Communications in Combinatorics and Optimization
Vol. xx, No. x (xxxx), pp. 1-14
https://doi.org/10.22049/cco.2024.28757.1702

CCO
Commun. Comb. Optim.

Research Article

Sharp bounds on additively weighted Mostar index of Cacti

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Received: 16 June 2023; Accepted: 29 March 2024

Abstract: Let $\mathcal{C}(n,t)$ denotes the collection of all cacti of order n with exactly t cycles and $\mathcal{C}_n^t$ denotes the collection of cacti of order n and t end vertices. In this paper, we compute three upper bounds of the additively weighted Mostar index of graphs in $\mathcal{C}(n,t)$. We also determine the upper bound of the additively weighted Mostar index for graphs in $\mathcal{C}_n^t$. We characterize all the graphs attaining the bounds.

Keywords: Mostar Index, additively weighted Mostar index, Cacti

AMS Subject classification: 05C35, 05C92.

1. Introduction

A graph $G = (V(G), E(G))$ is said to be simple if it has no loops or parallel edges, and if there is a path connecting every pair of vertices then it's connected. Throughout this paper, we consider only simple, finite, connected, undirected graphs. *Transmission* of a vertex u is the sum of all distances between u and other vertices of G, denoted by $\sigma_G(u)$ [1]. A graph G is said to be $k-$*transmission regular* if $\sigma_G(u) = k$ for all $u \in V(G)$ and for some $k \in \mathbb{N}$. Topological indices are numerical values associated with graphs, which are invariant under graph isomorphism. There is a multitude of topological indices which study structure-activity relations and structure-property relations of chemical compounds. Mostar index is one used to measure the degree peripherality of graphs and individual edges of graphs, it also measures the deviation

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of a graph from being transmission regular [1]. The Mostar index $Mo(G)$ of a graph G is defined as [5]

$$Mo(G) = \sum_{e=xy\in E(G)} |n_x(e|G) - n_y(e|G)| = \sum_{e=xy\in E(G)} |\sigma_G(x) - \sigma_G(y)|$$

where $n_x(e|G)$ denotes the number of vertices closer to x than to y. For a detailed literature on Mostar index, see [1, 4–6, 13, 19]. Various modified versions of Mostar index were proposed recently [2, 12], of which a prominent one is additively weighted Mostar index (also referred as the extended Mostar index). The additively weighted Mostar index $Mo_A(G)$ of a graph G is defined as [1]

$$Mo_A(G) = \sum_{e=xy\in E(G)} (d(x) + d(y))|n_x(e|G) - n_y(e|G)|$$

Cacti are connected graphs in which any two cycles have atmost one vertex in common. Computation of topological indices of different classes of graphs is an ongoing research problem, especially in the class of cacti. In [11], H Q Liu *et al.* presented a unified method to find extremal cacti with respect to some topological indices. In [9], Anhua Lin *et al.* computed the lower bounds of Randić index of cacti of a given order with k pendant vertices and characterized the graphs obtaining the bounds. In [8], Shuchao Li *et al.* characterized cacti of order n with r pendant vertices which attains extremal Zagreb indices. Wang *et al.* [16] determined the cacti with perfect matching which has the largest Harary index and established the upper bounds of the Harary index among cacti. Wang D F *et al.* [15] computed the upper bound of Hyper Wiener index for cacti. In 2016, Chen S [3] characterized the extremal cacti for the Gutman index and computed the first three lower bounds. The extremal PI index for cacti was determined by Wang C *et al.* [14]. Shujing Wang [17, 18] determined the lower bound of the Szeged index and the revised Szeged index for cacti of given order with fixed number of cycles. In 2019, Hayat *et al.* determined some sharp bounds of the Mostar index for cacti of a given order [7]. In [20], Yasmeen F *et al.* determined the upper bound of the edge Mostar index for $\mathcal{C}(n,t)$. In [10], Hechao Liu determined the extremal cacti for Sombar index.

In [1], Akbar Ali, Tomislav Došlić computed the extrema of additively weighted Mostar index for trees. In this paper, we determine the first three upper bounds of the additively weighted Mostar index for graphs in $\mathcal{C}(n,t)$. We also determine the upper bound of the additively weighted Mostar index of cacti in $\mathcal{C}_n^t$ and characterize the graphs attaining the bounds.

2. Notations

We use the following notations throughout this paper.

$\mathcal{C}(n,t)$	The collection of all cacti of order n with exactly t cycles.
$\mathcal{C}_n^t$	The collection of all cacti of order n with t end vertices.
$d_{xy}\|G$	The sum of degrees of end vertices of the edge xy.
$\eta_e(x,y\|G)$	$\|n_x(e\|G)-n_y(e\|G)\|$.
$N_G(v)$	The set of all vertices in G adjacent to the vertex v.
$C_0(n,k)$	The cacti bundle with k triangles along with $n-2k-1$ pendant edges incident with a single vertex.
$C^1(n,r,s)$	The cacti bundle with r- C_4 and s- C_3 along with $n-3r-2s-1$ pendant edges incident with the common vertex.

For the edge $e=xy$ in G, let $Mo_A(e|G)=(d_{xy}|G)\eta_e(x,y|G)$ be the contribution by the edge e onto the additively weighted Mostar index.

3. Upper bound for $\mathcal{C}(n,k)$

In this section, we determine the upper bound of additively weighted Mostar index of graphs in $\mathcal{C}(n,t)$. We use the following lemmas in our discussion.

Lemma 1. *[1] Let $e=uv$ be a non pendant bridge of G. Let G_1 be the graph obtained from G by deleting the edge e, identifying its end vertices to a new vertex z and adding a new pendant edge at z. Then*

$$Mo_A(G_1)>Mo_A(G).$$

Lemma 2. *Let G be a cacti with cycle $C_r=v_1v_2\dots v_rv_1$ such that $G-E(C_r)$ has exactly r components and G_i be the component of $G-E(C_r)$ at the vertex v_i, $i=1,2,\dots,r$. Let*

$$G'=G-\bigcup_{i=2}^{r}\bigcup_{u\in N_{G_i}(v_i)}uv_i+\bigcup_{i=2}^{r}\bigcup_{u\in N_{G_i}(v_i)}uv_1.$$

Then $Mo_A(G')\geq Mo_A(G)$ and the equality holds if and only if C_r is an end block, i.e. $G\cong G'$.

Proof. Let $|V(G_i)|=n_i, i=1,2,\dots,r$ and $\sum_{i=1}^{r}n_i=n$. Let d_i denotes the number of edges in G_i incident with the vertex v_i and $\sum_{i=1}^{r}d_i=d$. From the construction of the graph G' it is clear that for every edge $e=uv\in G_i$, every vertex which is closer to u in G should be closer to u in G'. Also, every vertex which is closer to v in G should be closer to v in G' and every vertex which is equi-distant from both the vertices u and v in G should be equi-distant from both u and v in G'. Thus for every $e=uv\in G_i$, $\eta_e(u,v|G)=\eta_e(u,v|G')$, $i=1,2,3,\dots,r$. For every edge $e=uv\in G_i$ such that $u,v\neq v_i, i=1,2,3,\dots,r$, $d_{uv}|G=d_{uv}|G'$. For the edges $uv\in G_i$ with $v=v_i$, $i=1,2,3,\dots,r$, we have $d_{uv}|G=d(u)+d_i+2$ and for the corresponding transformed edge in G', we have $d_{uv}|G'=d(u)+\sum_{j=1}^{r}d_j+2$. Then

$$\sum_{i=1}^{r}\sum_{e=uv\in G_i}(Mo_A(e|G')-Mo_A(e|G))=\sum_{i=1}^{r}\sum_{e=uv_i\in G_i}(Mo_A(e|G')-Mo_A(e|G)) \tag{3.1}$$
$$=\sum_{i=1}^{r}\sum_{e=uv_i\in G_i}(d-d_i)\eta_e(u,v_i|G_i)>0. \tag{3.2}$$

Now, we divide the rest into the following two cases.

Case I. r is even, $r=2k$.
For each edge $e_i=v_iv_{i+1}\in C_{2k}$, $i=1,2,\dots,2k-1$ and $e_{2k}=v_{2k}v_1$ we have $\eta_e(v_i,v_{i+1}|G')=n-2k$ and

$$\begin{aligned}\eta_e(v_i,v_{i+1}|G)&=((n_i+n_{i-1}+\cdots+n_{i-k+1})-(n_{i+1}+n_{i+2}+\cdots+n_{i+k}))\\&=(n-p_i)\le(n-2k)\end{aligned}$$

where $p_i\ge 2k$ with equality if and only if $n_j=1$ for $j=i,i-1,\dots,i-k+1$ or $n_j=1$ for $j=i+1,i+2,\dots,i+k$. For the edge $e_i=v_iv_{i+1}\in C_{2k}, i\ne 1$ or $2k$, $d_{v_iv_{i+1}}|G=d_i+d_{i+1}+4$ and $d_{v_iv_{i+1}}|G'=4$. For the remaining two edges in C_{2k}, $d_{v_iv_{i+1}}|G=d_i+d_{i+1}+4$ and $d_{v_iv_{i+1}}|G'=4+d$. Thus,

$$\begin{aligned}\sum_{i=1}^{2k}\sum_{e=v_iv_{i+1}\in C_{2k}}(Mo_A(e|G')-Mo_A(e|G))&=(8k+2d)(n-2k)-\sum_{i=1}^{2k}(d_i+d_{i+1}+4)(n-p_i)\\&\ge(8k+2d)(n-2k)-(8k+2d)(n-2k)\ge 0\end{aligned}$$

with equality holds if and only if there exist a j, $1\le j\le 2k$ such that $n_j=n-2k+1$ and $n_i=1$,for all $i\ne j$. Thus, $Mo_A(G')-Mo_A(G)\ge 0$ where the equality holds whenever $G\cong G'$.

Case II. r is odd, $r=2k+1$.
For each edge $e_i=v_iv_{i+1}\in C_{2k+1}$, $i=1,2,\dots,2k, i\ne k$ and $e_{2k+1}=v_{2k+1}v_1$ we have $\eta_e(v_i,v_{i+1}|G')=n-2k-1$ and for the edge $e=v_kv_{k+1}$, $\eta_e(v_k,v_{k+1}|G')=0$ and

$$\begin{aligned}\eta_e(v_i,v_{i+1}|G)&=((n_i+n_{i-1}+\cdots+n_{i-k+1})-(n_{i+1}+n_{i+2}+\cdots+n_{i+k}))\\&=(n-q_i)\\&\le(n-2k-n_{i-k})\end{aligned}$$

where $q_i\ge 2k+1$ with equality holds if and only if $n_j=1$ for $j=i,i-1,\dots,i-k+1$ or $n_j=1$ for $j=i+1,i+2,\dots,i+k$. For the edge $e_i=v_iv_{i+1}\in C_{2k+1}, i\ne 1$ or $2k+1$,

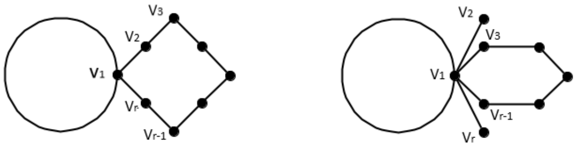

Figure 1. **The graphs G and G' in Lemma 3.**

$d_{v_iv_{i+1}}|G = d_i + d_{i+1} + 4$ and $d_{v_iv_{i+1}}|G' = 4$. For the remaining two edges in C_{2k+1}, $d_{v_iv_{i+1}}|G = d_i + d_{i+1} + 4$ and $d_{v_iv_{i+1}}|G' = 4 + d$. Thus,

$$\begin{aligned}\sum_{i=1}^{2k+1} \sum_{e=v_iv_{i+1}\in C_{2k}} (Mo_A(e|G') - Mo_A(e|G)) &= (8k+2d)(n-2k-1) - \sum_{i=1}^{2k+1}(d_i + d_{i+1} + 4)(n - q_i)\\ &\geq (8k+2d)(n-2k-1) - \sum_{i=1}^{2k+1}(d_i + d_{i+1} + 4)(n - 2k - n_{i-k})\\ &\geq \sum_{i=1}^{2k+1}(d_i + d_{i+1})n_{i-k} - 2d \geq 0,\end{aligned}$$

since $\sum_{i=1}^{2k+1} n_{i-k} = n$ and $n_{i-k} \geq 1$ for all i, with equality holds if and only if there exist a j, $1 \leq j \leq 2k+1$ such that $n_j = n - 2k - 1$ and $n_i = 1$, for all $i \neq j$. Thus, $Mo_A(G') - Mo_A(G) \geq 0$ where the equality holds whenever $G \cong G'$. □

Lemma 3. *Let G be a cacti with the end block $C_r = v_1v_2 \ldots v_rv_1$ such that $d(v_1) > 2$ and $G' = G - v_2v_3 - v_{r-1}v_r + v_3v_1 + v_{r-1}v_1$. Then $Mo_A(G') > Mo_A(G)$ (See Figure 1)*

Proof. Let $|V(G)| = |V(G')| = n$. From the construction of G' it is clear that for the edges uv with $u, v \notin C_r$, $\eta_e(u, v|G) = \eta_e(u, v|G')$ and $d_{uv}|G = d_{uv}|G'$. Now, we divide the rest into the following two cases.

Case I. r is even.

Let $r = 2k, k \geq 2$. For the edge $e = uv_1$ and $u \notin C_r$, $\eta_e(u, v_1|G) = \eta_e(u, v_1|G')$ and $d_{uv_1}|G' = d_{uv_1}|G + 2$. For the edge v_1v_2 and v_1v_r, $\eta_e(v_1, v_j|G) = (n - 2k)$ and $\eta_e(v_1, v_j|G') = (n - 2)$, $j = 2, r$, also $d_{v_1v_j}|G = d(v_1) + 2$ and $d_{v_1v_j}|G' = d(v_1) + 3$ for $j = 2, r$. For the edge v_1v_3 and v_1v_{r-1} in G', $\eta_e(v_1, v_j|G') = (n - (2k - 2))$ and $d_{v_1v_j}|G' = (d(v_1)) + 4$ for $j = 3, r - 1$. For all other edges $uv \in C_r$, $\eta_e(u, v|G) = (n - 2k)$, $\eta_e(u, v|G') = (n - (2k - 2))$ and $d_{uv}|G = d_{uv}|G' = 4$. Thus

$$\begin{aligned}Mo_A(G') - Mo_A(G) = &\sum_{uv_1, u\notin C_r} 2(\eta_e(u, v_1|G)) + 8(2k - 4) + 2(d(v_1) + 3)(n - 2)\\ &- 2(d(v_1) + 2)(n - 2k) + 2(d(v_1) + 4)(n - 2k + 2) - 8(n - 2k)\\ &\geq \sum_{uv_1, u\notin C_r} 2(\eta_e(u, v_1|G)) + 8(2k - 4)\\ &+ 2(n - 2) + 2(d(v_1))(n - 2k + 2) + 16 > 0.\end{aligned}$$

Since $n-2 > n-2k$ and all other quantities are positive.

Case II. r is odd.

Let $r = 2k+1, k \geq 2$ be odd. For the edge $e = uv_1$ and $u \notin C_r$, $\eta_e(u, v_1|G) = \eta_e(u, v_1|G')$ and $d_{uv_1}|G' = d_{uv_1}|G + 2$. For the edge v_1v_2 and v_1v_r, $\eta_e(v_1, v_j|G) = (n-2k-1)$ and $\eta_e(v_1, v_j|G') = (n-2)$ for $j = 2, r$, also $d_{v_1v_j}|G = d(v_1)+2$ and $d_{v_1v_j}|G' = d(v_1)+3$ for $j = 2, r$. For the edge v_1v_3 and v_1v_{r-1} in G', $\eta_e(v_1, v_j|G') = (n-2k+1)$ and $d_{v_1v_j} = (d(v_1)) + 4$ for $j = 3, r-1$. For all other edges $uv \in C_r$, $\eta_e(u, v|G) = (n-2k-1)$, $\eta_e(u, v|G') = (n-2k+1))$ and $d_{uv}|G = d_{uv}|G' = 4$. Thus

$$\begin{aligned}
Mo_A(G') - Mo_A(G) &= \sum_{uv_1, u \notin C_r} 2(\eta_e(u, v_1|G)) + 8(2k-4) + 2(d(v_1)+3)(n-2) \\
&- 2(d(v_1)+2)(n-2k-1) + 2(d(v_1)+4)(n-2k+1) - 8(n-2k-1) \\
&\geq \sum_{uv_1, u \notin C_r} 2(\eta_e(u, v_1|G)) + 8(2k-4) + 2(n-2) + 2(d(v_1))(n-2k+1) \\
&+ 16 > 0.
\end{aligned}$$

Since $n-2 > n-2k-1$, $n-2k+1 > n-2k-1$ and all other quantities are positive. Thus $Mo_A(G') > Mo_A(G)$.

□

Lemma 4. *Let $C_4 = v_1v_2v_3v_4v_1$ be the end block of G with $d(v_1) \geq 2$. Let $G' = G - v_3v_4 + v_1v_3$. Then $Mo_A(G') > Mo_A(G)$.*

Proof. Let $|V(G)| = |V(G')| = n$. Then for all the edges $uv \in G, u, v \notin C_4$, we have $\eta_e(u, v|G) = \eta_e(u, v|G')$ and $d_{uv}|G = d_{uv}|G'$. For the edge v_1u with $u \notin C_4$, $\eta_e(u, v_1|G) = \eta_e(u, v_1|G')$ and $d_{uv_1}|G' = d_{uv_1}|G + 1$. For every edge $uv \in C_4$, $\eta_e(u, v|G) = n-4$ and $\eta_e(u, v|G') = n-2$ for $u = v_1, v = v_4$ and $\eta_e(u, v|G') = n-3$ for $u = v_1, v = v_2$ or v_3 and $\eta_e(u, v|G') = 0$ for $u = v_2, v = v_3$. Also, $d_{v_1v_4}|G = d_{v_1v_4}|G'$ and $d_{v_1v_2}|G' = d_{v_1v_2}|G + 1$ and $d_{v_2v_3}|G = d_{v_3v_4}|G = 4 = d_{v_2v_3}|G'$ but $d_{v_1v_3}|G' = (d(v_1) + 3$. Thus,

$$\begin{aligned}
Mo_A(G') - Mo_A(G) &= \sum_{uv_1, u \notin C_4} (\eta_e(u, v_1|G)) + (d(v_1)+2)(n-2) + 2(d(v_1)+3)(n-3) \\
&- 8(n-4) - 2(d(v_1)+2)(n-4) \\
&= \sum_{uv_1, u \notin C_4} (\eta_e(u, v_1|G)) + 2(d(v_1)+3) + (d(v_1)+2)(n-2) - 6(n-4) > 0,
\end{aligned}$$

if $d(v_1) \geq 4$. If $d(v_1) = 2$ or 3 by direct calculations, $Mo_A(G') - Mo_A(G) > 18 > 0$. Thus, $Mo_A(G') - Mo_A(G) > 0$. □

Proposition 1. *If $n \geq 7$, then $Mo_A(C_0(n, k)) = n^3 - 3n^2 + 2n - 6k$.*

Proof. Let u be the vertex in $C_0(n,k)$ with $d(u) > 2$. For the $n-2k-1$ pendant edges $e = xy$, $\eta_e(x,y|C_0(n,k)) = n-2$ and $d_{xy}|C_0(n,k) = n-1+1 = n$. For the $2k$ edges $e = xy$ on the cycle incident at u, $\eta_e(x,y|C_0(n,k)) = n-3$ and $d_{xy}|C_0(n,k) = n-1+2 = n+1$. For the remaining k edges $e = xy$ on the cycles, $\eta_e(x,y|C_0(n,k)) = 0$ and $d_{xy}|C_0(n,k) = 4$. Thus, $Mo_A(C_0(n,k)) = (n-2k-1)n(n-2)+2k(n+1)(n-3) = n^3-3n^2+2n-6k$. ☐

Now we obtain the maximum value of additively weighted Mostar index of $\mathcal{C}(n,k)$.

Theorem 1. *Let $G \in \mathcal{C}(n,k)$. Then $Mo_A(G) \leq n^3-3n^2+2n-6k$ with equality holds if and only if $G \cong C_0(n,k)$.*

Proof. Let $G \in \mathcal{C}(n,k)$ be the graph with the maximum additively weighted Mostar index. By Lemma 1, all the bridges of G should be pendant edges. By Lemma 2, all the cycles and pendant edges should be attached to a single vertex, by Lemma 3, 4 every cycle in such a graph should be a triangle. Thus $G \cong C_0(n,k)$, by Proposition 1, $Mo_A(C_0(n,k)) = n^3-3n^2+2n-6k$. ☐

Proposition 2. *If $r,s \geq 1$, then $Mo_A(C^1(n,r,s)) = n^3-2n^2r-3n^2+nr^2+11nr+2n+2r^2+2rs-42r-6s$.*

Proof. Let u be the vertex in $C^1(n,r,s)$ with $d(u) > 2$. For the $n-3r-2s-1$ pendant edges $e = xy$, $\eta_e(x,y|C^1(n,r,s)) = n-2$ and $d_{xy}|C^1(n,r,s) = n-r$. For the $2r$ edges $e = xy$ on the $4-$ cycle incident on u, $\eta_e(x,y|C^1(n,r,s)) = n-4$ and $d_{xy}|C^1(n,r,s) = n-r+1$. For the remaining $2r$ edges $e = xy$ on the $4-$ cycle, $\eta_e(x,y|C^1(n,r,s)) = n-4$ and $d_{xy}|C^1(n,r,s) = 4$. For the $2s$ edges $e = xy$ on the $3-$ cycle incident on u, $\eta_e(x,y|C^1(n,r,s)) = n-3$ and $d_{xy}|C^1(n,r,s) = n-r+1$. For the remaining s edges $e = xy$ on the $3-$ cycle, $\eta_e(x,y|C^1(n,r,s)) = 0$ and $d_{xy}|C^1(n,r,s) = 4$. Thus, $Mo_A(C^1(n,r,s)) = (n-r)(n-2)(n-3r-2s-1)+(n-r+1)(n-4)2r+4(n-4)2r+(n-r+1)(n-3)2s = n^3-2n^2r-3n^2+nr^2+11nr+2n+2r^2+2rs-42r-6s$. ☐

Using Lemma 1- 4 and Proposition 2, we obtain the next result.

Corollary 1. *Let $G \in \mathcal{C}(n,k)$ with exactly r even cycles and s odd cycles where $k = r+s, r \geq 1, s \geq 1$. Then $Mo_A(G) \leq n^3-2n^2r-3n^2+nr^2+11nr+2n+2r^2+2rs-42r-6s$ and the equality holds if and only if $G \cong C^1(n,r,s)$.*

Proposition 3. *Let G_1, G_2, G_3, G_5, G_6 be graphs in $\mathcal{C}(n,k)$ plotted as in Figure 2 and Figure 3. Then*

(a.) $Mo_A(G_1) = n^3-7n^2+24n-2k-44$.

(b.) $Mo_A(G_2) = n^3-7n^2+24n-2k-42$.

(c.) $Mo_A(G_3) = n^3-5n^2+10n-4k-12$.

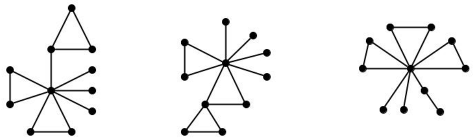

Figure 2. G_1, G_2, $G_3 = C^2(n,k)$ **of Proposition 3 and Theorem 2.**

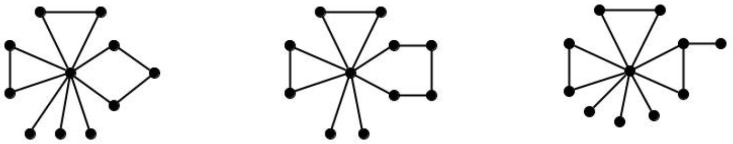

Figure 3. $G_4 = C^1(n,1,k-1)$, G_5 **and** $G_6 = C^3(n,k)$ **of Proposition 3 and Theorem 2.**

(d.) $Mo_A(G_5) = n^3 - 7n^2 + 20n - 2k - 48.$

(e.) $Mo_A(G_6) = n^3 - 5n^2 + 10n - 4k - 12.$

Proof. Let u be the central vertex where the cycles and pendant edges coincides. In G_1, for $n-2k-2$ pendant edges, $d_{xy}|G_1 = n-2$ and $\eta_e(x,y|G_1) = n-2$ and for $2k-2$ edges of the cycle incident on u, $d_{xy}|G_1 = n-1$ and $\eta_e(x,y|G_1) = n-3$. For one bridge $d_{xy}|G_1 = n$ and $\eta_e(x,y|G_1) = n-6$ and for two edges in the remaining cycle incident on the bridge, $d_{xy}|G_1 = 5$ and $\eta_e(x,y|G_1) = n-3$ and for the remaining edges, the contribution is zero. Thus, $Mo_A(G_1) = (n-2k-2)(n-2)(n-2) + 2(k-1)(n-1)(n-3) + (n-6)n + 10(n-3) = n^3 - 7n^2 + 24n - 2k - 44$. In G_2, for $n-2k-1$ pendant edges, $d_{xy}|G_1 = n-2$ and $\eta_e(x,y|G_1) = n-2$ and for $2k-4$ edges of the cycle incident on u, $d_{xy}|G_1 = n-1$ and $\eta_e(x,y|G_1) = n-3$. For the two edges in the cycle which are not incident at u, the contribution is $6(n-3)$. For the three edges in the remaining cycle, the contributions are $(n-1)(n-5)$, $(n+1)(n-7)$ and 12 respectively. For the remaining edges, the contribution is zero. Thus, $Mo_A(G_2) = (n-2k-1)(n-2)(n-2) + 2(k-2)(n-1)(n-3) + (n+1)(n-7) + (n-1)(n-5) + 12(n-3) + 12 = n^3 - 7n^2 + 24n - 2k - 42$.
Similarly, $Mo_A(G_3) = (n-2k-3)(n-1)(n-2) + 3(n-2) + n(n-4) + 2k(n-3)n = n^3 - 5n^2 + 10n - 4k - 12$ and $Mo_A(G_5) = (n-2k-3)(n-2)(n-2) + 2(k-1)(n-3)(n-1) + 2(n-1)(n-5) + 8(n-5) = n^3 - 7n^2 + 20n - 2k - 48$. Also, $Mo_A(G_6) = (n-2k-2)(n-2)(n-1) + 2(k-1)(n-3)(n) + (n+1)(n-5) + 4(n-2) + n(n-4) + 5 = n^3 - 5n^2 + 10n - 4k - 12$. □

Now we establish the next upper bound of additively weighted Mostar index for cacti in $\mathcal{C}(n,t)$.

Theorem 2. *Let* $G \in \mathcal{C}(n,k)|C_0(n,k)$ *with* $n \geq 7$. *Then* $Mo_A(G) \leq n^3 - 5n^2 + 14n - 4k - 36$ *and the equality holds if and only if* $G \cong C^1(n,1,k-1)$.

Proof. Let G be the cacti in $\mathcal{C}(n,k)|C_0(n,k)$ which attains the maximum additively weighted Mostar index. Then there are four cases.

Case I. G has a cycle which is not an end block.
Then there are the following two possibilities, either G has a cycle which is incident on a pendant vertex or G has a cycle which is incident on another cycle other than the common vertex. In both the subcases, by Lemma 2 all except one cycle should be incident on a single vertex. By Lemma 3 and Lemma 4 all the cycles should be C_3. If G has a cycle which is incident on a pendant vertex. By Lemma 1 except one bridge, all other bridges should be pendant edges and incident on the common vertex, thus G should be of the form G_1(see Figure 2) and by Proposition 3, $Mo_A(G_1) = n^3 - 7n^2 - 2k + 24n - 44$. If G has a cycle which is incident on another cycle other than the common vertex, G should be of the form G_2(see Figure 2) and by Proposition 3, $Mo_A(G_2) = n^3 - 7n^2 + 24n - 2k - 42$.

Case II. G has one bridge which is not a pendant edge.
Then by Lemma 1 to Lemma 4 all the cycles should be C_3 and are end blocks. Also, all except one edge are pendant edges and incident on the common vertex, thus G should be isomorphic to G_3(see Figure 3) and by Proposition 3, $Mo_A(G_3) = n^3 - 5n^2 - 4k + 10n - 12$.

Case III. G has a cycle which is not C_3.
Then by Lemma 1 all the bridges are pendant edges and by Lemma 2 all the cycles should be end blocks. Also, by Lemma 3 and Lemma 4 all except one cycle are C_3. Thus G must be either one of the form G_4 or G_5(see Figure 3). Now by Proposition 2, $Mo_A(G_4) = n^3 - 5n^2 + 14n - 4k - 36$ and by Proposition 3, $Mo_A(G_5) = n^3 - 7n^2 + 20n - 2k - 48$.

Case IV. G has a pendant edge which is not incident on the common vertex.
Then by Lemma 2 all the cycles and all except one pendant edges should be incident on a common vertex. By Lemma 3 and Lemma 4 all the cycles should be C_3. Thus G should be of the form G_6(see Figure 3) and by Proposition 3, $Mo_A(G_6) = n^3 - 5n^2 - 4k + 10n - 12$. Clearly, $Mo_A(G_4) \geq Mo_A(G_i), i = 1,2,3,4,5,6$ whenever $n \geq 7$, hence the result. □

As a consequence of the theorem, we get the third upper bound.

Corollary 2. *Let* $G \in \mathcal{C}(n,k)|\{C_0(n,k), C^1(n,1,k-1)\}$ *with* $n \geq 7$. *Then* $Mo_A(G) \leq n^3 - 5n^2 + 10n - 4k - 12$ *and the equality holds if and only if* $G \cong C^2(n,k)$ *or* $G \cong C^3(n,k)$

4. Upper bound for $\mathcal{C}_n^t$

In this section, we find the upper bound of the additively weighted Mostar index of cacti of order n with t pendant vertices.

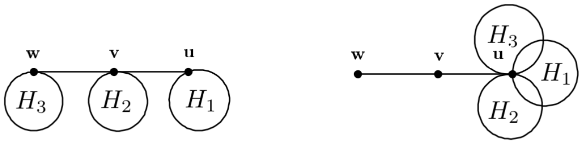

Figure 4. **Graphs G and G' in Lemma 5.**

Lemma 5. *Let G be a graph as in Figure 4 with two adjacent bridges $e_1 = uv$ and $e_2 = vw$ and H_1, H_2, H_3 be the components of $G - \{e_1, e_2\}$ at the vertices u, v, w respectively. Let G' be the graph obtained by moving the components H_2, H_3 of G to u with $|V(H_1)| \geq |V(H_3)|$. Then $Mo_A(G') \geq Mo_A(G)$(as in Figure 4).*

Proof. Let n_1, n_2, n_3 be the number of vertices of H_1, H_2, H_3 respectively and $n_1 + n_2 \geq n_3$ and let $d(u) = d_1 + 1$ and $d(v) = d_2 + 2$ and $d(w) = d_3 + 1$ be the degrees of vertices u, v, w respectively. Then

Edge	$\eta_e(u, v\|G)$	Sum of degrees
$ux, x \neq v$	$\eta_e(u, x\|G) = \eta_e(u, x\|G')$	$d_{ux}\|G + d_2 + d_3 = d_{ux}\|G'$
$vx, x \neq u, w$	$\eta_e(v, x\|G) = \eta_e(v, x\|G')$	$d_{vx}\|G + d_1 + d_3 - 1 = d_{vx}\|G'$
$wx, x \neq v$	$\eta_e(w, x\|G) = \eta_e(w, x\|G')$	$d_{wx}\|G + d_1 + d_2 = d_{wx}\|G'$
uv	$\eta_e(u, v\|G) = \|n_2 + n_3 - n_1\|$ $\eta_e(u, v\|G') = n - 4$	$d_{uv}\|G = d_1 + d_2 + 3$ $d_{uv}\|G' = d_1 + d_2 + d_3 + 3$
vw	$\eta_e(v, w\|G) = \|n_1 + n_2 - n_3\|$ $\eta_e(v, w\|G') = n - 2$	$d_{vw}\|G = d_2 + d_3 + 3$ $d_{vw}\|G' = 3$

$$\begin{aligned} Mo_A(G') - Mo_A(G) = & \sum_{ux, x\neq v} (d_2 + d_3)\eta_e(u, x|G) + \sum_{vx, x\neq u,w} (d_1 + d_3 - 1)\eta_e(v, x|G) \\ & + \sum_{wx, x\neq v} (d_1 + d_2)\eta_e(w, x|G) + (n - 4)(d_1 + d_2 + d_3 + 3) \\ & - |n_2 + n_3 - n_1|(d_1 + d_2 + 3) \\ & + 3(n - 2) - |n_1 + n_2 - n_3|(d_2 + d_3 + 3) > 0. \end{aligned}$$

Since $\eta_e(w, x|G) \geq |n_1 + n_2 - n_3|$ and $(n - 4) \geq |n_2 + n_3 - n_1|$. □

Lemma 6. *Let G' be a graph as in the previous lemma with two adjacent bridges $e_1 = uv$ and $e_2 = vw$ and $G'' = G' + uw$. Then $Mo_A(G'') > Mo_A(G')$(as in Figure 5).*

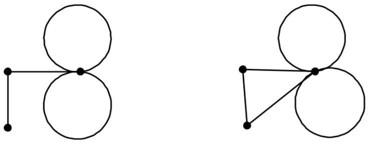

Figure 5. **Graphs G' and G'' in Lemma 6.**

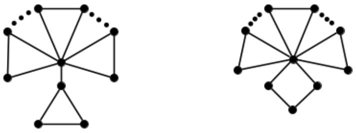

Figure 6. **Graphs G and G' in Lemma 7.**

Proof. From direct calculations we obtain,

$$\begin{aligned} Mo_A(G'') - Mo_A(G') &= \sum_{ux, x \neq v} \eta_e(u, x|G') + 2(d(u)+3)(n-3) - (d(u)+2)(n-4) - 3(n-2) \\ &= \sum_{ux, x \neq v} \eta_e(u, x|G') + (d(u)+1)(n-3) + (d(u)-1) > 0. \end{aligned}$$

□

Lemma 7. *Let G and G' be two graphs shown in Figure 6 with $n \geq 7$ vertices. Then $Mo_A(G') > Mo_A(G)$.*

Proof. From direct calculations we obtain,

$$Mo_A(G') - Mo_A(G) = (n^3 - 5n^2 + 12n - 32) - (n^3 - 7n^2 + 23n - 42) = 2n^2 - 11n + 10 > 0.$$

□

Lemma 8. *Let G and G' be two graphs shown in Figure 7 with $n \geq 7$ vertices and $t \geq 1$ pendant vertices. Then $Mo_A(G') > Mo_A(G)$.*

Proof. From direct calculations,

$$Mo_A(G') - Mo_A(G) = (n^3 - 5n^2 + 12n + 2t - 32) - (n^3 - 5n^2 + 8n + 2t - 8) = 4n - 24 > 0.$$

□

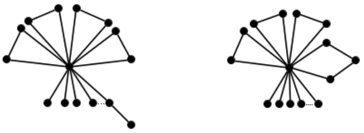

Figure 7. **Graphs G and G' in Lemma 8**

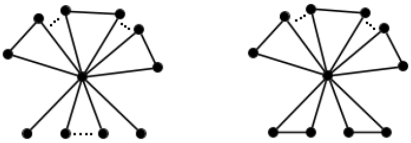

Figure 8. **Graphs G_0 and G_{10} in Theorem 3.**

Using these results we obtain the following.

Theorem 3. *Let $G \in \mathcal{C}_n^t$ be a cacti with $n \geq 7$ vertices and t pendant edges, then*

(a.) $Mo_A(G) \leq Mo_A(G_0)$ If n and t are of different parity.

(b.) $Mo_A(G) \leq Mo_A(G_{10})$, If n is odd and $t = 0$.

(c.) $Mo_A(G) \leq Mo_A(G_{20})$, If n is even $t = 0$.

(d.) $Mo_A(G) \leq Mo_A(G_{12})$, If both n and t are of same parity with $n > 5$,$t > 0$.

where $G_0, G_{10}, G_{20}, G_{12}$ are graphs shown in Figure 8,9.

Proof. Let $G \in \mathcal{C}_n^t$ be the graph with the maximum additively weighted Mostar index. Then by Lemma 2, all the cycles are end blocks and by Lemma 3, 4 all the cycles are triangles. Also by Lemma 6, 7 the graph G cannot have two adjacent non-trivial bridges. If the parity of n and t are different, then G should have at least one pendant edge, thus $G \cong G_0$. If n is odd and $t = 0$ then by Lemma 3, 4, 7, $G \cong G_{10}$. If n is even and $t = 0$ then G should have at least one bridge or G should have at

Figure 9. **Graphs G_{20} and G_{12} in Theorem 3.**

least one cycle which is not C_3, then by Lemma 7, $G \cong G_{20}$. If both n and t are odd or even with $t > 0$ then by Lemma 6, 8, $G \cong G_{12}$. □

When $n = 5$ and $t = 1$, then the graph $G = C_3 \boxdot P_3$, obtained by attaching P_3 onto a vertex of C_3 has the largest additively weighted Mostar index among $\mathcal{C}_5^1$.

Conflict of Interest. The authors declare that they have no conflict of interest.

Data Availability. Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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