Filomat 33:15 (2019), 4865–4873
https://doi.org/10.2298/FIL1915865H

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

On Cacti with Large Mostar Index

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Abstract. The Mostar index of a graph G is defined as the sum of absolute values of the differences between n_u and n_v over all edges $e = uv$ of G, where $n_u(e)$ and $n_v(e)$ are respectively, the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u. A cactus is a graph in which any two cycles have at most one common vertex. In this paper, we determine all the n-vertex cacti with the largest Mostar index, and we give a sharp upper bound of the Mostar index for cacti of order n with k cycles, and characterize all the cacti that achieve this bound.

1. Introduction

In this paper we consider only simple finite graphs. Let G be a connected graph on n vertices with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex v in G is the number of edges that are incident to v in G. A vertex is said to be a pendant vertex if its degree is one, and an edge is said to be a pendant edge if one of its end vertices is a pendant vertex. Let $d_G(u, v)$ denotes the distance between u and v in G . An edge e is a cut edge of G if $G - e$ (the graph obtained from G by deleting e) is disconnected. Let C_n and S_n denotes the cycle and star on n vertices, respectively. For $e = uv \in E(G)$, let $N_u(e)$ and $N_v(e)$ be respectively the set of vertices of G lying closer to vertex u than to vertex v and the set of vertices of G lying closer to vertex v than to vertex u. That is,

$$N_u(e) = \{x \in V(G) : d_G(u, x) < d_G(v, x)\},$$
$$N_v(e) = \{x \in V(G) : d_G(v, x) < d_G(u, x)\}.$$

The number of vertices of $N_u(e)$ and $N_v(e)$ are denoted by $n_u(e)$ and $n_v(e)$, respectively.

In order to distill and condense the information contained in connectivity patterns of graphs, a number of numerical quantities, variously known as structural invariants, molecular descriptors, topological descriptors, or topological indices, have been proposed and studied. We call them topological indices here. The Wiener index is one of the oldest and the most thoroughly studied topological indices [2, 5, 14, 16, 19].

Recall that the Wiener index $W(G)$ of G is, by definition, equal to the sum of distances between all pairs of vertices of graph. Obviously, for the direct calculation of $W(G)$ a total of $\binom{n}{2}$ distances needs to be determined [16]. If G is a tree, Wiener gave an efficient method to compute its Wiener index:

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

2010 *Mathematics Subject Classification*. Primary 05C12; Secondary 05C35
Keywords. Mostar index, cactus, extremal graph, unicyclic graph.
Received: 02 May 2019; Accepted: 05 September 2019
Communicated by Paola Bonacini
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where the right hand side consists of only $n-1$ summands, each of which is somewhat easily evaluated. For connected graphs G that are not necessarily trees, Gutman proposed the Szeged index as

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

Obviously, Szeged and Wiener indices coincide for trees, and for graphs with cycles we have $Sz(G) \geq W(G)$ with equality if and only if each block of G is complete. See [3, 6, 11, 18, 22] for various properties of the Szeged index of a graph. Some invariants such as edge Szeged index, revised Szeged index were also studied, see, e.g., [1, 7, 8, 12, 17, 20, 21]. Very recently, Doslić et al. [4] introduced a new invariant – the Mostar index, of a connected graph G, defined as

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

They determined its extremal values and characterized extremal trees and unicyclic graphs, and they also showed how it can be efficiently computed for various classes of chemically interesting graphs using a variant of the cut method proposed by Klavžar, Gutman and Mohar [10]. The Mostar index of bicyclic graphs was studied by Tepeh [15]. As pointed out in [4], the Mostar index measures how far is a graph from being distance-balanced and may be viewed of as a quantitative refinement of the distance-non-balancedness of a graph. For the distance-balanced graphs and generalizations, one may refer to [9, 13].

A cactus is a graph in which any block is either a cut edge or a cycle, or equivalently, a graph in which any two cycles have at most one common vertex. In this paper, we give an upper bound for the Mostar index of cacti of order n with k cycles, and also characterize those cacti that achieve the bound. Then we use this result to determine all cacti with largest Mostar index in the class of cacti on n vertices.

2. Preliminaries

In this section, we give some preliminary results which will be used in the subsequent sections.

Lemma 2.1. *Let G be a connected graph of order n with a cut edge $e = uv$. Then $|n_u(e) - n_v(e)| \leq n-2$ with equality if and only if $e = uv$ is a pendant edge.*

Proof. Let G_1 and G_2 be the components of $G - uv$ that contain u and v, respectively. Note that $N_u(e) = V(G_1)$ and $N_v(e) = V(G_2)$. Thus $n_u(e) + n_v(e) = |V(G_1)| + |V(G_2)| = |V(G)| = n$. Assume that $n_u(e) \geq n_v(e)$. As $n_v(e) \geq 1$, we have $|n_u(e) - n_v(e)| = n - 2n_v(e) \leq n-2$ with equality if and only if $n_v(e) = 1$, i.e., $N_v(e) = \{v\}$, i.e., v is a pendant vertex. □

A cycle in a connected graph is called an end-block if all but one vertex of this cycle have degree 2.

Lemma 2.2. *Let G be a graph with a cycle C of length $2\ell+1$ such that $G - E(C)$ has exactly $2\ell+1$ components. Then*

$$\sum_{e=uv\in E(C)} |n_u(e) - n_v(e)| \leq 2\ell(n - 2\ell - 1)$$

with equality if and only if C is an end-block.

Proof. It is trivial if $G = C$. Suppose that $G \neq C$. Let $C = u_1u_2\dots u_{2\ell+1}u_1$. For $1 \leq i \leq 2\ell+1$, let G_i be the component of $G - E(C)$ that contains u_i. Let $V_i = V(G_i) \setminus \{u_i\}$ and $n_i = |V_i| \geq 0$ for $i \in \{1, \dots, 2\ell+1\}$. Then $\sum_{i=1}^{2\ell+1} n_i = n - 2\ell - 1$. Note that $N_{u_1}(u_{2\ell+1}u_1) = V_1 \cup \dots \cup V_\ell \cup \{u_1, \dots, u_\ell\}$ and $N_{u_{2\ell+1}}(u_{2\ell+1}u_1) =$

$V_{\ell+2} \cup \cdots \cup V_{2\ell+1} \cup \{u_{\ell+2}, \ldots, u_{2\ell+1}\}$. If $\sum_{i=1}^{\ell} n_i \le \sum_{i=\ell+2}^{2\ell+1} n_i$, then

$$\begin{aligned} |n_{u_1}(u_{2\ell+1}u_1) - n_{u_{2\ell+1}}(u_{2\ell+1}u_1)| &= \left|\sum_{i=1}^{\ell} n_i - \sum_{i=\ell+2}^{2\ell+1} n_i\right| \\ &= \sum_{i=1}^{2\ell+1} n_i - n_{\ell+1} - 2\sum_{i=1}^{\ell} n_i \\ &= n - 2\ell - 1 - n_{\ell+1} - 2\sum_{i=1}^{\ell} n_i \\ &\le n - 2\ell - 1 - n_{\ell+1}, \end{aligned}$$

where equality holds if and only if $n_i = 0$ for all $i \in \{1, \ldots, \ell\}$; otherwise, we have

$$\begin{aligned} |n_{u_1}(u_{2\ell+1}u_1) - n_{u_{2\ell+1}}(u_{2\ell+1}u_1)| &= \left|\sum_{i=1}^{\ell} n_i - \sum_{i=\ell+2}^{2\ell+1} n_i\right| \\ &= \sum_{i=1}^{2\ell+1} n_i - n_{\ell+1} - 2\sum_{i=\ell+2}^{2\ell+1} n_i \\ &= n - 2\ell - 1 - n_{\ell+1} - 2\sum_{i=\ell+2}^{2\ell+1} n_i \\ &\le n - 2\ell - 1 - n_{\ell+1}, \end{aligned}$$

where equality holds if and only if $n_i = 0$ for all $i \in \{\ell + 2, \ldots, 2\ell + 1\}$. Hence, we have

$$|n_{u_1}(u_{2\ell+1}u_1) - n_{u_{2\ell+1}}(u_{2\ell+1}u_1)| \le n - 2\ell - 1 - n_{\ell+1}$$

with equality if and only if $n_i = 0$ for all $i \in \{1, \ldots, \ell\}$ or for all $i \in \{\ell + 2, \ldots, 2\ell + 1\}$. Similarly, for $1 \le j \le 2\ell$, we have

$$|n_{u_j}(u_j u_{j+1}) - n_{u_{j+1}}(u_j u_{j+1})| \le n - 2\ell - 1 - n_{\ell+j+1}$$

with equality if and only if $n_i = 0$ for all $i \in \{j + 1, \ldots, j + \ell\}$ or for all $i \in \{j + \ell + 2, \ldots, j + 2\ell + 1\}$, where the subscript i in n_i is of modulo $2\ell + 1$ in $\{1, \ldots, 2\ell + 1\}$. So we have

$$\begin{aligned} \sum_{e=uv\in E(C)} |n_u(e) - n_v(e)| &\le \sum_{i=1}^{2\ell+1} (n - 2\ell - 1 - n_i) \\ &= (2\ell + 1)(n - 2\ell - 1) - \sum_{i=1}^{2\ell+1} n_i \\ &= 2\ell(n - 2\ell - 1). \end{aligned}$$

Suppose that $\sum_{e=uv\in E(C)} |n_u(e)-n_v(e)| = 2\ell(n-2\ell-1)$. Then by the above arguments, we have $|n_{u_1}(u_{2\ell+1}u_1) - n_{u_{2\ell+1}}(u_{2\ell+1}u_1)| = |n_{u_j}(u_j u_{j+1}) - n_{u_{j+1}}(u_j u_{j+1})| = n - 2\ell - 1 - n_{\ell+j+1}$ for each $j \in \{1, \ldots, 2\ell\}$, and thus $n_i = 0$ for all $i \in \{1, \ldots, \ell\}$ or for all $i \in \{\ell+2, \ldots, 2\ell+1\}$, and $n_i = 0$ for all $i \in \{j+1, \ldots, j+\ell\}$ or for all $i \in \{j+\ell+2, \ldots, j+2\ell+1\}$ for each $j \in \{1, \ldots, 2\ell\}$, where, as early, the subscript i in n_i is of modulo $2\ell + 1$ in $\{1, \ldots, 2\ell + 1\}$. Note that $G \ne C$. We may assume $n_{\ell+1} \ge 1$ and $n_1 = \cdots = n_\ell = 0$. Then we have $n_1 = n_{2\ell+1} = \cdots = n_{\ell+3} = 0$ by considering $j = 1$. Now setting $j = \ell + 1$, we have $n_{\ell+2} = 0$. Therefore, $n_{\ell+1} = n - 2\ell + 1$ and $n_i = 0$ for $i \ne \ell + 1$, i.e., $G - E(C)$ contains only one nontrivial component $G_{\ell+1}$, i.e., C is an end-block of G.

Conversely, if C is an end-block of G, i.e., there is a k with $1 \le k \le 2\ell + 1$ such that $n_k = n - 2\ell - 1$ and $n_i = 0$ for $i \ne k$, then by the above proof, it is easy to see that $\sum_{e=uv\in E(C)} |n_u(e) - n_v(e)| = 2\ell(n - 2\ell - 1)$. □

The proof of the following lemma is almost parallel to the proof of Lemmas 2.2, except that there are no equidistant vertices as in the odd case.

Lemma 2.3. *Let G be a connected graph with an even cycle C of length 2ℓ such that $G - E(C)$ has exactly 2ℓ components. Then*

$$\sum_{e=uv\in E(C)} |n_u(e) - n_v(e)| \le 2\ell(n - 2\ell)$$

with equality if and only if C is an end-block.

Let $C(n, k)$ be the class of all cacti of order n with k cycles.

A bundle is a cactus in which all cycles have exactly one common vertex. Let $G_n(\ell_1, \dots, \ell_k)$ be a bundle obtained from the bundle consisting precisely of k cycles of lengths $\ell_1, \dots, \ell_k$ (with a unique common vertex v) by attaching $n - 1 + k - \sum_{i=1}^{k} \ell_i$ pendant vertices at v.

Let $C^0_{n,k} = G_n(\ell_1, \dots, \ell_k)$ with $\ell_1 = \cdots = \ell_k = 3$, i.e., the bundle of k triangles (with a unique common vertex v) and $n - 2k - 1$ pendant edges at v. Let $C^1_{n,k} = G_n(\ell_1, \dots, \ell_k)$ with $\ell_1 = \cdots = \ell_k = 4$, i.e., the bundle of k quadrangles (with a unique common vertex v) and $n - 3k - 1$ pendant edges at v.

For odd integers $\ell_1, \dots, \ell_r$ and even integers $\ell_{r+1}, \dots, \ell_k$, let

$$f(\ell_1, \dots, \ell_k) = (n-2)(n-1+k) - rn - \left(\sum_{i=1}^{r}(\ell_i^2 - 3\ell_i) + \sum_{i=r+1}^{k}(\ell_i^2 - 2\ell_i)\right).$$

3. Cactus with large Mostar index in $C(n, k)$

We first want to determine the graphs in $C(n, k)$ with maximum Mostar index.

Lemma 3.1. *Suppose that $G \in C(n, k)$ with cycles $C_1, \dots, C_k$. Let $\ell_i = |C_i|$ for $i = 1, 2, \dots, k$, where $\ell_1, \dots, \ell_r$ are odd, and $\ell_{r+1}, \dots, \ell_k$ are even. Then $Mo(G) \le f(\ell_1, \dots, \ell_k)$ equality holding if and only if $G \cong G_n(\ell_1, \dots, \ell_k)$.*

Proof. Obviously, $|E(G)| = n - 1 + k$. Thus, there are exactly $n - 1 + k - \sum_{i=1}^{k} \ell_i$ cut edges in G. Considering the contributions of cut edges, edges on the odd cycles and edges on the even cycles, we have by Lemmas 2.1, 2.2 and 2.3 that

$$\begin{aligned} Mo(G) &\le (n-2)\left(n-1+k-\sum_{i=1}^{k}\ell_i\right) + \sum_{i=1}^{r}(\ell_i - 1)(n - \ell_i) + \sum_{i=r+1}^{k}\ell_i(n - \ell_i) \\ &= (n-2)(n-1+k) - \sum_{i=1}^{k}\ell_i(n-2) + \sum_{i=1}^{k}\ell_i(n-\ell_i) - \sum_{i=1}^{r}(n-\ell_i) \\ &= (n-2)(n-1+k) - \sum_{i=1}^{k}\ell_i(\ell_i - 2) - \sum_{i=1}^{r}(n - \ell_i) \\ &= (n-2)(n-1+k) - rn - \left(\sum_{i=1}^{r}(\ell_i^2 - 3\ell_i) + \sum_{i=r+1}^{k}(\ell_i^2 - 2\ell_i)\right) \\ &= f(\ell_1, \dots, \ell_k), \end{aligned}$$

where equality holds if and only if all the cut edges are pendant edges and all the cycles are end-blocks, i.e., $G \cong G_n(\ell_1, \dots, \ell_k)$. □

Theorem 3.2. *For any graph $G \in C(n, k)$ with $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$.*

(i) If $n = 8$, then

$$Mo(G) \leq 42 - 2k$$

with equality if and only if G is a bundle with cycle lengths to be 3 or 4.

(ii) If $n < 8$ or $8 < n \leq 3k$, then

$$Mo(G) \leq (n-2)(n-1) - 2k$$

with equality if and only if $G \cong C^0_{n,k}$.

(iii) If $n > 8$ and $n \geq 3k+1$, then

$$Mo(G) \leq (n-2)(n-1) + (n-10)k$$

with equality if and only if $G \cong C^1_{n,k}$.

Proof. Let $C_1, \ldots, C_k$ be k cycles of G and $\ell_i = |C_i|$ for $i = 1, \ldots, k$. Then by Lemma 3.1, we have $Mo(G) \leq f(\ell_1, \ldots, \ell_k)$ with equality if and only if $G \cong G_n(\ell_1, \ldots, \ell_k)$. Let $h(\ell_1, \ldots, \ell_k) = \sum_{i=1}^{r}(\ell_i^2 - 3\ell_i) + \sum_{i=r+1}^{k}(\ell_i^2 - 2\ell_i)$. Obviously, $f(\ell_1, \ldots, \ell_k)$ achieves its maximum if and only if $h(\ell_1, \ldots, \ell_k)$ achieves its minimum. It is easy to see that $h(\ell_1, \ldots, \ell_k)$ is increasing for each $\ell_i \geq 3$. As $\ell_1, \ldots, \ell_r \geq 3$ and $\ell_{r+1}, \ldots, \ell_k \geq 4$, we have

$$\begin{aligned} f(\ell_1, \ldots, \ell_k) &\leq f(\underbrace{3, \ldots, 3}_{r}, \underbrace{4, \ldots, 4}_{k-r}) \\ &= (n-2)(n-1+k) - rn - 8(k-r) \\ &= (n-2)(n-1+k) - 8k + r(8-n) \end{aligned}$$

with equality if and only if $\ell_1 = \cdots = \ell_r = 3$ and $\ell_{r+1} = \cdots = \ell_k = 4$.

Let $F(r) = (n-2)(n-1+k) - 8k + r(8-n)$ for $0 \leq r \leq k$.

If $n = 8$, then

$$\begin{aligned} Mo(G) &\leq f(\ell_1, \ldots, \ell_k) \\ &\leq F(r) = (n-2)(n-1+k) - 8k = 42 - 2k \end{aligned}$$

with equalities if and only if $G \cong G_n(\ell_1, \ldots, \ell_k)$ with $\ell_1 = \cdots = \ell_r = 3$ and $\ell_{r+1} = \cdots = \ell_k = 4$, where $0 \leq r \leq k$, i.e., G is any bundle of cycle lengths to be 3 or 4.

If $n < 8$ or $8 < n \leq 3k$, then

$$\begin{aligned} Mo(G) &\leq f(\ell_1, \ldots, \ell_k) \\ &\leq F(r) \\ &\leq F(k) = (n-2)(n-1) - 2k \end{aligned}$$

with equalities if and only if $r = k$, $G \cong G_n(\ell_1, \ldots, \ell_k)$ with $\ell_1 = \cdots = \ell_k = 3$, i.e., $G \cong G_n(3, \ldots, 3) = C^0_{n,k}$

If $n > 8$ and $n \geq 3k+1$, then

$$\begin{aligned} Mo(G) &\leq f(\ell_1, \ldots, \ell_k) \\ &\leq F(r) \\ &\leq F(0) = (n-2)(n-1) + (n-10)k \end{aligned}$$

with equalities if and only if $r = 0$, $G \cong G_n(\ell_1, \ldots, \ell_k)$ with $\ell_1 = \cdots = \ell_k = 4$, i.e., $G \cong G_n(4, \ldots, 4) = C^1_{n,k}$. □

Note that $C(n, 1)$ for $n \geq 3$ is the set of n-vertex unicyclic graphs. By previous theorem, we immediately have the following corollary; see also [4].

Corollary 3.3. *Suppose that G is a unicyclic graph on $n \geq 3$ vertices. Then* *(i) If* $n = 8$*, then*

$$Mo(G) \leq 40$$

with equality if and only if G is a bundle with a triangle and five pendant vertices attached to some vertex or with a quadrangle and four pendant vertices attached to some vertex.

(ii) If $n < 8$*, then*

$$Mo(G) \leq n^2 - 3n$$

with equality if and only if $G \cong C^0_{n,1}$*.*

(iii) If $n > 8$*, then*

$$Mo(G) \leq n^2 - 2n - 8$$

with equality if and only if $G \cong C^1_{n,1}$*.*

In the following theorem we determine all the cacti with the largest Mostar index among all cacti of order n.

Theorem 3.4. *Let G be a cactus of order* $n \geq 3$*, then*

(i) If $n \leq 10$*, then*

$$Mo(G) \leq (n-1)(n-2)$$

with equality for $n \leq 9$ *if and only if* $G \cong S_n$ *and with equality for* $n = 10$ *if and only if* $G \cong S_n$ *or G is a bundle with one, two, or three cycles of length* 4*.*

(ii) If $n \geq 11$*, then*

$$Mo(G) \leq (n-2)(n-1) + (n-10)\left\lfloor \frac{n-1}{3} \right\rfloor$$

with equality if and only if $G \cong C^1_{n,\lfloor \frac{n-1}{3} \rfloor}$*.*

Proof. If G is a tree, then $Mo(G) \leq (n-2)(n-1)$ with equality if and only if $G \cong S_n$.

Next suppose that G is not a tree. Then G contains at least one cycle. By Theorem 3.2, we have $Mo(G) \leq 40 < 42 = (n-2)(n-1)$ if $n = 8$, and $Mo(G) \leq (n-2)(n-1) - 2$ if $n < 8$.

Suppose that $n \geq 9$. Let k be the number of cycles in G. If $n < 3k$, then, by Theorem 3.2, $Mo(G) < (n-2)(n-1)$. So we may assume that $n \geq 3k+1$. By Theorem 3.2, we have $Mo(G) \leq (n-2)(n-1) - 1$ for $n = 9$, $Mo(G) \leq (n-2)(n-1)$ with equality if and only if $G \cong C^1_{n,k}$ with $k = 1, 2, 3$ for $n = 10$, and

$$Mo(G) \leq (n-2)(n-1) + (n-10)\left\lfloor \frac{n-1}{3} \right\rfloor$$

with equality if and only if $G \cong C^1_{n,\lfloor \frac{n-1}{3} \rfloor}$ for $n \geq 11$.

Now the result follows easily. □

In the following, we determine the graphs in $\mathcal{C}(n,k) \setminus \{C^1_{n,k}\}$ with maximum Mostar index for $n \geq 9$ and $n \geq 3k+1$. Let $B_{n,k}$ be the graph that is obtained from $C^1_{n-1,k}$ by adding a pendant edge at a pendant vertex.

Lemma 3.5. *Let* $G \in \mathcal{C}(n,k)$ *such that there exists a cut edge that is not a pendant edge, where* $n \geq 9$*. Then*

$$Mo(G) \leq (n-2)(n-1+k) - 8k - 2$$

with equality if and only if $G \cong B_{n,k}$*.*

Proof. Let $e = uv$ be the cut edge that is not a pendant edge in G. Then $2 \leq n_u(e), n_v(e) \leq n-2$, and thus

$$|n_u(e) - n_v(e)| \leq n - 4$$

with equality if and only if one component of $G - uv$ contains a single edge.

Let $C_1, \ldots, C_k$ be k disjoint cycles of G and $\ell_i = |C_i|$ for $i = 1, \ldots, k$. Suppose that $\ell_1, \ldots, \ell_r$ are odd, and $\ell_{r+1}, \ldots, \ell_k$ are even. Then by similar argument as in the proof of Lemma 3.1 and Theorem 3.2, we have

$$\begin{aligned}
Mo(G) &\leq n - 4 + (n-2)\left(n - 1 + k - \sum_{i=1}^{k} \ell_i - 1\right) \\
&\quad + \sum_{i=1}^{r} (\ell_i - 1)(n - \ell_i) + \sum_{i=r+1}^{k} \ell_i(n - \ell_i) \\
&= (n-2)(n-1+k) - \sum_{i=1}^{k} \ell_i(n-2) + \sum_{i=1}^{k} \ell_i(n-\ell_i) - \sum_{i=1}^{r}(n-\ell_i) - 2 \\
&= (n-4)(n-1+k) - \sum_{i=1}^{k} \ell_i(\ell_i - 2) - \sum_{i=1}^{r}(n-\ell_i) \\
&= f(\ell_1, \ldots, \ell_k) - 2 \\
&\leq f(\underbrace{3, \ldots, 3}_{r}, \underbrace{4, \ldots, 4}_{k-r}) - 2 \\
&= (n-2)(n-1+k) - rn - 8(k-r) - 2 \\
&= (n-2)(n-1+k) - 8k + r(8-n) - 2 \\
&\leq (n-2)(n-1+k) - 8k - 2
\end{aligned}$$

with equalities if and only if uv is the only cut edge that is not a pendant edge, one component of $G - uv$ containing a single edge, all the cycles are end-blocks, $r = 0$, and $\ell_1 = \cdots = \ell_k = 4$, i.e., $G \cong B_{n,k}$. □

Lemma 3.6. *Let $G \in \mathcal{C}(n,k)$ such that there is a cycle that is not a quadrangle. Then either $Mo(G) < (n-2)(n-1+k) - 8k - 2$ or $Mo(G) \leq (n-2)(n-1) - 8k + 8 - n$ with equality if and only if $G \cong G_n(3, \underbrace{4, \ldots, 4}_{k-1})$.*

Proof. Let $C_1, \ldots, C_k$ be k disjoint cycles of G and $\ell_i = |C_i|$ for $i = 1, \ldots, k$. Suppose that $\ell_1, \ldots, \ell_r$ are odd, and $\ell_{r+1}, \ldots, \ell_k$ are even. By Lemma 3.1, we have $Mo(G) \leq f(\ell_1, \ldots, \ell_k)$ with equality if and only if $G \cong G_n(\ell_1, \ldots, \ell_k)$.

Suppose first that G has an odd cycle. Then $r \geq 1$. By the proof of Lemma 3.1 and Theorem 3.2, we have

$$\begin{aligned}
f(\ell_1, \ldots, \ell_k) &\leq f(\underbrace{3, \ldots, 3}_{r}, \underbrace{4, \ldots, 4}_{k-r}) \\
&= (n-2)(n-1+k) - 8k + r(8-n) \\
&\leq (n-2)(n-1) - 8k + 8 - n
\end{aligned}$$

with equalities if and only if $\ell_1 = 3$ and $\ell_2 = \cdots = \ell_k = 4$. Thus $Mo(G) \leq (n-2)(n-1) - 8k + 8 - n$ with equality if and only if $G \cong G_n(3, \underbrace{4, \ldots, 4}_{k-1})$.

Now suppose that all cycle of G are even. Then $r = 0$. As there is a cycle that is not C_4, we may assume that $\ell_1 \geq 6$. By the proof of Theorem 3.2, we have

$$\begin{aligned} Mo(G) &\leq f(\ell_1, \ldots, \ell_k) \\ &\leq f(6, \underbrace{4, \ldots, 4}_{k-1}) \\ &= (n-2)(n-1+k) - 8k - 16 \\ &< (n-2)(n-1+k) - 8k - 2. \end{aligned}$$

The result follows easily. □

Lemma 3.7. *Let G be a graph in $\mathcal{C}(n,k)$ such that there exists a cycle that is not an end-block. Then $Mo(G) < (n-2)(n-1+k) - 8k - 2$ or $Mo(G) < (n-2)(n-1) - 8k + 8 - n$.*

Proof. If there is a cycle that is not a quadrangle, then by Lemma 3.6, we have $Mo(G) < (n-2)(n-1)-8k+8-n$ or $Mo(G) < (n-2)(n-1+k)-8k-2$. So we may assume that all cycles are quadrangles. Let $C = u_1u_2u_3u_4u_1$ be a quadrangle that is not an end-block, that is, there are at least two of u_1, u_2, u_3, u_4 have degree more than 2 in G. If $d_G(u_1) \geq 3$ and $d_G(u_2) \geq 3$, then

$$\sum_{e=uv \in E(C)} |n_u(e) - n_v(e)| \leq 2(n-4) + 2(n-6) = 4(n-4) - 4,$$

and if $d_G(u_1) \geq 3$ and $d_G(u_3) \geq 3$, then

$$\sum_{e=uv \in E(C)} |n_u(e) - n_v(e)| \leq 6(n-4) < 4(n-4) - 4.$$

Thus, by Lemmas 2.1 and 2.3, we have

$$\begin{aligned} Mo(G) &\leq (n-2)(n-1+k-4k) + 4(n-4)(k-1) + 4(n-4) - 4 \\ &= (n-2)(n-1+k) - 8k - 4 \\ &< (n-2)(n-1+k) - 8k - 2, \end{aligned}$$

as desired. □

By Lemmas 3.5-3.7, we have the following theorem.

Theorem 3.8. *Let G be a graph in $\mathcal{C}(n,k)$ that is not isomorphic to $C^1_{n,k}$, where $n > 8$ and $n \geq 3k+1$.*

(i) If $n = 9$, then $Mo(G) \leq (n-2)(n-1+k) - 8k - 1$ with equality if and only $G \cong G_n(3, \underbrace{4, \ldots, 4}_{k-1})$.

(ii) If $n = 10$, then $Mo(G) \leq (n-2)(n-1+k) - 8k - 2$ with equality if and only if $G \cong G_n(3, \underbrace{4, \ldots, 4}_{k-1})$ or $G \cong B_{n,k}$.

(iii) If $n \geq 11$, then $Mo(G) \leq (n-2)(n-1+k) - 8k - 2$ with equality if and only $G \cong B_{n,k}$.

Proof. As $G \in \mathcal{C}(n,k)$ and G is not isomorphic to $C^1_{n,k}$, there are three cases.
Case 1. G has a cut edge that is not a pendant edge. By Lemma 3.5, we have

$$Mo(G) \leq (n-2)(n-1+k) - 8k - 2$$

with equality if and only if $G \cong B_{n,k}$.
Case 2. There is a cycle that is not a quadrangle. By Lemma 3.6, $Mo(G) < (n-2)(n-1+k) - 8k - 2$ or $Mo(G) \leq (n-2)(n-1) - 8k + 8 - n$ with equality if and only if $G \cong G_n(3, \underbrace{4, \ldots, 4}_{k-1})$.

Case 3. There is a cycle that is not an end-block. By Lemma 3.7, we have $Mo(G) < (n-2)(n-1+k) - 8k - 2$ or $Mo(G) < (n-2)(n-1) - 8k + 8 - n$.

Combining Cases 1–3, the maximum of $Mo(G)$ is equal to $(n-2)(n-1+k)-8k-2$ or $(n-2)(n-1)-8k+8-n$. Note that their difference is $n-10$, which is negative for $n = 9$, zero for $n = 10$, and positive for $n \geq 11$. Now the result follows easily. □

Acknowledgment. The authors would like to thank the referees for their helpful comments and suggestions.

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