} + 4) + 8(q_1 + 1)](n - 4) \\ & + b_2(d_{u_2} + 1)(n - 2) + 2t_2(d_{u_2} + 2)(n - 3) + [2q_2(d_{u_2} + 2) + 8q_2](n - 4) \\ & + b_3(d_{u_3} - 1)(n - 2) + 2t_3d_{u_3}(n - 3) + [2(q_3 - 1)d_{u_3} + 8(q_3 - 1)](n - 4) \\ & + (d_{u_1} + d_{u_2} + 2)|n_1 + 3 - n_2| + (d_{u_2} + d_{u_3} - 2)|n_2 - n_3 + 3| + (d_{u_1} + d_{u_3})|n_1 + 3 - n_3 + 3|. \end{aligned}$$

Since $n_1 \geq n_3 \geq n_2$ and $q_i \in \{0, 1\}$, it follows that $d_{u_1} - d_{u_3} = n_1 - n_3 + q_3 - q_1 \geq -1$, $|n_1 + i - n_2| - |n_2 - n_3 + i| \geq 0$, and $|n_2 - n_3 + i| - |n_2 - n_3| \geq -i$ for $i = 1, 2, 3$. Therefore,

$$
\begin{aligned}
&w^+Mo(G') - w^+Mo(H)\\
&= b_1(n-2) + (d_{u_1}+2)(n-2) + 2t_1(n-3) + 2q_1(n-4) - b_3(n-2) - d_{u_3}(n-2) - 2t_3(n-3) - 2q_3(n\\
&\quad - 4) + d_{u_1} + d_{u_2} + |n_1 + 1 - n_2| - |n_2 - n_3 + 1| + (d_{u_2} + d_{u_3})(|n_2 - n_3 + 1| - |n_2 - n_3|) + 2(d_{u_1} + d_{u_3})\\
&= (n-4)\left[(b_1 + 2t_1 + 3q_1) - (b_3 + 2t_3 + 3q_3)\right] + \left[2b_1 + 2t_1 - q_1(n-4)\right] - \left[2b_3 + 2t_3 - q_3(n-4)\right]\\
&\quad + (d_{u_1} - d_{u_3})(n-2) + 2(n-2) + 3d_{u_1} + d_{u_2} + 2d_{u_3} + |n_1 + 1 - n_2| - |n_2 - n_3 + 1|\\
&\quad + (d_{u_2} + d_{u_3})(|n_2 - n_3 + 1| - |n_2 - n_3|)\\
&\geq (n-4)(n_1 - n_3) + (q_3 - q_1)(n-4) + 2(b_1 - b_3) + 2(t_1 - t_3) - (n-2) + 2(n-2) + 3d_{u_1} + d_{u_2} + 2d_{u_3}\\
&\quad - (d_{u_2} + d_{u_3})\\
&= (n_1 - n_3)(n-4) + (q_3 - q_1)(n-4) + 2(b_1 - b_3) + 2(t_1 - t_3) + (n-2) + 3d_{u_1} + d_{u_3}\\
&\geq 0 - (n-4) + (n-2) + (5b_1 + 8t_1 + 6q_1 - b_3 + 2q_3 + 8)\\
&= (5b_1 + 8t_1 + 6q_1) - (b_3 - 2q_3) + 10 \geq 2n_1 - n_3 + 10 > 0,
\end{aligned}
$$

$$
\begin{aligned}
&w^+Mo(G'') - w^+Mo(H)\\
&= 2b_1(n-2) + 2(d_{u_1}+4)(n-3) + 4t_1(n-3) + 4q_1(n-4) - 2b_3(n-2) - 2d_{u_3}(n-3) - 4t_3(n-3)\\
&\quad - 4q_3(n-4) + 2(d_{u_1} + d_{u_2}) + 2(|n_1 + 2 - n_2| - |n_2 - n_3 + 2|) + (d_{u_2} + d_{u_3})(|n_2 - n_3 + 2| - |n_2 - n_3|)\\
&\quad + 4(d_{u_1} + d_{u_3})\\
&= 2(n-4)\left[(b_1 + 2t_1 + 3q_1) - (b_3 + 2t_3 + 3q_3)\right] + 2\left[2b_1 + 2t_1 - q_1(n-4)\right] - 2[2b_3 + 2t_3 - q_3(n-4)]\\
&\quad + 2(d_{u_1} - d_{u_3})(n-3) + 8(n-3) + 6d_{u_1} + 2d_{u_2} + 4d_{u_3} + 2(|n_1 + 2 - n_2| - |n_2 - n_3 + 2|)\\
&\quad + (d_{u_2} + d_{u_3})(|n_2 - n_3 + 2| - |n_2 - n_3|)\\
&\geq 2(n-4)(n_1 - n_3) + 2(q_3 - q_1)(n-4) + 4(b_1 - b_3) + 4(t_1 - t_3) - 2(n-3) + 8(n-3) + 6d_{u_1} + 2d_{u_2}\\
&\quad + 4d_{u_3} - 2(d_{u_2} + d_{u_3})\\
&\geq 2(n_1 - n_3)(n-4) - 2(n-4) + 6(n-3) + 4(b_1 - b_3) + 4(t_1 - t_3) + 6d_{u_1} + 2d_{u_3}\\
&\geq 2 \times 0 + 4n - 10 + (10b_1 + 16t_1 + 12q_1 - 2b_3 + 4q_3 + 16)\\
&= 4n + 6 + (10b_1 + 16t_1 + 12q_1) - (2b_3 - 4q_3) \geq 4n + 6 + 4n_1 - 2n_3 > 0,
\end{aligned}
$$

$$
\begin{aligned}
&w^+Mo(G''') - w^+Mo(H)\\
&= 2b_1(n-2) + 2(d_{u_1}+4)(n-4) + 4t_1(n-3) + 4q_1(n-4) + 8(n-4) - 2b_3(n-2) - 2d_{u_3}(n-4)\\
&\quad - 4t_3(n-3) - 4q_3(n-4) - 8(n-4) + 3(d_{u_1} + d_{u_2}) + 2(|n_1 + 3 - n_2| - |n_2 - n_3 + 3|) + (d_{u_2} +\\
&\quad d_{u_3})(|n_2 - n_3 + 3| - |n_2 - n_3|) + 6(d_{u_1} + d_{u_3})\\
&= 2(n-4)[(b_1 + 2t_1 + 3q_1) - (b_3 + 2t_3 + 3q_3)] + 2[2b_1 + 2t_1 - q_1(n-4)] - 2[2b_3 + 2t_3 - q_3(n-4)]\\
&\quad + 2(d_{u_1} - d_{u_3})(n-4) + 8(n-4) + 9d_{u_1} + 3d_{u_2} + 6d_{u_3} + 2(|n_1 + 3 - n_2| - |n_2 - n_3 + 3|)\\
&\quad + (d_{u_2} + d_{u_3})(|n_2 - n_3 + 3| - |n_2 - n_3|)\\
&\geq 2(n-4)(n_1 - n_3) + 2(q_3 - q_1)(n-4) + 4(b_1 - b_3) + 4(t_1 - t_3) - 2(n-4) + 8(n-4) + 9d_{u_1} + 3d_{u_2}\\
&\quad + 6d_{u_3} - 3(d_{u_2} + d_{u_3})\\
&\geq 2(n_1 - n_3)(n-4) - 2(n-4) + 6(n-4) + 4(b_1 - b_3) + 4(t_1 - t_3) + 9d_{u_1} + 3d_{u_3}
\end{aligned}
$$

$\geq 2 \times 0 + 4(n-4) + (13b_1 + 22t_1 + 18q_1 + 18 - b_3 + 2t_3 + 6q_3 + 6)$

$= 4(n+2) + (13b_1 + 22t_1 + 18q_1) - (b_3 - 2t_3 - 6q_3) \geq 4(n+2) + 6n_1 - n_3 > 0.$

By the above transformations and the maximality of H, we deduce that $n_2 = 0$ and $b_3 + t_3 + q_3 = 1$ in H.

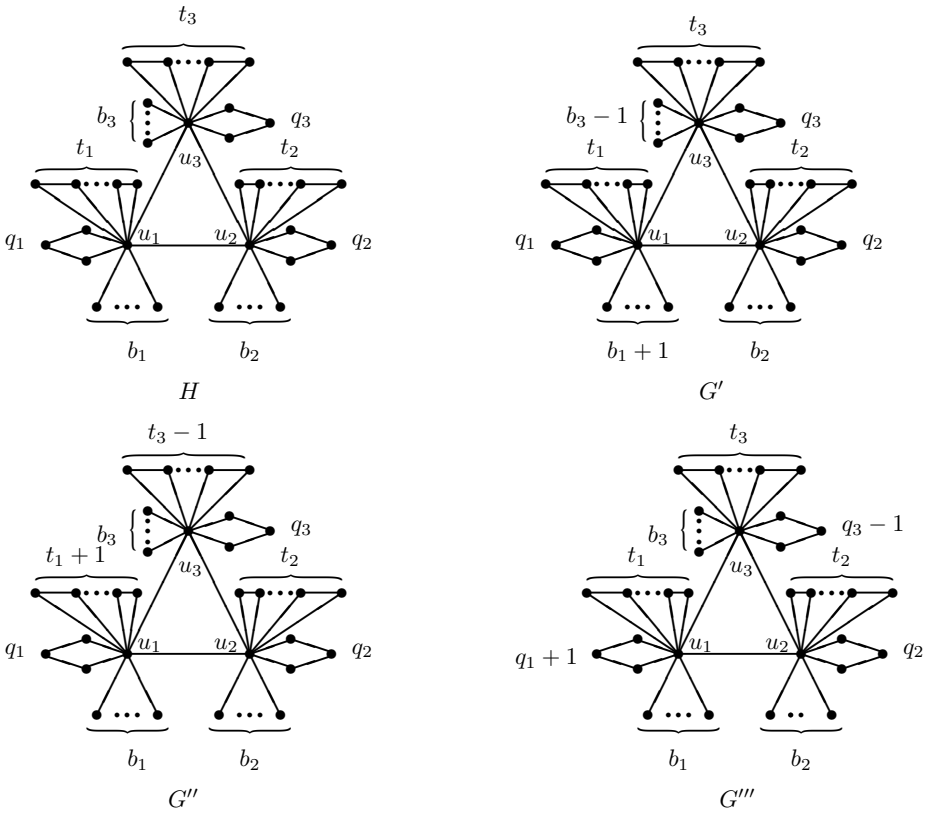


Figure 6. Figures H, G', G'', and G''' in the proof of Case 2.

Subcase 2.1. $q_3 = 1$.

Since $n - b$ is odd, it follows that $q_1 = 1$, and thus $n - b \geq 9$. By Remark 2.1, $w^+Mo(H) < w^+Mo(G_n^b(\underbrace{3, \ldots, 3}_{\frac{n-b-7}{2}}, 4, 4)) = n^3 - 7n^2 + 27n + b - 69$ when $n - b \geq 9$. This indicates $w^+Mo(H) < n^3 - 7n^2 + 27n - 69$ if $b = 0$ and $n \geq 9$. Furthermore, since $(n^3 - 5n^2 + 8n + 2b - 10) - (n^3 - 7n^2 + 27n + b - 69) = 2n^2 - 19n + b + 59 > 0$ for $n, b \geq 0$, we have $w^+Mo(H) < n^3 - 7n^2 + 27n + b - 69 < n^3 - 5n^2 + 8n + 2b - 10 = w^+Mo(H_1)$ if $b \geq 1$ and $n - b \geq 9$.

Subcase 2.2. $q_3 = 0$.

As $n - b$ is odd, we have $q_1 = 0$. Then

$$H \cong \begin{cases} H_1, & \text{if } n - b = 3, n \geq 5, \\ H_1 \text{ or } H_2, & \text{if } n - 5 \geq b \geq 1, \\ H_2, & \text{if } b = 0 \text{ and } n \geq 9, \end{cases}$$

where H_1 and H_2 are shown in Figure 5. By direct calculation, we obtain

$w^+Mo(H_1) = n^3 - 5n^2 + 8n + 2b - 10$ for $n - 3 \geq b \geq 1$ and $n \geq 5$,

$$w^+Mo(H_2) = \begin{cases} n^3 - 7n^2 + 23n + b - 41, & \text{if } n - 5 \geq b \geq 0, n \geq 7, \\ 76, & \text{if } n = 6, b = 1. \end{cases}$$

If $n - 5 \geq b \geq 1$, then

$$w^+Mo(H_1) - w^+Mo(H_2) = \begin{cases} 2n^2 - 15n + b + 31 > 0, & \text{if } n \geq 7, \\ 0, & \text{if } n = 6, b = 1. \end{cases}$$

This implies that $w^+Mo(H_1) \geq w^+Mo(H_2)$, with equality if and only if $n = 6,\ b = 1$ (in which case $H_1 \cong H_2$). Hence, $H \cong H_1$.

If $b = 0$ and $n \geq 9$, then $w^+Mo(H) = w^+Mo(H_2) = n^3 - 7n^2 + 23n - 41$. Since $(n^3 - 7n^2 + 27n - 69) - (n^3 - 7n^2 + 23n - 41) = 4n - 28 > 0$ for $n \geq 9$, it follows that $w^+Mo(H) < n^3 - 7n^2 + 27n - 69$ if $b = 0$ and $n \geq 9$.

In summary, under the assumptions that $n - b$ is odd and $l = 3$, the maximality of H implies (i) if $n - 3 \geq b \geq 1$ and $n \geq 5$, then $q_3 = 0$ and hence $H \cong H_1$; (ii) if $b = 0$ and $n \geq 9$, then $w^+Mo(H) < n^3 - 7n^2 + 27n + b - 69$.

Combining the analysis of Case 1 and Case 2, we conclude that if $n - b$ is odd, then the maximality of H implies $l = 3$, and hence $H \cong H_1$ for $n - 3 \geq b \geq 1$ and $n \geq 5$. Besides, if $b = 0$ and $n \geq 9$, then $w^+Mo(H) < n^3 - 7n^2 + 27n + b - 69$. Consequently, the result holds if $n - b$ is odd.

Case 3. $n - b$ is even, $l = 3$.

Without loss of generality, suppose $n_1 \geq n_3 \geq n_2$. Since $\sum_{i=1}^{3}(2t_i + 3q_i) = n - 3 - b$, it follows that $3(q_1 + q_2 + q_3 + 1) \equiv n - b \pmod 2$. Since $n - b$ is even, we deduce $q_1 + q_2 + q_3 \in \{1, 3\}$.

Subcase 3.1. $q_1 + q_2 + q_3 = 3$.

Then $n - b = 3 + \sum_{i=1}^{3}(2t_i + 3q_i) \geq 12$. By Remark 2.1, $w^+Mo(H) < w^+Mo(G_n^b(\underbrace{3, \ldots, 3}_{\frac{n-b-10}{2}}, 4, 4, 4) = n^3 - 9n^2 + 44n - 108$. Furthermore, since $(n^3 - 7n^2 + 23n + b - 45) - (n^3 - 9n^2 + 44n - 108) = 2n^2 - 21n + b + 63 > 0$ for $n, b \geq 0$, we have $w^+Mo(H) < n^3 - 7n^2 + 23n + b - 45 = w^+Mo(G_1)$ if $b \geq 1$.

Subcase 3.2. $q_1 + q_2 + q_3 = 1$.

Applying the transformations illustrated in Figure 6, we obtain $n_2 = 0$ and $b_3 + t_3 + q_3 = 1$ in H. Consequently,

$$H \cong \begin{cases} G_1, G_2 \text{ or } G_3, & \text{if } b \geq 1, n - b \geq 8, \\ G_1 \text{ or } G_3, & \text{if } b \geq 1, n - b = 6, \\ G_2 \text{ or } G_3, & \text{if } b = 0, n \geq 10, \\ G_2 \cong G_3, & \text{if } b = 0, n = 8, \end{cases}$$

where G_1, G_2, and G_3 are shown in Figure 5. Direct computation gives

$w^+Mo(G_1) = n^3 - 7n^2 + 23n + b - 45$ for $n - b \geq 6,\ b \geq 1$,

$w^+Mo(G_2) = n^3 - 9n^2 + 40n - 78$ for $n - b \geq 8,\ b \geq 0$,

$$w^+Mo(G_3) = \begin{cases} n^3 - 9n^2 + 36n - 86, & \text{if } n - b \geq 6, n \geq 9, \\ n^3 - 11n^2 + 57n - 86, & \text{if } n - b \geq 6, n < 9. \end{cases}$$

If $b \geq 1$ and $n - b \geq 8$, then $w^+Mo(G_1) - w^+Mo(G_2) = (2n-11)(n-3) + b > 0$ and $w^+Mo(G_2) - w^+Mo(G_3) = 4n + 8 > 0$. By the maximality of H, $H \cong G_1$.

If $b \geq 1$ and $n - b = 6$, then

$$w^+Mo(G_1) - w^+Mo(G_3) = \begin{cases} 2n^2 - 13n + b + 41 > 0, & \text{if } n \geq 9, \\ 27, & \text{if } n = 8, b = 2, \\ 0, & \text{if } n = 7, b = 1. \end{cases}$$

This indicates that $w^+Mo(G_1) \geq w^+Mo(G_3)$, with equality if and only if $n = 7, b = 1$ (in which case $G_3 \cong G_1$). Therefore, $H \cong G_1$.

If $b = 0$, $n \geq 10$, then $w^+Mo(G_2) - w^+Mo(G_3) = 4n + 8 > 0$ and hence $H \cong G_2$. Since $(n^3 - 9n^2 + 44n - 108) - w^+Mo(G_2) = 4n - 30 > 0$, we have $w^+Mo(H) = w^+Mo(G_2) < n^3 - 9n^2 + 44n - 108$.

In summary, under the assumptions that $n - b$ is even and $l = 3$, the maximality of H implies (i) if $b \geq 1$ and $n - b \geq 6$, then $q_1 + q_2 + q_3 = 1$ and hence $H \cong G_1$; (ii) if $b = 0$ and $n \geq 10$, then $w^+Mo(H) < n^3 - 9n^2 + 44n - 108$; (iii) if $b = 0$ and $n = 8$, then $H \cong G_2$ with $w^+Mo(H) = 178$.

Case 4. $n - b$ is even, $l = 4$.

From the equality $\sum_{i=1}^{4}(2t_i + 3q_i) = n - 4 - b$, it follows that $3\sum_{i=1}^{4} q_i \equiv n - b \pmod 2$. Since $n - b$ is even, we obtain $\sum_{i=1}^{4} q_i \in \{0, 2, 4\}$.

Subcase 4.1. $q_1 + q_2 + q_3 + q_4 = 2$ or 4.

Then $n - b = 4 + \sum_{i=1}^{4}(2t_i + 3q_i) \geq 4 + 3 \cdot 2 = 10$, and hence H contains exactly 3 or 5 quadrangles. By Remark 2.1 and Lemma 2.4, $w^+Mo(H) < w^+Mo(G_n^b(\underbrace{3, \ldots, 3}_{\frac{n-b-10}{2}}, 4, 4, 4)) = n^3 - 9n^2 + 44n - 108$. Notice that if $b \geq 1$, then $(n^3 - 7n^2 + 25n + b - 64) - (n^3 - 9n^2 + 44n - 108) = 2n^2 - 19n + b + 44 = (2n-11)(n-4) + b > 0$. Thus, $w^+Mo(H) < n^3 - 9n^2 + 44n - 108 < n^3 - 7n^2 + 25n + b - 64 = w^+Mo(G_4)$ if $b \geq 1$.

Subcase 4.2. $q_1 + q_2 + q_3 + q_4 = 0$.

Then $q_i = 0$ for all $i \in \{1, 2, 3, 4\}$. Consequently, $n_i = b_i + 2t_i$ and $d_{u_i} = n_i + 2$ for $i = 1, 2, 3, 4$. Without loss of generality, assume $n_1 \geq n_3$. By symmetry, we can further assume that $n_2 \geq n_4$ and $n_1 \geq n_2$.

Define $\mathcal{A} = |n_1 + n_2 + 2 - (n_3 + n_4)| - |n_1 + n_2 - (n_3 + n_4)| + |n_1 + n_4 + 2 - (n_2 + n_3)| - |n_1 + n_4 - (n_2 + n_3)|$ and $\mathcal{B} = |n_1 + n_2 + 4 - (n_3 + n_4)| - |n_1 + n_2 - (n_3 + n_4)| + |n_1 + n_4 + 4 - (n_2 + n_3)| - |n_1 + n_4 - (n_2 + n_3)|$.

We now prove the following claim.

Claim 1. $\mathcal{A}, \mathcal{B} \geq 0$

Proof of Claim 1. We verify $\mathcal{A} \geq 0$ case by case under the assumptions $n_1 \geq n_3$, $n_2 \geq n_4$, and $n_1 \geq n_2$.

(i) $n_1 + n_2 \geq n_3 + n_4$, $n_1 + n_4 \geq n_2 + n_3$.

Then $\mathcal{A} = (n_1 + n_2 + 2 - n_3 - n_4) - (n_1 + n_2 - n_3 - n_4) + (n_1 + n_4 + 2 - n_2 - n_3) - (n_1 + n_4 - n_2 - n_3) = 4$.

(ii) $n_1 + n_2 \geq n_3 + n_4$, $n_2 + n_3 > n_1 + n_4 \geq n_2 + n_3 - 2$.

Then $\mathcal{A} = (n_1 + n_2 + 2 - n_3 - n_4) - (n_1 + n_2 - n_3 - n_4) + (n_1 + n_4 + 2 - n_2 - n_3) - (n_2 + n_3 - n_1 - n_4) = 2 + 2(n_1 + n_4) - 2(n_2 + n_3) + 2 \geq 2 + 2 \times (-2) + 2 = 0$.

(iii) $n_1 + n_2 \geq n_3 + n_4$, $n_1 + n_4 < n_2 + n_3 - 2$.

Then $\mathcal{A} = (n_1 + n_2 + 2 - n_3 - n_4) - (n_1 + n_2 - n_3 - n_4) + (n_2 + n_3 - n_1 - n_4 - 2) - (n_2 + n_3 - n_1 - n_4) = 2 - 2 = 0$.

In all cases, $\mathcal{A} \geq 0$. By replacing the constant 2 with 4 throughout the above argument, we deduce $\mathcal{B} \geq 0$. This completes the proof of Claim 1.

Let G' (resp. G'') denote the graph obtained from H by moving one cut edge (resp. one triangle) from vertex u_3 to vertex u_1, provided that $b_3 \neq 0$ (resp. $t_3 \neq 0$); see Figure 7. Then

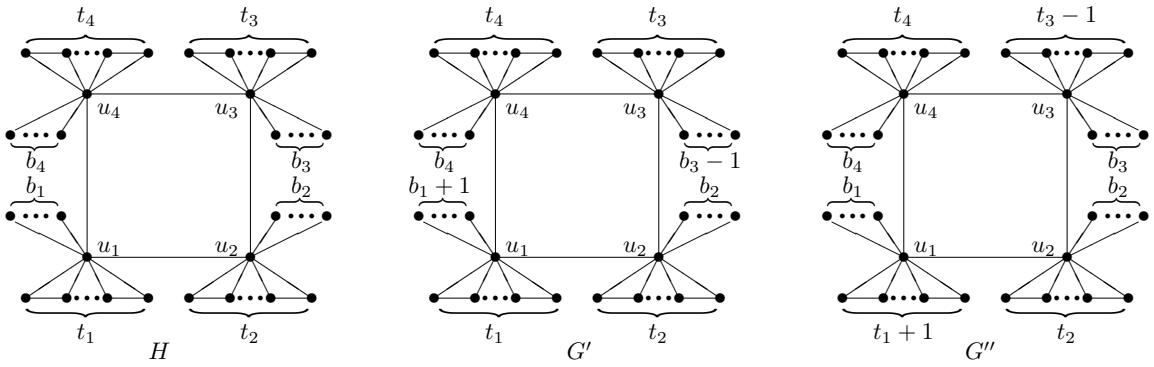


Figure 7. Graphs H, G', and G'' in the proof of Case 4.

$$\begin{aligned} w^+Mo(H) = {} & b_1(d_{u_1}+1)(n-2) + 2t_1(d_{u_1}+2)(n-3) + b_2(d_{u_2}+1)(n-2) + 2t_2(d_{u_2}+2)(n-3) \\ & + b_3(d_{u_3}+1)(n-2) + 2t_3(d_{u_3}+2)(n-3) + b_4(d_{u_4}+1)(n-2) + 2t_4(d_{u_4}+2)(n-3) \\ & + (d_{u_1}+d_{u_2})\,|n_1+n_4-(n_2+n_3)| + (d_{u_2}+d_{u_3})\,|n_1+n_2-(n_3+n_4)| \\ & + (d_{u_3}+d_{u_4})\,|n_1+n_4-(n_2+n_3)| + (d_{u_1}+d_{u_4})\,|n_1+n_2-(n_3+n_4)|\,, \end{aligned}$$

$$\begin{aligned} w^+Mo(G') = {} & (b_1+1)(d_{u_1}+2)(n-2) + 2t_1(d_{u_1}+3)(n-3) + b_2(d_{u_2}+1)(n-2) + 2t_2(d_{u_2}+2)(n-3) \\ & + (b_3-1)d_{u_3}(n-2) + 2t_3(d_{u_3}+1)(n-3) + b_4(d_{u_4}+1)(n-2) + 2t_4(d_{u_4}+2)(n-3) \\ & + (d_{u_1}+d_{u_2}+1)\,|n_1+n_4+2-(n_2+n_3)| + (d_{u_2}+d_{u_3}-1)\,|n_1+n_2+2-(n_3+n_4)| \\ & + (d_{u_3}+d_{u_4}-1)\,|n_1+n_4+2-(n_2+n_3)| + (d_{u_1}+d_{u_4}+1)\,|n_1+n_2+2-(n_3+n_4)|\,, \end{aligned}$$

$$\begin{aligned} w^+Mo(G'') = {} & b_1(d_{u_1}+3)(n-2) + 2(t_1+1)(d_{u_1}+4)(n-3) + b_2(d_{u_2}+1)(n-2) + 2t_2(d_{u_2}+2)(n-3) \\ & + b_3(d_{u_3}-1)(n-2) + 2(t_3-1)d_{u_3}(n-3) + b_4(d_{u_4}+1)(n-2) + 2t_4(d_{u_4}+2)(n-3) \\ & + (d_{u_1}+d_{u_2}+2)\,|n_1+n_4+4-n_2-n_3| + (d_{u_2}+d_{u_3}-2)\,|n_1+n_2+4-n_3-n_4| \\ & + (d_{u_3}+d_{u_4}-2)\,|n_1+n_4+4-n_2-n_3| + (d_{u_1}+d_{u_4}+2)\,|n_1+n_2+4-n_3-n_4|\,. \end{aligned}$$

By Claim 1,

$$\begin{aligned} & w^+Mo(G') - w^+Mo(H) \\ = {} & b_1(n-2) + (d_{u_1}+2)(n-2) + 2t_1(n-3) - b_3(n-2) - d_{u_3}(n-2) - 2t_3(n-3) + (d_{u_1}+d_{u_2}+d_{u_3}+ \\ & d_{u_4})[|n_1+n_2+2-(n_3+n_4)| - |n_1+n_2-(n_3+n_4)| + |n_1+n_4+2-(n_2+n_3)| - |n_1+n_4-(n_2+n_3)|] \\ = {} & (n-3)[(b_1+2t_1)-(b_3+2t_3)] + b_1 - b_3 + (d_{u_1}-d_{u_3})(n-2) + 2(n-2) + (d_{u_1}+d_{u_2}+d_{u_3}+d_{u_4})\mathcal{A} \end{aligned}$$

$$
\begin{aligned}
&= (n-3)(n_1-n_3) + (n_1-n_3)(n-2) + 2(n-2) + b_1 - b_3 + (d_{u_1} + d_{u_2} + d_{u_3} + d_{u_4})\mathcal{A} \\
&\geq (n-3)(n_1-n_3) + (n_1-n_3)(n-2) + 2(n-2) + b_1 - b_3 \\
&\geq 2(n-2) + b_1 - b_3 > 0,
\end{aligned}
$$

$$
\begin{aligned}
&w^+Mo(G'') - w^+Mo(H) \\
&= 2b_1(n-2) + 2(d_{u_1}+4)(n-3) + 4t_1(n-3) - 2b_3(n-2) - 2d_{u_3}(n-3) - 4t_3(n-3) + (d_{u_1} + d_{u_2} + d_{u_3} \\
&\quad + d_{u_4})[|n_1+n_2+4-n_3-n_4| - |n_1+n_2-(n_3+n_4)| + |n_1+n_4+4-n_2-n_3| - |n_1+n_4-(n_2+n_3)|] \\
&= 2(n-3)\left[(b_1+2t_1) - (b_3+2t_3)\right] + 2(b_1-b_3) + 2(d_{u_1}-d_{u_3})(n-3) + 8(n-3) \\
&\quad + (d_{u_1} + d_{u_2} + d_{u_3} + d_{u_4})\mathcal{B} \\
&\geq 2(n-3)(n_1-n_3) + 2(n_1-n_3)(n-3) + 8(n-3) + 2(b_1-b_3) \\
&\geq 8(n-3) + 2(b_1-b_3) > 0.
\end{aligned}
$$

Suppose $n_2 = 0$. Then $n_4 = 0$. By the transformations shown in Figure 7, exactly one pendant edge or exactly one triangle is incident to u_3. Consequently,

$$
H \cong \begin{cases} G_4', & \text{if } n = b+4 \geq 6, \\ G_4' \text{ or } G_5', & \text{if } n-b \geq 6, b \geq 1, \\ G_5', & \text{if } b = 0, n \geq 8, \end{cases}
$$

where G_4' and G_5' are shown in Figure 8. Direct computation yields

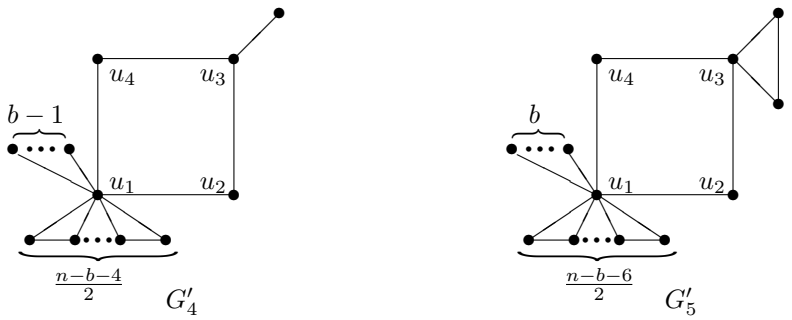


Figure 8. Figures G_4' and G_5'.

$$
w^+Mo(G_4') = n^3 - 7n^2 + 23n + b - 72 \text{ for } n-4 \geq b \geq 1 \text{ and } n \geq 6,
$$

$$
w^+Mo(G_5') = \begin{cases} n^3 - 9n^2 + 40n - 136, & \text{if } n-6 \geq b \geq 0, n \geq 8, \\ n^3 - 13n^2 + 56n - 8, & \text{if } n-6 \geq b \geq 0, n < 8. \end{cases}
$$

If $b \geq 1$ and $n - b \geq 6$, then

$$
w^+Mo(G_4') - w^+Mo(G_5') = \begin{cases} 2n^2 - 17n + b + 64 > 0, & \text{if } n-6 \geq b \geq 1, n \geq 8, \\ 0, & \text{if } n = 7, b = 1. \end{cases}
$$

This implies $w^+Mo(G_5') \leq w^+Mo(G_4')$, with equality if and only if $n = 7$, $b = 1$ (in which case $G_4' \cong G_5'$).

By the maximality of H, if $n-4 \geq b \geq 1$ and $n \geq 6$, then $H \cong G_4'$ and $w^+Mo(H) = n^3 - 7n^2 + 23n + b - 72 < w^+Mo(G_4) = n^3 - 7n^2 + 25n + b - 64$. If $b = 0$, $n \geq 10$, then $w^+Mo(H) = n^3 - 9n^2 + 40n - 136 < n^3 - 9n^2 + 44n - 108$. If $b = 0$, $n = 8$, then $H \cong G_5'$ and $w^+Mo(H) = 120$.

Now assume $n_2 > 0$. Applying the transformations in Figure 7 again yields $n_3 = n_4 = 0$, and the structure of H is depicted in Figure 9.

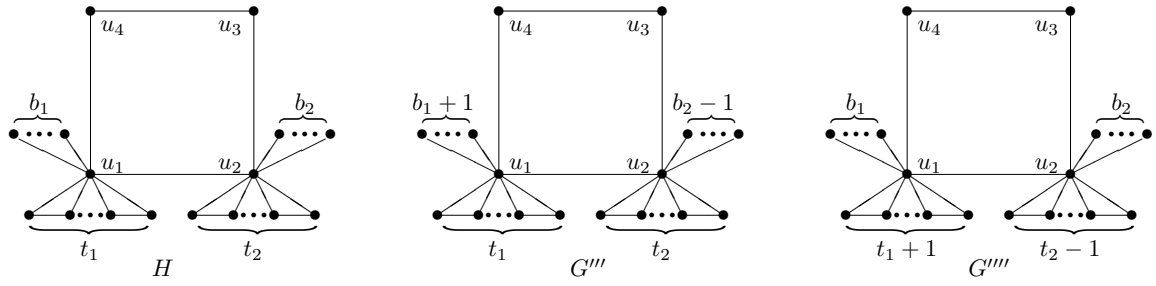


Figure 9. Figures H, G''', and G''''.

Let G''' (resp. G'''') denote the graph obtained from H by moving a cut edge (resp. a triangle) from u_2 to u_1, provided that $b_2 > 0$ (resp. $t_2 > 0$); see Figure 9. Then

$$\begin{aligned} w^+Mo(H) = {} & b_1(d_{u_1}+1)(n-2) + 2t_1(d_{u_1}+2)(n-3) + b_2(d_{u_2}+1)(n-2) + 2t_2(d_{u_2}+2)(n-3) \\ & + (d_{u_1}+d_{u_2})\,|n_1-n_2| + (d_{u_2}+d_{u_3})\,|(n_1+n_2+1)-1| + (d_{u_3}+d_{u_4})\,|n_1-n_2| \\ & + (d_{u_1}+d_{u_4})\,|(n_1+n_2+1)-1|\,, \end{aligned}$$

$$\begin{aligned} w^+Mo(G''') = {} & (b_1+1)(d_{u_1}+2)(n-2) + 2t_1(d_{u_1}+3)(n-3) + (b_2-1)d_{u_2}(n-2) \\ & + 2t_2(d_{u_2}+1)(n-3) + (d_{u_1}+d_{u_2})\,|(n_1+2)-n_2| + (d_{u_2}-1+d_{u_3})\,|(n_1+n_2+1)-1| \\ & + (d_{u_3}+d_{u_4})\,|(n_1+2)-n_2| + (d_{u_1}+1+d_{u_4})\,|(n_1+n_2+1)-1|\,, \end{aligned}$$

$$\begin{aligned} w^+Mo(G'''') = {} & b_1(d_{u_1}+3)(n-2) + 2(t_1+1)(d_{u_1}+4)(n-3) + b_2(d_{u_2}-1)(n-2) + 2(t_2 \\ & - 1)d_{u_2}(n-3) + (d_{u_1}+d_{u_2})\,|(n_1+3)-(n_2-1)| + (d_{u_2}-2+d_{u_3})\,|(n_1+n_2+1)-1| \\ & + (d_{u_3}+d_{u_4})\,|(n_1+3)-(n_2-1)| + (d_{u_1}+2+d_{u_4})\,|(n_1+n_2+1)-1|\,. \end{aligned}$$

Therefore,

$$\begin{aligned} & w^+Mo(G''') - w^+Mo(H) \\ = {} & b_1(n-2) + (d_{u_1}+2)(n-2) + 2t_1(n-3) - b_2(n-2) - d_{u_2}(n-2) - 2t_2(n-3) + (d_{u_1}+d_{u_2} \\ & + d_{u_3}+d_{u_4})\,[|n_1+2-n_2| - |n_1-n_2|] \\ = {} & (n-3)\,[(b_1+2t_1)-(b_2+2t_2)] + b_1 - b_2 + (d_{u_1}-d_{u_2}+2)(n-2) + 2(d_{u_1}+d_{u_2}+d_{u_3}+d_{u_4}) \\ > {} & (n-3)(n_1-n_2) + (n_1-n_2+2)(n-2) + b_1 - b_2 \\ \geq {} & 2(n-2) + b_1 - b_2 > 0, \end{aligned}$$

$$
\begin{aligned}
&w^+Mo(G'''') - w^+Mo(H)\\
&= 2b_1(n-2) + 2(d_{u_1}+4)(n-3) + 4t_1(n-3) - 2b_2(n-2) - 2d_{u_2}(n-3) - 4t_2(n-3) + (d_{u_1}+d_{u_2}\\
&\quad + d_{u_3}+d_{u_4})\,[|n_1+3-(n_2-1)| - |n_1-n_2|]\\
&= 2(n-3)\,[(b_1+2t_1)-(b_2+2t_2)] + 2(b_1-b_2) + 2(d_{u_1}-d_{u_2}+4)(n-3) + 4(d_{u_1}+d_{u_2}+d_{u_3}+d_{u_4})\\
&> 2(n-3)(n_1-n_2) + 2(n_1-n_2+4)(n-3) + 2(b_1-b_2)\\
&\geq 8(n-3) + 2(b_1-b_2) > 0.
\end{aligned}
$$

By iteratively applying the graph transformations illustrated in Figure 9, we deduce that exactly one cut edge or exactly one triangle is incident to u_2, i.e.,

$$
H \cong \begin{cases} G_4, & \text{if } n = b+4 \geq 6,\\ G_4 \text{ or } G_5, & \text{if } n-6 \geq b \geq 1,\\ G_5, & \text{if } b = 0, n \geq 8, \end{cases}
$$

where G_4 and G_5 are depicted in Figure 5. Direct computation yields

$w^+Mo(G_4) = n^3 - 7n^2 + 25n + b - 64$ for $n-4 \geq b \geq 1$ and $n \geq 6$,

$$
w^+Mo(G_5) = \begin{cases} n^3 - 9n^2 + 44n - 120, & \text{if } n-6 \geq b, n \geq 8,\\ n^3 - 11n^2 + 52n - 56, & \text{if } n-6 \geq b, n < 8. \end{cases}
$$

If $n-6 \geq b \geq 1$, then

$$
w^+Mo(G_4) - w^+Mo(G_5) = \begin{cases} 2n^2 - 19n + b + 56 > 0, & \text{if } n \geq 8,\\ 0, & \text{if } n = 7, b = 1. \end{cases}
$$

This implies $w^+Mo(G_5) \leq w^+Mo(G_4)$, with equality if and only if $n = 7$, $b = 1$ (in which case $G_4 \cong G_5$).

By the maximality of H, if $n-4 \geq b \geq 1$ and $n \geq 6$, then $H \cong G_4$ and $w^+Mo(H) = n^3 - 7n^2 + 25n + b - 64$. If $b = 0$, $n \geq 10$, then $w^+Mo(H) = n^3 - 9n^2 + 44n - 120 < n^3 - 9n^2 + 44n - 108$. If $b = 0$, $n = 8$, then $H \cong G_5$ and $w^+Mo(H) = 168$.

In summary, under the assumptions that $n-b$ is even and $l = 4$, the maximality of H implies (i) if $n-4 \geq b \geq 1$ and $n \geq 6$, then $q_1 + q_2 + q_3 + q_4 = 0$, $n_2 > 0$, and thus $H \cong G_4$; (ii) if $b = 0$ and $n \geq 10$, then $w^+Mo(H) < n^3 - 9n^2 + 44n - 108$; (iii) if $b = 0$ and $n = 8$, then $w^+Mo(H) = \max\{120, 168\} = 168$ and thus $H \cong G_5$.

Observe that $w^+Mo(G_4) - w^+Mo(G_1) = 2n - 19$. Combining the analysis of Case 3 and Case 4, we conclude that if $n-b$ is even, then the maximality of H implies $H \cong G_1$ if $n-6 \geq b \geq 1$ and $n \leq 9$, and $H \cong G_4$ in the following two cases: (i) $n-6 \geq b \geq 1$ and $n \geq 10$, or (ii) $n-4 = b \geq 2$. Besides, if $b = 0$ and $n \geq 10$, then $w^+Mo(H) < n^3 - 9n^2 + 44n - 108$; if $b = 0$ and $n = 8$, then $w^+Mo(H) = \max\{178, 168\} = 178$ and thus $H \cong G_2$. Consequently, if $b = 0$ and $n = 8$, or $n-b$ is even, the result holds. This completes the proof. □

Lemma 4.4. *Let G be a cactus in $\mathcal{F}_4(n,b)$, where $n-3 \geq b \geq 1$. Let H_1', H_2', G_1', and G_2' denote the graphs illustrated in Figure 10.*

(1) If $b = 1$ and $n \geq 6$ is even, then $w^+Mo(G) \leq n^3 - 7n^2 + 23n + b - 43$, with equality if and only if $G \cong H'_2$.

(2) If $b = 1$ and $n \geq 7$ is odd, then $w^+Mo(G) \leq n^3 - 9n^2 + 40n - 82$, with equality if and only if $G \cong G'_2$.

(3) If $2 \leq b \leq n-3$ and $n-b$ is odd, then $w^+Mo(G) \leq n^3 - 5n^2 + 8n + 2b - 10$, with equality if and only if $G \cong H'_1$.

(4) If $2 \leq b \leq n-4$ and $n-b$ is even, then $w^+Mo(G) \leq n^3 - 7n^2 + 23n + b - 46$, with equality if and only if $G \cong G'_1$.

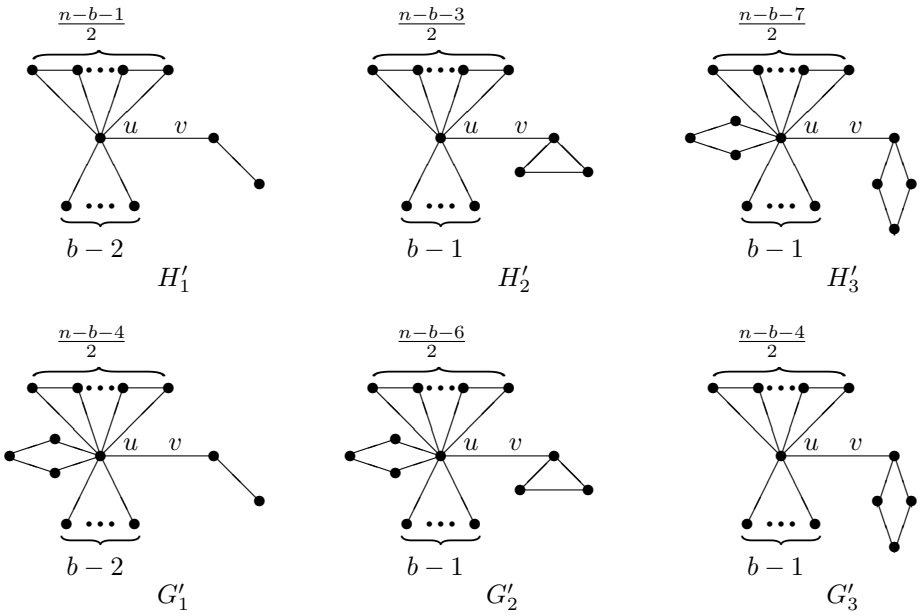


Figure 10. Figures $H'_1, H'_2, H'_3, G'_1, G'_2$, and G'_3.

Proof. Among the graphs in $\mathcal{F}_4(n, b)$, let H be one with the maximum additively weighted Mostar index. By Lemma 2.1, H contains exactly one such non-pendant cut edge, denoted by $e = uv$. Furthermore, by Remark 2.1 and Lemma 2.3, every cycle in H is an end-block and is of length 3 or 4.

Let t'_1, q'_1, and b'_1 (respectively, t'_2, q'_2, and b'_2) denote the number of triangles, quadrangles, and pendant edges incident to u (respectively, to v) in H. According to Lemma 2.4, $q'_i \in \{0, 1\}$ for $i = 1, 2$. The resulting structure of H is depicted in Figure 11. Define $n'_i = b'_i + 2t'_i + 3q'_i$ for $i = 1, 2$. For brevity, denote $d_H(u)$ and $d_H(v)$ by d_u and d_v, respectively. Then $d_u = b'_1 + 2t'_1 + 2q'_1 + 1$, $d_v = b'_2 + 2t'_2 + 2q'_2 + 1$.

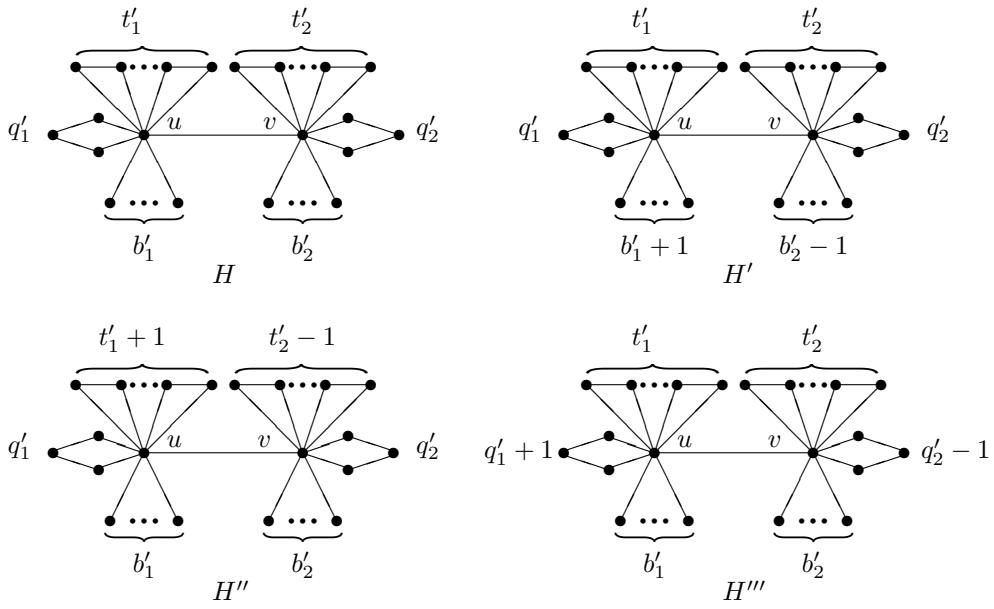


Figure 11. Graphs H, H', H'', and H''' in the proof of Lemma 4.4.

Without loss of generality, assume $n'_1 \geq n'_2$. Let H' (H'', H''') be the graph obtained from H by moving one pendant edge (one triangle, one quadrangle) from v to u, provided $b'_2 > 0$ ($t'_2 > 0$, $q'_2 > 0$); see Figure 11. By direct calculation, we get

$$\begin{aligned} w^+Mo(H) = {} & b'_1(d_u+1)(n-2) + 2t'_1(d_u+2)(n-3) + 2q'_1(d_u+2)(n-4) + 8q'_1(n-4) + b'_2(d_v+ \\ & 1)(n-2) + 2t'_2(d_v+2)(n-3) + 2q'_2(d_v+2)(n-4) + 8q'_2(n-4) + (d_u+d_v)(n'_1-n'_2), \end{aligned}$$

$$\begin{aligned} w^+Mo(H') = {} & (b'_1+1)(d_u+2)(n-2) + 2t'_1(d_u+3)(n-3) + 2q'_1(d_u+3)(n-4) + 8q'_1(n-4) \\ & + (b'_2-1)d_v(n-2) + 2t'_2(d_v+1)(n-3) + 2q'_2(d_v+1)(n-4) + 8q'_2(n-4) \\ & + (d_u+d_v)(n'_1-n'_2+2), \end{aligned}$$

$$\begin{aligned} w^+Mo(H'') = {} & b'_1(d_u+3)(n-2) + 2(t'_1+1)(d_u+4)(n-3) + 2q'_1(d_u+4)(n-4) + 8q'_1(n-4) \\ & + b'_2(d_v-1)(n-2) + 2(t'_2-1)d_v(n-3) + 2q'_2d_v(n-4) + 8q'_2(n-4) \\ & + (d_u+d_v)(n'_1-n'_2+4), \end{aligned}$$

$$\begin{aligned} w^+Mo(H''') = {} & b'_1(d_u+3)(n-2) + 2t'_1(d_u+4)(n-3) + 2(q'_1+1)(d_u+4)(n-4) + 8(q'_1+1)(n-4) \\ & + b'_2(d_v-1)(n-2) + 2t'_2d_v(n-3) + 2(q'_2-1)d_v(n-4) + 8(q'_2-1)(n-4) \\ & + (d_u+d_v)(n'_1-n'_2+6). \end{aligned}$$

Since $n'_1 \geq n'_2$ and $d_u - d_v = n'_1 - n'_2 + q'_2 - q'_1$, it follows that $d_u - d_v \geq q'_2 - q'_1 \geq -1$. Therefore,

$$\begin{aligned} & w^+Mo(H') - w^+Mo(H) \\ = {} & b'_1(n-2) + (d_u+2)(n-2) + 2t'_1(n-3) + 2q'_1(n-4) - b'_2(n-2) - d_v(n-2) - 2t'_2(n-3) \\ & - 2q'_2(n-4) + 2(d_u+d_v) \\ = {} & (d_u+2-d_v)(n-2) + b'_1(n-4) + 2t'_1(n-4) + 2q'_1(n-4) + 2b'_1 + 2t'_1 - b'_2(n-4) - 2t'_2(n-4) \end{aligned}$$

$$
\begin{aligned}
&\quad - 2q_2'(n-4) - 2b_2' - 2t_2' + 2(d_u + d_v)\\
&= (d_u + 2 - d_v)(n-2) + (n-4)(d_u - d_v) + 2(d_u + d_v + b_1' + t_1' - b_2' - t_2')\\
&\geq (-1+2)(n-2) + (n-4)(-1) + 2(d_u + b_1' + t_1' + d_v - b_2' - t_2')\\
&= 2 + 2(d_u + b_1' + t_1' + d_v - b_2' - t_2') > 0,
\end{aligned}
$$

$$
\begin{aligned}
&\quad w^+Mo(H'') - w^+Mo(H)\\
&= 2b_1'(n-2) + 2(d_u+4)(n-3) + 4t_1'(n-3) + 4q_1'(n-4) - 2b_2'(n-2) - 2d_v(n-3) - 4t_2'(n-3)\\
&\quad - 4q_2'(n-4) + 4(d_u + d_v)\\
&= 2(d_u + 4 - d_v)(n-3) + 2b_1'(n-4) + 4t_1'(n-3) + 4q_1'(n-4) + 4b_1' + 4t_1' - 2b_2'(n-4) - 4t_2'(n-4)\\
&\quad - 4q_2'(n-4) - 4b_2' - 4t_2' + 4(d_u + d_v)\\
&= 2(d_u + 4 - d_v)(n-3) + 2(n-4)(d_u - d_v) + 4(d_u + d_v + b_1' + t_1' - b_2' - t_2')\\
&\geq 2(-1+4)(n-3) + 2(n-4)(-1) + 4(d_u + b_1' + t_1' + d_v - b_2' - t_2')\\
&= 4n - 10 + 4(d_u + b_1' + t_1' + d_v - b_2' - t_2') > 0,
\end{aligned}
$$

$$
\begin{aligned}
&\quad w^+Mo(H''') - w^+Mo(H)\\
&= 2b_1'(n-2) + 4t_1'(n-3) + 4q_1'(n-4) + 2(d_u+4)(n-4) + 8(n-4) - b_2'(n-2) - 4t_2'(n-3)\\
&\quad - 4q_2'(n-4) - 2d_v(n-4) - 8(n-4) + 6(d_u + d_v)\\
&= 2(d_u + 4 - d_v)(n-4) + 2b_1'(n-4) + 4t_1'(n-4) + 4q_1'(n-4) + 4b_1' + 4t_1' - 2b_2'(n-4)\\
&\quad - 4t_2'(n-4) - 4q_2'(n-4) - 4b_2' - 4t_2' + 6(d_u + d_v)\\
&= 2(d_u + 4 - d_v)(n-4) + 2(n-4)(d_u - d_v) + 4(d_u + d_v + b_1' + t_1' - b_2' - t_2') + 2(d_u + d_v)\\
&\geq 2(-1+4)(n-4) + 2(n-4)(-1) + 4(d_u + b_1' + t_1' + d_v - b_2' - t_2') + 2(d_u + d_v)\\
&= 4(n-4) + 4(d_u + b_1' + t_1' + d_v - b_2' - t_2') + 2(d_u + d_v) > 0.
\end{aligned}
$$

By applying the graph transformations shown in Figure 11, we deduce that $b_2' + t_2' + q_2' = 1$ in H.

Case 1. $n - b$ is odd.

Since $q_1' \in \{0, 1\}$, it follows that

$$
H \cong \begin{cases} H_1', H_2' \text{ or } H_3', & \text{if } n - b \geq 7, b \geq 2,\\ H_2' \text{ or } H_3', & \text{if } n - b \geq 7, b = 1,\\ H_1' \text{ or } H_2', & \text{if } n - b = 3 \text{ or } 5, b \geq 2,\\ H_2', & \text{if } n = 6, b = 1, \end{cases}
$$

where H_1', H_2', and H_3' are depicted in Figure 10. Direct computation yields

$w^+Mo(H_1') = n^3 - 5n^2 + 8n + 2b - 10$ for $n - 1 \geq b \geq 2$ and $n \geq 4$,

$$
w^+Mo(H_2') = \begin{cases} n^3 - 7n^2 + 23n + b - 43, & \text{if } n - 3 \geq b \geq 1, n \geq 6,\\ 34, & \text{if } n = 5, b = 2, \end{cases}
$$

$w^+Mo(H_3') = n^3 - 11n^2 + 59n - b - 135$ for $n - 7 \geq b \geq 1$.

If $n-b \geq 7, b \geq 2$, then $w^+Mo(H_1') - w^+Mo(H_2') = 2n^2 - 15n + b + 33 > 0$ and $w^+Mo(H_2') - w^+Mo(H_3') = 4n^2 - 36n + 2b + 92 > 0$.

If $n-b \geq 7, b = 1$, then $w^+Mo(H_2') - w^+Mo(H_3') = 4n^2 - 36n + 2b + 92 > 0$.

If $n-b \in \{3,5\}, b \geq 2$, then

$$w^+Mo(H_1') - w^+Mo(H_2') = \begin{cases} 2n^2 - 15n + b + 33, & \text{if } n \geq 6, \\ 0, & \text{if } n = 5, b = 2. \end{cases}$$

This implies $w^+Mo(H_1') \geq w^+Mo(H_2')$, with equality if and only if $n = 5$, $b = 2$ (in which case $H_1' \cong H_2'$).

Therefore, under the assumption $n-b$ is odd, the maximality of H implies $H \cong H_1'$ if $b \geq 2$ and $n-b \geq 3$, and $H \cong H_2'$ if $b = 1$ and $n \geq 6$. Hence, statements (1) and (3) hold.

Case 2. $n-b$ is even.

Since $q_1' \in \{0,1\}$, it follows that

$$H \cong \begin{cases} G_1', G_2' \text{ or } G_3', & \text{if } n-b \geq 6, b \geq 2, \\ G_1' \text{ or } G_3', & \text{if } n-4 = b \geq 2, \\ G_2' \text{ or } G_3', & \text{if } b = 1, n \geq 7, \end{cases}$$

where G_1', G_2', and G_3' are depicted in Figure 10. Direct computation yields

$w^+Mo(G_1') = n^3 - 7n^2 + 23n + b - 46$ for $n-4 \geq b \geq 2$,

$w^+Mo(G_2') = n^3 - 9n^2 + 40n - 82$ for $n-6 \geq b \geq 1$,

$$w^+Mo(G_3') = \begin{cases} n^3 - 9n^2 + 40n - 94, & \text{if } n-4 \geq b \geq 1, n \geq 8, \\ n^3 - 11n^2 + 58n - 110, & \text{if } n-4 \geq b \geq 1, n < 8. \end{cases}$$

If $n-b \geq 6, b \geq 2$, then $w^+Mo(G_1') - w^+Mo(G_2') = (2n-9)(n-4) + b > 0$ and $w^+Mo(G_2') - w^+Mo(G_3') = 12 > 0$.

If $n-4 = b \geq 2$, then

$$w^+Mo(G_1') - w^+Mo(G_3') = \begin{cases} 2n^2 - 17n + b + 48 > 0, & \text{if } n \geq 8, \\ 0, & \text{if } n = 6, b = 2, \\ 18, & \text{if } n = 7, b = 3. \end{cases}$$

This implies that $w^+Mo(G_1') \geq w^+Mo(G_3')$, with equality if and only if $n = 6, b = 2$ (in which case $G_1' \cong G_3'$).

If $b = 1, n \geq 7$, then

$$w^+Mo(G_2') - w^+Mo(G_3') = \begin{cases} 12, & \text{if } n \geq 8, \\ 0, & \text{if } n = 7. \end{cases}$$

This implies that $w^+Mo(G_2') \geq w^+Mo(G_3')$, with equality if and only if $n = 7, b = 1$ (in which case $G_2' \cong G_3'$).

Consequently, under the assumption $n-b$ is even, the maximality of H implies $H \cong G_1'$ if $b \geq 2$ and $n-b \geq 4$, and $H \cong G_2'$ if $b = 1$ and $n \geq 7$. Thus, statements (2) and (4) hold. This completes the proof. □

By Lemmas 4.1–4.4, we easily obtain the following theorem.

Theorem 4.2. *Let $G \in C^*(n,b)$ be a graph with the maximum additively weighted Mostar index, where $0 \le b \le n-3$ and $n \ge 5$. Let $H_1, H_2, G_1, G_2, G_4, H_1'$, and G_1' denote the graphs depicted in Figures 5 and 10. Then the structure of G and the corresponding value of $w^+Mo(G)$ are summarized in Table 2.*

Table 2. Structure and $w^+Mo(G)$ of G in Theorem 4.2.

Case	Conditions	Structure of G	$w^+Mo(G)$
$b \ge 2$	$n-b$ is odd	H_1 or H_1'	$n^3-5n^2+8n+2b-10$
	$n-b$ is even, $n \ge 10$	G_4	$n^3-7n^2+25n+b-64$
	$(n,b) = (9,3)$ or $(8,2)$	G_1	$n^3-7n^2+23n+b-45$
	$(n,b) = (9,5)$	G_4 or G_1'	328
	$(n,b) = (6,2), (7,3)$ or $(8,4)$	G_1'	$n^3-7n^2+23n+b-46$
$b = 1$	n is even, $n \ge 6$	H_1	n^3-5n^2+8n-8
	$n = 7$ or 9	G_1	$n^3-7n^2+23n-44$
	n is odd, $n \ge 11$	G_4	$n^3-7n^2+25n-63$
$b = 0$	$n = 5$	C_5	0
	$n = 6$	C_6	0
	$n = 7$	$G_7^0(4,4)$ or H_2	120
	$n = 8$	G_2	178
	$n \ge 9$, n is odd	$G_n^0(\underbrace{3,\ldots,3}_{(n-7)/2},4,4)$	$n^3-7n^2+27n-69$
	$n \ge 10$, n is even	$G_n^0(\underbrace{3,\ldots,3}_{(n-10)/2},4,4,4)$	$n^3-9n^2+44n-108$

Proof. For $i = 1,2,3,4$, let $\mathcal{F}_i(n,b)$ be the families of cacti defined in Lemmas 4.1–4.4.

Case 1. $b \ge 2$ and $n-b$ is odd.

By Lemmas 4.1–4.4, the following hold:

- If $G \in \mathcal{F}_1(n,b)$, then $G \cong G_n^b(\underbrace{3,\ldots,3}_{(n-b-5)/2},5)$ with $n-b \ge 5$ and $w^+Mo(G) = n^3-7n^2+19n+b-45 \triangleq M_1$.
- If $G \in \mathcal{F}_2(n,b)$, then $G \cong G_n^b(\underbrace{3,\ldots,3}_{(n-b-7)/2},4,4)$ with $n-b \ge 7$ and $w^+Mo(G) = n^3-7n^2+27n+b-69 \triangleq M_2$.
- If $G \in \mathcal{F}_3(n,b)$, then $G \cong H_1$ and $w^+Mo(G) = n^3-5n^2+8n+2b-10 \triangleq M_3$.
- If $G \in \mathcal{F}_4(n,b)$, then $G \cong H_1'$ and $w^+Mo(G) = M_3$.

If $n-b = 3$, then $G \cong H_1$ or H_1'. If $n-b = 5$, then $G \cong G_n^b(\underbrace{3,\ldots,3}_{(n-b-5)/2},5)$, H_1, or H_1'. If $n-b \ge 7$, then $G \cong G_n^b(\underbrace{3,\ldots,3}_{(n-b-5)/2},5), G_n^b(\underbrace{3,\ldots,3}_{(n-b-7)/2},4,4), H_1,$ or H_1'.

Since $M_3 - M_2 = 2n^2 - 19n + b + 59 > 0$ and $M_3 - M_1 = 2n^2 - 11n + b + 35 > 0$ for any nonnegative integers n and b, it follows that $w^+Mo(G) = M_3 = n^3 - 5n^2 + 8n + 2b - 10$, and consequently $G \cong H_1$ or H_1'.

Case 2. $b \geq 2$ and $n - b$ is even.

By Lemmas 4.1–4.4, the following hold:

- If $G \in \mathcal{F}_1(n, b)$, then

$$G \cong \begin{cases} G_n^b(6), & \text{if } n - b = 6, \\ G_n^b(\underbrace{3, 3, \ldots, 3}_{(n-b-8)/2}, 4, 5), & \text{if } n - b \geq 8, \end{cases}$$

  and $w^+Mo(G) = M_1$, where

$$M_1 = \begin{cases} n^3 - 9n^2 + 36n - 108, & \text{if } n - b = 6, \\ n^3 - 9n^2 + 36n - 84, & \text{if } n - b \geq 8. \end{cases}$$

- If $G \in \mathcal{F}_2(n, b)$, then $G \cong G_n^b(\underbrace{3, \ldots, 3}_{(n-b-10)/2}, 4, 4, 4)$ with $n - b \geq 10$ and $w^+Mo(G) = n^3 - 9n^2 + 44n - 108 \triangleq M_2$.
- If $G \in \mathcal{F}_3(n, b)$, then

$$G \cong \begin{cases} G_4, & \text{if } n - b \geq 6 \text{ and } n \geq 10, \text{ or } n - b = 4, \\ G_1, & \text{if } n - b \geq 6 \text{ and } n \leq 9, \end{cases}$$

  and $w^+Mo(G) = M_3$, where

$$M_3 = \begin{cases} n^3 - 7n^2 + 25n + b - 64, & \text{if } n - b \geq 6 \text{ and } n \geq 10, \text{ or } n - b = 4, \\ n^3 - 7n^2 + 23n + b - 45, & \text{if } n - b \geq 6 \text{ and } n \leq 9. \end{cases}$$

- If $G \in \mathcal{F}_4(n, b)$, then $G \cong G_1'$ with $n - b \geq 4$ and $w^+Mo(G) = n^3 - 7n^2 + 23n + b - 46 \triangleq M_4$.

Now assume $n \geq 10$. If $n - b \geq 10$, then $G \cong G_n^b(\underbrace{3, 3, \ldots, 3}_{(n-b-8)/2}, 4, 5)$, $G_n^b(\underbrace{3, \ldots, 3}_{(n-b-10)/2}, 4, 4, 4)$, G_4, or G_1'. If $n - b = 8$, then $G \cong G_n^b(4, 5)$, G_4, or G_1'. If $n - b = 6$, then $G \cong G_n^b(6)$, G_4, or G_1'. If $n - b = 4$, then $G \cong G_4$ or G_1'.

Since $n \geq 10$, we have $M_3 = n^3 - 7n^2 + 25n + b - 64$. Moreover, $M_3 - M_1 \geq 2n^2 - 11n + b + 20 > 0$, $M_3 - M_2 = 2n^2 - 19n + b + 44 > 0$, and $M_3 - M_4 = 2n - 18 > 0$. Consequently, $w^+Mo(G) = M_3 = n^3 - 7n^2 + 25n + b - 64$ and $G \cong G_4$.

Next, consider the case $n \leq 9$. Since $n - 3 \geq b \geq 2$ and $n - b$ is even, we have

$$(n, b) \in \{(9, 3), (8, 2), (9, 5), (6, 2), (7, 3), (8, 4)\}.$$

If $(n, b) \in \{(9, 3), (8, 2)\}$, then $G \cong G_n^b(6)$, G_1, or G_1', with $M_1 = n^3 - 9n^2 + 36n - 108$, $M_3 = n^3 - 7n^2 + 23n + b - 45$, and $M_4 = n^3 - 7n^2 + 23n + b - 46$. Since $M_3 - M_1 = 2n^2 - 13n + b + 63 > 0$ and $M_3 > M_4$, it follows that $w^+Mo(G) = M_3 = n^3 - 7n^2 + 23n + b - 45$ and $G \cong G_1$.

If $(n,b) \in \{(9,5),(6,2),(7,3),(8,4)\}$, then $G \cong G_4$ or G_1', with $M_3 = n^3 - 7n^2 + 25n + b - 64$ and $M_4 = n^3 - 7n^2 + 23n + b - 46$. Direct computation yields $M_3 = M_4 = 328$ when $(n,b) = (9,5)$, and $M_3 - M_4 = 2n - 18 < 0$ when $(n,b) \in \{(6,2),(7,3),(8,4)\}$. Therefore, if $(n,b) = (9,5)$, then $w^+Mo(G) = 328$ and $G \cong G_4$ or G_1'; if $(n,b) \in \{(6,2),(7,3),(8,4)\}$, then $w^+Mo(G) = M_4 = n^3 - 7n^2 + 23n + b - 46$ and $G \cong G_1'$.

Case 3. $b = 1$.

Subcase 3.1. n is even.

By Lemmas 4.1–4.4, the following hold:

- If $G \in \mathcal{F}_1(n,b)$, then $G \cong G_n^1(\underbrace{3,\ldots,3}_{(n-6)/2},5)$ with $n \geq 6$ and $w^+Mo(G) = n^3 - 7n^2 + 19n - 44 \triangleq M_1$.
- If $G \in \mathcal{F}_2(n,b)$, then $G \cong G_n^1(\underbrace{3,\ldots,3}_{(n-8)/2},4,4)$ with $n \geq 8$ and $w^+Mo(G) = n^3 - 7n^2 + 27n - 68 \triangleq M_2$.
- If $G \in \mathcal{F}_3(n,b)$, then $G \cong H_1$ with $n \geq 6$ and $w^+Mo(G) = n^3 - 5n^2 + 8n - 8 \triangleq M_3$.
- If $G \in \mathcal{F}_4(n,b)$, then $G \cong H_2'$ with $n \geq 6$ and $w^+Mo(G) = n^3 - 7n^2 + 23n - 42 \triangleq M_4$.

Based on the above, if $n = 6$, then $G \cong G_6^1(5), H_1$, or H_2'; if $n \geq 8$, then $G \cong G_n^1(\underbrace{3,\ldots,3}_{(n-6)/2},5), G_n^1(\underbrace{3,\ldots,3}_{(n-8)/2},4,4), H_1$, or H_2'. Since for any integer n, $M_3 - M_1 = 2n^2 - 11n + 36 > 0$, $M_3 - M_2 = 2n^2 - 19n + 60 > 0$, and $M_3 - M_4 = 2n^2 - 15n + 34 > 0$, it follows that $w^+Mo(G) = M_3 = n^3 - 5n^2 + 8n - 8$ and $G \cong H_1$.

Subcase 3.2. n is odd.

By Lemmas 4.1–4.4, the following hold:

- If $G \in \mathcal{F}_1(n,b)$, then

$$G \cong \begin{cases} G_7^1(6), & \text{when } n = 7, \\ G_n^1(\underbrace{3,\ldots,3}_{(n-9)/2},4,5), & \text{when } n \geq 9, \end{cases}$$

  and $w^+Mo(G) = M_1$, where

$$M_1 = \begin{cases} n^3 - 9n^2 + 36n - 108, & \text{when } n = 7, \\ n^3 - 9n^2 + 36n - 84, & \text{when } n \geq 9. \end{cases}$$

- If $G \in \mathcal{F}_2(n,b)$, then $G \cong G_n^1(\underbrace{3,\ldots,3}_{(n-11)/2},4,4,4)$ with $n \geq 11$ and $w^+Mo(G) = n^3 - 9n^2 + 44n - 108 \triangleq M_2$.
- If $G \in \mathcal{F}_3(n,b)$, then

$$G \cong \begin{cases} G_4, & \text{when } n \geq 11, \\ G_1, & \text{when } n \in \{7,9\}, \end{cases}$$

  and $w^+Mo(G) = M_3$, where

$$M_3 = \begin{cases} n^3 - 7n^2 + 25n - 63, & \text{when } n \geq 11, \\ n^3 - 7n^2 + 23n - 44, & \text{when } n \in \{7,9\}. \end{cases}$$

- If $G \in \mathcal{F}_4(n, b)$, then $G \cong G_2'$ with $n \geq 7$ and $w^+Mo(G) = n^3 - 9n^2 + 40n - 82 \triangleq M_4$.

Based on the above, if $n = 7$, then $G \cong G_7^1(6)$, G_1, or G_2'; if $n = 9$, then $G \cong G_9^1(4, 5)$, G_1, or G_2'.

For $n \in \{7, 9\}$, we have $M_3 - M_1 \geq 2n^2 - 13n + 40 > 0$ and $M_3 - M_4 = 2n^2 - 17n + 38 > 0$. Hence, $w^+Mo(G) = M_3 = n^3 - 7n^2 + 23n - 44$ and $G \cong G_1$.

If $n \geq 11$, then $G \cong G_n^1(\underbrace{3, \ldots, 3}_{(n-9)/2}, 4, 5)$, $G_n^1(\underbrace{3, \ldots, 3}_{(n-11)/2}, 4, 4, 4)$, G_4, or G_2'. Since for all integers $n \geq 11$, $M_3 - M_1 = 2n^2 - 11n + 21 > 0$, $M_3 - M_2 = 2n^2 - 19n + 45 > 0$, and $M_3 - M_4 = 2n^2 - 15n + 19 > 0$, it follows that $w^+Mo(G) = M_3 = n^3 - 7n^2 + 25n - 63$ and $G \cong G_4$.

Case 4. $b = 0$.

In this case, $\mathcal{F}_4(n, 0) = \emptyset$. Hence, $G \in \mathcal{F}_1(n, 0) \cup \mathcal{F}_2(n, 0) \cup \mathcal{F}_3(n, 0)$.

Subcase 4.1. n is odd.

By Lemmas 4.1–4.4, the following hold:

- If $G \in \mathcal{F}_1(n, 0)$, then $G \cong G_n^0(\underbrace{3, \ldots, 3}_{(n-5)/2}, 5)$ with $n \geq 5$ and $w^+Mo(G) = n^3 - 7n^2 + 19n - 45 \triangleq M_1$.
- If $G \in \mathcal{F}_2(n, 0)$, then $G \cong G_n^0(\underbrace{3, \ldots, 3}_{(n-7)/2}, 4, 4)$ with $n \geq 7$ and $w^+Mo(G) = n^3 - 7n^2 + 27n - 69 \triangleq M_2$.
- If $G \in \mathcal{F}_3(n, 0)$, then $G \cong H_2$ only when $n = 7$, in which case $w^+Mo(G) = M_2$; whereas for $n \geq 9$, $w^+Mo(G) < M_2$.

If $n = 5$, then $G \cong G_5^0(5) \cong C_5$ and $w^+Mo(G) = 0$.

If $n = 7$, then $G \cong G_7^0(3, 5), G_7^0(4, 4)$, or H_2. Direct computation yields $M_1 = 88$ and $M_2 = 120$. Therefore, $w^+Mo(G) = 120$, and $G \cong G_7^0(4, 4)$ or H_2.

If $n \geq 9$, then $M_2 - M_1 = 8n - 24 > 0$. Therefore, $w^+Mo(G) = M_2 = n^3 - 7n^2 + 27n - 69$ and $G \cong G_n^0(\underbrace{3, \ldots, 3}_{(n-7)/2}, 4, 4)$.

Subcase 4.2. n is even.

By Lemmas 4.1–4.4, the following hold:

- If $G \in \mathcal{F}_1(n, 0)$, then

$$G \cong \begin{cases} G_6^0(6), & \text{when } n = 6, \\ G_n^0(\underbrace{3, \ldots, 3}_{(n-8)/2}, 4, 5), & \text{when } n \geq 8, \end{cases}$$

  and $w^+Mo(G) = M_1$, where

$$M_1 = \begin{cases} 0, & \text{when } n = 6, \\ n^3 - 9n^2 + 36n - 84, & \text{when } n \geq 8. \end{cases}$$

- If $G \in \mathcal{F}_2(n, 0)$, then $G \cong G_n^0(\underbrace{3, \ldots, 3}_{(n-10)/2}, 4, 4, 4)$ with $n \geq 10$ and $w^+Mo(G) = n^3 - 9n^2 + 44n - 108 \triangleq M_2$.
- If $G \in \mathcal{F}_3(n, 0)$, then $G \cong G_2$ only when $n = 8$, in which case $w^+Mo(G) = n^3 - 9n^2 + 40n - 78 = 178$; whereas for $n \geq 10$, $w^+Mo(G) < M_2$.

If $n = 6$, then $G \cong G_6^0(6) \cong C_6$ and $w^+Mo(G) = 0$.

If $n = 8$, then $G \cong G_8^0(4, 5)$ or G_2, with $M_1 = n^3 - 9n^2 + 36n - 84 = 140$. Since $w^+Mo(G_2) = 178 > 140$, it follows that $w^+Mo(G) = 178$ and $G \cong G_2$.

If $n \geq 10$, then $G \cong G_n^0(\underbrace{3, \ldots, 3}_{(n-8)/2}, 4, 5)$ or $G_n^0(\underbrace{3, \ldots, 3}_{(n-10)/2}, 4, 4, 4)$. Since $M_2 - M_1 = 8n - 24 > 0$, we get $w^+Mo(G) = M_2 = n^3 - 9n^2 + 44n - 108$ and $G \cong G_n^0(\underbrace{3, \ldots, 3}_{(n-10)/2}, 4, 4, 4)$.

This completes the proof. □

5. Conclusions

A novel distance-based topological index called the Mostar index was introduced recently to measure the peripherality in graphs. As a natural generalization, the additively weighted Mostar index has attracted substantial theoretical attention. In this paper, we address the extremal problems for the additively weighted Mostar index over the class of cacti with given graph parameters. Specifically, we determine the maximum value of the additively weighted Mostar index over all cacti of order n containing exactly p pendant vertices. Additionally, we establish both the largest and the second largest values of the additively weighted Mostar index among all n-vertex cacti with precisely b cut edges. For each extremal value, the corresponding extremal cacti are fully characterized. The extremal cacti characterized in this paper correspond to molecular frameworks where cyclic fragments are as small as possible and pendant substituents are densely localized around a small number of central vertices. Such configurations maximize the distance imbalance captured by the additively weighted Mostar index, thereby establishing a theoretical foundation for understanding structure-property relationships and enabling rational molecular design. It would be interesting to investigate the corresponding extremal problems for other restrictions on cacti, as well as related distance-based indices (e.g., the edge Mostar index and its variants). We will consider it for future study.

Author contributions

Wenjie Ning: Supervision, project administration, writing–review & editing; Yao Lu: Investigation, writing–original draft; Kun Wang: Conceptualization, validation. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

All authors declare no conflicts of interest in this paper.

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