

# Difference of Zagreb Indices and Reduced Second Zagreb Index of Cyclic Graphs with Cut Edges

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## Abstract

The classical first and second Zagreb indices of a graph  $G$  are defined as  $M_1(G) = \sum_{v \in V} d_G(v)^2$  and  $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$ , where  $d_G(v)$  is the degree of the vertex  $v$  of graph  $G$ . The reduced second Zagreb index of a graph  $G$  is defined as  $MR_2(G) = \sum_{uv \in E(G)} (d_G(u) - 1)(d_G(v) - 1)$ . Recently, the reduced second Zagreb index and difference of Zagreb indices of trees were studied. In this paper, we determine the graphs having maximum and minimum reduced second Zagreb index in the class of cyclic graphs of order  $n$  with  $k$  cut edges. Moreover difference of the classical Zagreb indices are studied.

## 1 Introduction

Let  $G = (V, E)$  be a connected graph with vertex set  $V(G)$  and edge set  $E(G)$ . Denote by  $d_G(u)$ , the degree of the vertex  $u$  of  $G$ . A pendant vertex is a vertex of degree

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one. An edge of a graph is said to be pendant if one of its end vertices is a pendant vertex. For  $v \in V(G)$ ,  $N_G(v)$  denotes the neighbors of  $v$ . The maximum degree of  $G$  is denoted by  $\Delta(G)$ . A cut edge in a graph  $G$  is an edge whose removal increases the number of connected components of  $G$ . The cyclomatic number of a connected graph is equal to  $\nu = m - n + 1$ , i. e., its number of independent cycles. If  $\nu > 1$  for a graph  $G$  then it is called cyclic graph. If a graph  $G$  has  $\nu = 0$  and  $\nu = 1$  then it is called tree and unicyclic, respectively. For a subset  $E$  of  $E(G)$ , we denote by  $G - E$  the subgraph of  $G$  obtained by deleting the edges in  $E$ . Similarly, the graph obtained from  $G$  by adding a set of edges  $E$  is denoted by  $G + E$ . If  $E = \{e\}$  we write  $G - e$  and  $G + e$ .

The classical first Zagreb index  $M_1$  and second Zagreb index  $M_2$  of graph  $G$  are among the oldest and the most famous topological indices and they are defined as

$$M_1(G) = \sum_{u \in V(G)} (d_G(u))^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

In 1972, the quantities the Zagreb indices were found to occur within certain approximate expressions for the total  $\pi$ -electron energy [19]. In 1975, these graph invariants were proposed to be measures of branching of the carbon-atom skeleton [18]. For details of the mathematical theory and chemical applications of the Zagreb indices, see [4, 10, 12, 16, 17, 25, 27, 29, 35] and the references cited therein. The Zagreb indices were independently studied in the mathematical literature under other names [3, 9, 28].

Caporossi and Hansen [5, 6] conjectured that, for all connected graphs  $G$  it holds that

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \tag{1}$$

and the bound is tight for complete graphs. Although this conjecture is disproved for general graphs [20], it was just the beginning of a long series of studies [1, 2, 21, 24, 26, 33, 34] in which the validity or non-validity of (1) was considered for various classes of graphs.

Recently, much attention is being paid to the comparison of  $M_1$  and  $M_2$  of graph  $G$ . Direct comparisons were obtained on the Zagreb indices for trees [11, 31] and cyclic graphs [7, 22, 30]. The difference of the Zagreb indices of a graph  $G$  has been

studied in [15, 23]. Recently, Furtula et al. [15] showed that the difference of the Zagreb indices is closely related to the vertex-degree-based graph invariant

$$MR_2(G) = \sum_{uv \in E(G)} (d_G(u) - 1)(d_G(v) - 1)$$

and determined a few basic properties of  $MR_2$ .

The extremal first and second Zagreb indices of graphs of order  $n$  with  $k$  cut edges were studied in [8, 13, 14, 32]. Note that a connected graph of order  $n$  has at most  $n - 1$  cut edges and if  $k = n - 1$  then it is a tree. Trees with extremal  $RM_2$  were studied in [15, 23]. For nonnegative integers  $n$  and  $k$  with  $0 \leq k < n - 1$ , we denote by  $\mathcal{G}_n^k$  the set of connected cyclic graphs of order  $n$  with  $k$  cut edges. In this paper, we determine the graphs that have maximum and minimum reduced second Zagreb indices  $RM_2$  in  $\mathcal{G}_n^k$ . Moreover, the graphs with extremal  $M_2 - M_1$ -value are characterized.

## 2 Graphs with maximum $RM_2$ or $M_2 - M_1$

For  $u \in V(G)$ , the set of all pendant neighbors of  $u$  is denoted by  $N_G^1(u)$ .

**Lemma 1.** *Let  $G$  be a connected graph and  $uv$  be a non-pendant cut edge in  $G$ . Let  $N_G^1(u) = N_G(u) \setminus \{v\}$ . Also let  $u_0 \in N_G(u) \setminus \{v\}$  and  $v_0 \in N_G(v) \setminus \{u\}$ . Consider the graph  $G' = G - \{u_0u\} + \{u_0v_0\}$ . Then*

$$RM_2(G') \geq RM_2(G)$$

*with equality holding if and only if  $N_G^1(v_0) = N_G(v_0) \setminus \{v\}$ .*

*Proof.* We have  $d_{G'}(\omega) = d_G(\omega)$  for  $\omega \neq u, v_0$  whereas  $d_{G'}(u) = d_G(u) - 1$  and  $d_{G'}(v_0) = d_G(v_0) + 1$ . Since  $uv$  is a cut edge in  $G$ , we have  $uv_0 \notin E(G)$ . Hence by the definition of the reduced second Zagreb index, we get

$$\begin{aligned} & RM_2(G') - RM_2(G) \\ &= \sum_{u_i \in N_G(u) \setminus \{v\}} (d_G(u_i) - 1)(d_G(u) - 2) + (d_G(u) - 2)(d_G(v) - 1) \\ &+ \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1)d_G(v_0) + d_G(v_0)(d_G(v) - 1) \end{aligned}$$

$$\begin{aligned}
 & - \sum_{u_i \in N_G(u) \setminus \{v\}} (d_G(u_i) - 1)(d_G(u) - 1) - (d_G(u) - 1)(d_G(v) - 1) \\
 & - \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1)(d_G(v_0) - 1) - (d_G(v_0) - 1)(d_G(v) - 1) \\
 & = \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1) - \sum_{u_i \in N_G(u) \setminus \{v\}} (d_G(u_i) - 1) \\
 & = \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1) \geq 0. \tag{2}
 \end{aligned}$$

since  $d_G(u_i) = 1$  for all  $u_i \in N_G(u) \setminus \{v\}$  and  $d_G(x) \geq 1$  for all  $x \in N_G(v_0) \setminus \{v\}$ .

Suppose now that equality holds in (2). Then we must have

$$\sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1) = 0.$$

Hence  $d_G(x) = 1$  for all  $x \in N_G(v_0) \setminus \{v\}$ , that is  $N_G^1(v_0) = N_G(v_0) \setminus \{v\}$ . This completes the proof. ■

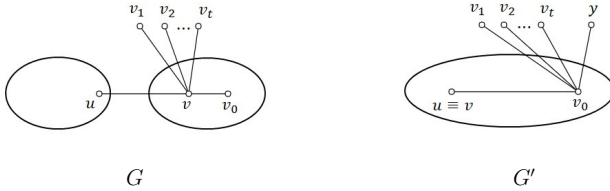


Fig. 1. The graphs  $G$  and  $G'$

An edge  $uv$  of a graph  $G$  is said to be contracted if it is deleted and its end vertices  $u$  and  $v$  are identified, the obtained graph is denoted by  $G \cdot uv$ . Also the identified vertex in  $G \cdot uv$  is denoted by one of  $u$  and  $v$ . Denote by  $\mathcal{G}_{n,m}$ , the set of connected cyclic graphs of order  $n$  with  $m$  edges.

**Proposition 2.** *Let  $G$  be a graph in  $\mathcal{G}_{n,m}$ . If  $RM_2(G)$  is maximum, then all cut edges of  $G$  are pendant.*

*Proof.* Conversely, suppose that  $uv$  is a non-pendant cut edge in  $G$ . We distinguish the following two cases.

*Case (1) :*  $N_G^1(u) = N_G(u) \setminus \{v\}$  or  $N_G^1(v) = N_G(v) \setminus \{u\}$ .

Assume that  $N_G^1(u) = N_G(u) \setminus \{v\}$ . If  $N_G^1(v_i) = N_G(v_i) \setminus \{v\}$  for all  $v_i$  in  $N_G(v)$ , then

$G$  is a tree with diameter at most four and it contradicts the assumption that  $\mathcal{G}_{n,m}$ . Hence there exists a vertex  $v_0 \in N_G(v) \setminus \{u\}$  such that  $N_G^1(v_0) \neq N_G(v_0) \setminus \{v\}$ . Let  $u_0 \in N_G(u) \setminus \{v\}$ . We consider the graph  $G' = G - \{u_0u\} + \{u_0v_0\}$ . Then  $G' \in \mathcal{G}_{n,m}$  and by Lemma 1, we have

$$RM_2(G') > RM_2(G).$$

But it contradicts the fact that  $RM_2(G)$  is maximum in  $\mathcal{G}_{n,m}$ .

*Case (2) :*  $N_G^1(u) \neq N_G(u) \setminus \{v\}$  and  $N_G^1(v) \neq N_G(v) \setminus \{u\}$ .

Assume that  $|N_G^1(u)| \geq |N_G^1(v)|$ . Then we prove that a connected component containing vertex  $v$  is a tree in the graph  $G - uv$ . Let  $N_G^1(v) = \{v_1, v_2, \dots, v_t\}$  and  $v_0$  be a vertex in  $N_G(v) \setminus (N_G^1(v) \cup \{u\})$  such that  $\sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1)$  is maximum. Also let  $G^*$  be the obtained graph by joining a pendant vertex  $y$  to the vertex  $v_0$  of  $G - uv$ . Consider the graph (see Fig. 1).

$$G' = G^* - \{vv_1, vv_2, \dots, vv_t\} + \{v_0v_1, v_0v_2, \dots, v_0v_t\}.$$

Then  $G' \in \mathcal{G}_{n,m}$ . Also we have  $d_{G'}(y) = 1$  and  $d_{G'}(\omega) = d_G(\omega)$  for  $\omega \neq u, v_0$  whereas  $d_{G'}(u) = d_G(u) + d_G(v) - t - 2$ ,  $d_{G'}(v_0) = d_G(v_0) + t + 1$ . For convinience, set  $S = \{v_1, v_2, \dots, v_t, u, v_0\}$ . Then by the definition of the reduced second Zagreb index, we get

$$\begin{aligned} RM_2(G') - RM_2(G) &= \sum_{x \in N_G(u) \setminus \{v\}} (d_G(x) - 1)(d_G(u) + d_G(v) - t - 3) \\ &+ \sum_{x \in N_G(v) \setminus S} (d_G(x) - 1)(d_G(u) + d_G(v) - t - 3) \\ &+ (d_G(u) + d_G(v) - t - 3)(d_G(v_0) + t) \\ &+ \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1)(d_G(v_0) + t) \\ &- \sum_{x \in N_G(u) \setminus \{v\}} (d_G(x) - 1)(d_G(u) - 1) - (d_G(u) - 1)(d_G(v) - 1) \\ &- \sum_{x \in N_G(v) \setminus S} (d_G(x) - 1)(d_G(v) - 1) - (d_G(v_0) - 1)(d_G(v) - 1) \\ &- \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1)(d_G(v_0) - 1) \end{aligned}$$

that is,

$$\begin{aligned}
 RM_2(G') - RM_2(G) &= \sum_{x \in N_G(u) \setminus \{v\}} (d_G(x) - 1)(d_G(v) - t - 2) \\
 &+ \sum_{x \in N_G(v) \setminus S} (d_G(x) - 1)(d_G(u) - t - 2) \\
 &+ \sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1)(t + 1) \\
 &- (d_G(u) - t - 2)(d_G(v) - t - 2) \\
 &+ (d_G(u) - t - 2)(d_G(v_0) - 1). \tag{3}
 \end{aligned}$$

Since  $uv$  is a non-pendant cut edge in  $G$ ,  $N_G^1(u) \neq N_G(u) \setminus \{v\}$  and  $N_G^1(v) \neq N_G(v) \setminus \{u\}$ , we have

$$d_G(u) \geq t + 2 \quad \text{and} \quad d_G(v) \geq t + 2. \tag{4}$$

Now from (4) and  $d_G(x) \geq 2$  for all  $x \in N_G(v) \setminus S$ , one can easily see that

$$\sum_{x \in N_G(v) \setminus S} (d_G(x) - 1)(d_G(u) - t - 2) - (d_G(u) - t - 2)(d_G(v) - t - 2) \geq 0. \tag{5}$$

Therefore from (4), (3) and (5), we get

$$RM_2(G') \geq RM_2(G). \tag{6}$$

If the above inequality is strict, then it contradicts the fact that  $RM_2(G)$  is maximum in  $\mathcal{G}_{n,m}$ .

Suppose now that equality holds in (6). Then the equality holds in (5) and the remaining summands in (3) must be zero. Thus from (3), we have

$$\sum_{x \in N_G(u) \setminus \{v\}} (d_G(x) - 1)(d_G(v) - t - 2) = (d_G(u) - t - 2)(d_G(v_0) - 1) = 0 \tag{7}$$

and

$$\sum_{x \in N_G(v_0) \setminus \{v\}} (d_G(x) - 1) = 0. \tag{8}$$

Since  $N_G^1(u) \neq N_G(u) \setminus \{v\}$ , there exists a vertex  $x$  in  $N_G(u) \setminus \{v\}$  such that  $d_G(x) \geq 2$ . Also since the vertex  $v_0$  in  $N_G(v) \setminus (N_G^1(v) \cup \{u\})$ , we have  $d_G(v_0) \geq 2$ . Thus from (7), we get

$$d_G(u) = d_G(v) = t + 2. \tag{9}$$

From (8),  $d_G(x) = 1$  for all  $x \in N_G(v_0) \setminus \{v\}$ , that is  $N_G^1(v_0) = N_G(v_0) \setminus \{v\}$ . By the choice of the vertex of  $v_0$ , we have

$$N_G^1(v_i) = N_G(v_i) \setminus \{v\} \quad \text{for all } v_i \in N_G(v) \setminus \{u\}. \quad (10)$$

From this, we conclude that a connected component containing vertex  $v$  is a tree in  $G - uv$ .

On the other hand from (9),  $|N_G^1(u)| = t$  because  $d_G(v) \geq 2$  and there exists a vertex  $x$  in  $N_G(u) \setminus \{v\}$  such that  $d_G(x) \geq 2$ . Thus we have  $N_G^1(v) = N_G^1(u)$ . Therefore, similarly the above we can prove that a connected component containing vertex  $u$  is also a tree in  $G - uv$ . Hence,  $G$  is a tree with diameter at most 5. But it contradicts the assumption that  $G \in \mathcal{G}_{n,m}$ . ■

The number of cut edges of the considered graph  $G'$  in each case of the proof of Proposition 2 is equal to the number of cut edges of  $G$ . i.e., If  $G \in \mathcal{G}_n^k$ , then also  $G' \in \mathcal{G}_n^k$ . Hence we have the following corollary.

**Corollary 3.** *Let  $G$  be a graph in  $\mathcal{G}_n^k$ . If  $RM_2(G)$  is maximum, then all  $k$  cut edges of  $G$  are pendant.*

**Lemma 4.** *Let  $G$  be a connected graph and  $uv \notin E(G)$ . Consider the graph  $G' = G + uv$ . Then  $RM_2(G') > RM_2(G)$ .*

*Proof.* We have  $d_G(w) = d_{G'}(w)$  for  $w \neq u, v$  whereas  $d_{G'}(u) = d_G(u) + 1$  and  $d_{G'}(v) = d_G(v) + 1$ . Hence by the definition of  $RM_2$ , we get

$$\begin{aligned} & RM_2(G') - RM_2(G) \\ &= d_G(u) \sum_{x \in N_G(u)} (d_G(x) - 1) + d_G(v) \sum_{x \in N_G(v)} (d_G(x) - 1) + d_G(u)d_G(v) \\ &\quad - (d_G(u) - 1) \sum_{x \in N_G(u)} (d_G(x) - 1) - (d_G(v) - 1) \sum_{x \in N_G(v)} (d_G(x) - 1) \\ &= \sum_{x \in N_G(u)} (d_G(x) - 1) + \sum_{x \in N_G(v)} (d_G(x) - 1) + d_G(u)d_G(v) > 0 \end{aligned}$$

since  $G$  is connected. Thus  $RM_2(G') > RM_2(G)$ . ■

Let  $N$  be positive integer,  $N \geq 2$ .  $K_N$  be a complete graph of order  $N$ , and let  $v_1, v_2, \dots, v_N$  be its vertices. For  $i = 1, 2, \dots, N$ , let  $r_i$  be non-negative integers,

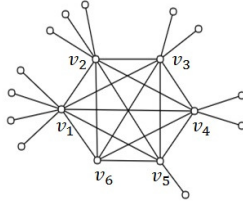


Fig. 2. The graph  $G(4, 3, 2, 2, 1, 0)$  in  $\mathcal{G}(18, 6) \subseteq \mathcal{G}_{18}^{12}$ .

labeled so that  $r_1 \geq r_2 \geq \dots \geq r_N$ . Construct the graph  $G(r_1, r_2, \dots, r_N)$  by attaching  $r_i$  pendent vertices to the vertex  $v_i$  of  $K_N$ . The graph  $G(r_1, r_2, \dots, r_N)$  has thus  $n = N + \sum_{i=1}^N r_i$  vertices. For given values  $N \geq 2$  and  $n \geq N$ , the set of all graphs  $G(r_1, r_2, \dots, r_N)$  constructed in the above described manner is denoted by  $\mathcal{G}(n, N)$  (see Fig. 2). Obviously  $\mathcal{G}(n, N) \subseteq \mathcal{G}_n^{n-N}$ .

**Proposition 5.** *Let  $G$  be a graph in  $\mathcal{G}_n^k$ . If  $G$  has maximum the reduced second Zagreb index, then  $G \in \mathcal{G}(n, n - k)$ .*

*Proof.* By Corollary 3, all  $k$  cut edges of  $G$  are pendent. If  $G \notin \mathcal{G}(n, n - k)$  then there exist two non-adjacent vertices of degrees greater than one in the graph  $G$ . We join these two non-adjacent vertices and denote by  $G'$  the obtained graph. Then  $G' \in \mathcal{G}_n^k$  and  $RM_2(G') > RM_2(G)$  by Lemma 4. But it contradicts the fact that  $RM_2(G)$  is maximum in  $\mathcal{G}_n^k$ . ■

**Theorem 1.** *Let  $G$  be a graph in  $\mathcal{G}_n^k$ . If  $RM_2(G)$  is maximum then  $G \cong G(r_1, r_2, \dots, r_{n-k})$ , where  $|r_p - r_q| \leq 1$  for  $1 \leq p, q \leq n - k$ .*

*Proof.* By Proposition 5, we have  $G \in \mathcal{G}(n, n - k)$ . Hence there exist nonnegative integers  $r_1, r_2, \dots, r_{n-k}$ , labeled so that  $r_1 \geq r_2 \geq \dots \geq r_{n-k}$  with  $r_1 + r_2 + \dots + r_{n-k} = k$  and  $G = G(r_1, r_2, \dots, r_{n-k})$ . Now we show that  $|r_p - r_q| \leq 1$  for  $1 \leq p, q \leq n - k$ .

Let  $v_1, v_2, \dots, v_{n-k}$  be vertices of the graph  $G(r_1, r_2, \dots, r_{n-k})$  whose degrees are greater than one. Then  $d_G(v_i) = r_i + n - k - 1$  for  $i = 1, 2, \dots, n - k$ . By definition of the reduced second Zagreb index, we get

$$RM_2(G) = \sum_{1 \leq i < j \leq n-k} (r_i + n - k - 2)(r_j + n - k - 2)$$



$$\begin{aligned}
 &= \sum_{1 \leq i < j \leq n-k} r_i r_j + (n-k-2) \sum_{1 \leq i < j \leq n-k} (r_i + r_j) + (n-k-2)^2 \binom{n-k}{2} \\
 &= \sum_{1 \leq i < j \leq n-k} r_i r_j + (n-k-1)(n-k-2) \left( k + \frac{(n-k)(n-k-2)}{2} \right)
 \end{aligned}$$

since  $r_1 + r_2 + \dots + r_{n-k} = k$ . Therefore  $RM_2(G)$  is maximum if and only if  $\sum_{1 \leq i < j \leq n-k} r_i r_j$  is maximum. Let now  $\sum_{1 \leq i < j \leq n-k} r_i r_j$  with  $r_1 + r_2 + \dots + r_{n-k} = k$  is maximum.

Suppose that there are integers  $r_p$  and  $r_q$  in  $G(r_1, r_2, \dots, r_{n-k})$  such that  $r_p - r_q \geq 2$ . Then we transform  $G(r_1, r_2, \dots, r_{n-k})$  into another graph  $G(r'_1, r'_2, \dots, r'_{n-k})$  with  $r'_p = r_p - 1$ ,  $r'_q = r_q + 1$  and  $r'_i = r_i$  for all  $i \neq p, q$ .

An elementary calculation gives

$$\begin{aligned}
 \sum_{1 \leq i < j \leq n-k} r'_i r'_j - \sum_{1 \leq i < j \leq n-k} r_i r_j &= (r_p - 1) \left( 1 + \sum_{i \neq p} r_i \right) + (r_q + 1) \sum_{i \neq p, q} r_i \\
 &\quad - r_p \sum_{i \neq p} r_i - r_q \sum_{i \neq p, q} r_i = r_p - r_q - 1 > 0
 \end{aligned}$$

and it contradicts that  $\sum_{1 \leq i < j \leq n-k} r_i r_j$  is maximum. Thus we have  $|r_p - r_q| \leq 1$ . ■

The reduced second Zagreb index satisfies the identity [15]

$$RM_2(G) - |E(G)| = M_2(G) - M_1(G). \tag{11}$$

By using the identity (11), similarly as above we prove that all results in this section hold for the difference of  $M_2$  and  $M_1$ . Hence we have the following theorem.

**Theorem 2.** *Let  $G$  be a graph in  $\mathcal{G}_n^k$ . If  $M_2(G) - M_1(G)$  is maximum then  $G \cong G(r_1, r_2, \dots, r_{n-k})$ , where  $|r_p - r_q| \leq 1$  for  $1 \leq p, q \leq n-k$ .*

### 3 Graphs with minimum $RM_2$ or $M_2 - M_1$

The vertex independence number of a graph, often called simply the independence number, is the cardinality of the largest independent vertex set, i.e., the size of a maximum independent vertex set. The cycle graph with  $n$  vertices is called  $C_n$ . Let

$\Gamma$  be a class of graphs  $H = (V, E)$  in  $\mathcal{G}_\nu$  such that  $2 \leq d_i \leq 3$  (there exists a vertex  $v_k$  in  $H$  such that  $d_k = 3$ ) for all  $v_i \in V(H)$  and the set of vertices of degree three is an independent set in  $H$ . The cycle of a graph  $G$  is denoted by  $C(G)$ . We denote the class of connected graphs with cyclomatic number  $\nu \geq 1$  by  $\mathcal{G}_\nu$ .

**Lemma 6.** [30] Let  $G$  be a graph in  $\mathcal{G}_\nu$ . Then

$$M_2(G) - M_1(G) \geq 6(\nu - 1)$$

with equality holding if and only if  $G \cong C_n$  or  $G \in \Gamma$

$S(m_1, m_2, \dots, m_p)$  is a unicyclic graph of order  $n$  with girth  $p$  and  $n - p$  pendant vertices, where  $m_i$  is the number of pendant vertices adjacent to  $i$ -th vertex of the cycle. We consider that the vertices in the cycle are numbered clockwise. Clearly  $\sum_{i=1}^p m_i = n - p$  and  $S(0, 0, \dots, 0) = C_n$ . Denote  $\mathcal{S} = \{S(m_1, m_2, \dots, m_p) \mid m_{i-1} = m_{i+1} = 0 \text{ for } m_i \neq 0, 2 \leq i \leq p, m_{p+1} = m_1\}$ .

**Lemma 7.** [22] Let  $G$  be a unicyclic graph with cycle length  $p$ . Then

$$M_2(G) - M_1(G) \geq \sum_{u \in V(C(G))} d_G(u) - 2p \tag{12}$$

with equality if and only if  $G \in \mathcal{S}$ .

Let  $B_n^p$  ( $p \leq n$ ) be the unicyclic graph with  $n - p$  pendant vertices and its each pendant vertex is adjacent to one vertex of  $C_p$ . In particular,  $B_n^n = C_n$ , a cycle of order  $n$ . Denote by  $C_{n,\Delta}^p$  ( $\Delta \geq 4$ ) a unicyclic graph obtained by identifying two pendant vertices of the path  $P_{n-\Delta-p+2}$  with the center of star  $K_{1,\Delta-1}$  and one vertex of cycle  $C_p$ , respectively. Denote  $\mathcal{C}_\Delta = \{C_{n,\Delta}^p \mid 3 \leq p \leq n - \Delta - 1\}$ .

**Lemma 8.** [22] Let  $G$  be a unicyclic graph of order  $n$  with maximum degree  $\Delta$ . Then

$$M_2(G) - M_1(G) \geq \begin{cases} \Delta - 2 & \text{if } d = 0 \\ \Delta & \text{if } d = 1 \\ 2 & \text{if } d > 1, \end{cases} \tag{13}$$

where  $d$  is the length of the shortest path from the maximum degree vertex  $u$  to the cycle  $C(G)$ . The equalities hold in (13) if and only if  $G \cong B_n^p$ ,  $G \cong C_{n,\Delta}^p$ ,  $\Delta + p = n$ , and  $G \in \mathcal{C}_\Delta$ , respectively.

Denote by  $C_{n,3}^p$  ( $n - p \geq 4$ ) a unicyclic graph obtained by identifying two pendant vertices of the path  $P_{n-p-1}$  with the center of star  $K_{1,2}$  and one vertex of cycle  $C_p$ , respectively. Also denote by  $C_{n,2}^p$  ( $n - p \geq 2$ ) a unicyclic graph obtained by identifying one pendant vertex of the path  $P_{n-p+1}$  with one vertex of cycle  $C_p$ . Denote  $\mathcal{U}_n^p = \mathcal{C}_\Delta \cup \{C_{n,2}^p, C_{n,3}^p\}$ , where  $p \geq 3$ . Obviously  $\mathcal{U}_n^p \subseteq \mathcal{G}_n^{n-p}$  and each unicyclic graph  $G$  in  $\mathcal{U}_n^p$  has  $n - p$  cut edges.

Now we are ready to characterize lower bound on  $M_2 - M_1$  and  $RM_2$  in  $\mathcal{G}_n^k$ . From the identity (11), it follows that  $RM_2(G)$  is minimum if and only if  $M_2(G) - M_1(G)$  is minimum in  $\mathcal{G}_n^k$ . Therefore, we give the proof of the following results for only  $M_2 - M_1$ .

**Proposition 9.** *Let  $G$  be a graph in  $\mathcal{G}_n^k$ . If  $M_2(G) - M_1(G)$  or  $RM_2$  is minimum, then  $G$  is unicyclic.*

*Proof.* Since  $G \in \mathcal{G}_n^k$ , we have  $\nu \geq 1$ . It is easy to see that  $M_2(H) - M_1(H) = 2$  for all  $H \in \mathcal{U}_n^{n-k} \subseteq \mathcal{G}_n^k$ . Hence  $M_2(G) - M_1(G) \leq 2$  since  $M_2(G) - M_1(G)$  is minimum. If  $G$  is not unicyclic graph, then  $\nu \geq 2$  and by Lemma 6, we get

$$M_2(G) - M_1(G) \geq 6(\nu - 1) \geq 6.$$

This completes the proof. ■

We denote by  $\mathcal{A}_n^2$ , a class of unicyclic graphs of order  $n$  obtained by attaching two pendant edges to the two non-adjacent vertices of the cycle  $C_{n-2}$ .

**Theorem 3.** *Let  $G$  be a graph in  $\mathcal{G}_n^k$ . Also let  $M_2(G) - M_1(G)$  or  $RM_2(G)$  be minimum.*

- (i) If  $k = 0$ , then  $G \cong C_n$ .
- (ii) If  $k = 1$ , then  $G \cong B_n^{n-1}$ .
- (iii) If  $k = 2$ , then  $G \cong C_{n,2}^{n-1}$ ,  $G \cong B_n^{n-2}$ , or  $G \in \mathcal{A}_n^2$
- (iv) If  $k \geq 3$ , then  $G \in \mathcal{U}_n^{n-k}$ .

*Proof.* We mentioned that  $RM_2(G)$  is minimum if and only if  $M_2(G) - M_1(G)$  is minimum in  $\mathcal{G}_n^k$ . Therefore we characterize the graphs such that  $M_2(G) - M_1(G)$  is minimum.

Since  $M_2(G) - M_1(G)$  is minimum in  $\mathcal{G}_n^k$ ,  $G$  is unicyclic graph by Proposition 9. Hence, the first two parts of Theorem 3 are trivial.

(iii) If  $G \cong C_{n,2}^{n-1}$ ,  $G \cong B_n^{n-2}$ , or  $G \in \mathcal{A}_n^2$  then one can easily see that  $M_2(G) - M_1(G) = 2$ . Otherwise  $G$  is a unicyclic graph of order  $n$  obtained by attaching two pendant edges to the two adjacent vertices of the cycle  $C_{n-2}$  and in this case  $M_2(G) - M_1(G) = 3$ .

(iv) If  $G \in \mathcal{U}_n^{n-k}$  then  $M_2(G) - M_1(G) = 2$ . Suppose that  $G \notin \mathcal{U}_n^{n-k}$ . To show that  $M_2(G) - M_1(G) > 2$ , we distinguish the following two cases. Let  $d$  be the length of the shortest path from the maximum degree vertex to the cycle  $C(G)$ .

*Case (1) :*  $d \geq 1$ . If  $d = 1$  then  $\Delta \geq 3$  and  $M_2(G) - M_1(G) \geq \Delta \geq 3$  by Lemma 8. If  $d > 1$  then  $M_2(G) - M_1(G) > 2$  because  $\mathcal{C}_\Delta$  is a subset of  $\mathcal{U}_n^{n-k}$ .

*Case (2) :*  $d = 0$ . If  $\Delta \geq 5$  then  $M_2(G) - M_1(G) \geq \Delta - 2 \geq 3$  by Lemma 8. If  $\Delta = 4$  then  $M_2(G) - M_1(G) \geq \Delta - 2 = 2$  with equality if and only if  $G \cong B_n^{n-k}$ . From the definition of  $B_n^{n-k}$ , we have  $k = \Delta - 2 = 2$  and it contradicts the assumption that  $k \geq 3$ . Let now  $\Delta = 3$ . Then all vertices of degree 3 must be on the cycle. Since  $G \notin \mathcal{U}_n^{n-k}$ , there are at least two vertices of degree three on the cycle. Then by Lemma 7

$$M_2(G) - M_1(G) \geq \sum_{u \in V(C(G))} d_G(u) - 2(n - k) \geq 2$$

with equality if and only if  $G \in \mathcal{A}_n^2$ . Hence if  $M_2(G) - M_1(G) = 2$ , then it contradicts the assumption that  $k \geq 3$ . ■

**Corollary 10.** *Let  $G$  be a cyclic graph. Then*

- (i)  $M_2(G) - M_1(G) = 0$  or  $RM_2(G) = n$  if and only if  $G \cong C_n$ .
- (ii)  $M_2(G) - M_1(G) = 1$  or  $RM_2(G) = n + 1$  if and only if  $G \cong B_n^{n-1}$ .
- (iii)  $M_2(G) - M_1(G) = 2$  or  $RM_2(G) = n + 2$  if and only if  $G \cong C_{n,2}^{n-1}$ ,  $G \cong B_n^{n-2}$ ,  $G \in \mathcal{A}_n^2$  or  $G \in \mathcal{U}_n^{n-k}$ .

## References

- [1] H. Abdo, D. Dimitrov, I. Gutman, On the Zagreb indices equality, *Discr. Appl. Math.* **160** (2012) 1–8.
- [2] V. Andova, S. Bogojev, D. Dimitrov, M. Pilipczuk, R. Škrekovski, On the Zagreb index inequality of graphs with prescribed vertex degrees, *Discr. Appl. Math.* **159** (2011) 852–858.

- [3] B. Bollobás, P. Erdős, A. Sarkar, Extremal graphs for weights, *Discr. Math.* **200** (1999) 5–19.
- [4] B. Borovičanin, T. Aleksić Lampert, On the maximum and minimum Zagreb indices of trees with a given number of vertices of maximum degree, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 81–96.
- [5] G. Caporossi, P. Hansen, Variable neighborhood search for extremal graphs: 1 The AutoGraphiX system, *Discr. Math.* **212** (2000) 29–44.
- [6] G. Caporossi, P. Hansen, Variable neighborhood search for extremal graphs. 5. Three ways to automate finding conjectures, *Discr. Math.* **276** (2004) 81–94.
- [7] G. Caporossi, P. Hansen, D. Vukičević, Comparing Zagreb indices of cyclic graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 441–451.
- [8] S. Chen, W. Liu, Extremal Zagreb indices of graphs with a given number of cut edges, *Graphs Comb.* **30** (2014) 109–118.
- [9] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, *Discr. Math.* **285** (2004) 57–66.
- [10] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52**(2004) 103–112.
- [11] K. C. Das, I. Gutman, B. Horoldagva, Comparison between Zagreb indices and Zagreb coindices of trees, *MATCH Commun. Math. Comput. Chem.* **68**(2012) 189–198.
- [12] C. Elphick, T. Réti, On the relations between the Zagreb indices, clique numbers and walks in graphs, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 19–34.
- [13] Y. Feng, X. Hu, S. Li, On the extremal Zagreb indices of graphs with cut edges, *Acta Appl. Math.* **110** (2010) 667–684.
- [14] Y. Feng, X. Hu, S. Li, Erratum to: On the extremal Zagreb indices of graphs with cut edges, *Acta Appl. Math.* **110** (2010) 685–685.
- [15] B. Furtula, I. Gutman, S. Ediz, On difference of Zagreb indices, *Discr. Appl. Math.* **178** (2014) 83–88.
- [16] I. Gutman, K. C. Das, The first Zagreb indices 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
- [17] I. Gutman, B. Furtula, C. Elphick, Three new/old vertex–degree–based topological indices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 617–682.
- [18] I. Gutman, B. Rušćić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals, XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.
- [19] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total  $\pi$ -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1971) 535–538.

- [20] P. Hansen, D. Vukičević, Comparing the Zagreb indices, *Croat. Chem. Acta* **80** (2007) 165–168.
- [21] B. Horoldagva, K. C. Das, On comparing Zagreb indices of graphs, *Hacetate J. Math. Statist.* **41** (2012) 223–230.
- [22] B. Horoldagva, K. C. Das, Sharp lower bounds for the Zagreb indices of unicyclic graphs, *Turk. J. Math.* **39** (2015) 595–603.
- [23] B. Horoldagva, K. C. Das, T. Selenge, Complete characterization of graphs for direct comparing Zagreb indices, *Discr. Appl. Math.* **215** (2016) 146–154.
- [24] B. Horoldagva, S. G. Lee, Comparing Zagreb indices for connected graphs, *Discr. Appl. Math.* **158** (2010) 1073–1078.
- [25] S. Li, H. Zhou, On the maximum and minimum Zagreb indices of graphs with connectivity at most  $k$ , *Appl. Math. Lett.* **23** (2010) 128–132.
- [26] B. Liu, On a conjecture about comparing Zagreb indices, in: I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008, pp. 205–209.
- [27] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
- [28] U. N. Peled, R. Petreschi, A. Sterbini,  $(n, e)$ -graphs with maximum sum of squares of degrees, *J. Graph Theory* **31** (1999) 283–295.
- [29] T. Selenge, B. Horoldagva, Maximum Zagreb indices in the class of  $k$ -apex trees, *Korean J. Math.* **23** (2015) 401–408.
- [30] T. Selenge, B. Horoldagva, K. C. Das, Direct comparison of the variable Zagreb indices of cyclic graphs, *MATCH Commun. Math. Comput. Chem.*, in press.
- [31] D. Stevanović, M. Milanić, Improved inequality between Zagreb indices of trees, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 147–156.
- [32] L. Sun, A simple proof on the extremal Zagreb indices of graphs with cut edges, *Appl. Math. E-Notes* **11** (2011) 232–237.
- [33] L. Sun, T. Chen, Comparing the Zagreb indices for graphs with small difference between the maximum and minimum degrees, *Discr. Appl. Math.* **157** (2009) 1650–1654.
- [34] D. Vukičević, A. Graovac, Comparing Zagreb  $M_1$  and  $M_2$  indices for acyclic molecules, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 587–590.
- [35] K. Xu, K. C. Das, S. Balachandran, Maximizing the Zagreb indices of  $(n, m)$ -graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 641–654.