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Sharp bounds on Zagreb indices of cacti with k pendant vertices

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Abstract. For a (molecular) graph, the first Zagreb index M_1 is equal to the sum of squares of its vertex degrees, and the second Zagreb index M_2 is equal to the sum of products of degrees of pairs of adjacent vertices. A connected graph G is a cactus if any two of its cycles have at most one common vertex. In this paper, we investigate the first and the second Zagreb indices of cacti with k pendant vertices. We determine sharp bounds for M_1-, M_2-values of n-vertex cacti with k pendant vertices. As a consequence, we determine the n-vertex cacti with maximal Zagreb indices and we also determine the cactus with a perfect matching having maximal Zagreb indices.

1. Introduction

A single number that can be used to characterize some property of the graph of a molecule is called a *topological index*. For quite some time there has been rising interest in the field of computational chemistry in topological indices that capture the structural essence of compounds. The interest in topological indices is mainly related to their use in nonempirical quantitative structure-property relationships and quantitative structure-activity relationships. One of the most important topological indices is the well-known Randić index.

In 1975, Randić proposed a structural descriptor called *branching index* [57] that later became well-known *Randić connectivity index*, which is the most used molecular descriptor in QSPR and QSAR; see [20, 33, 34, 55, 63]. The name connectivity index that replaced the original Randić term branching index has been suggested by Kier as stated by Randić [58]. The first paper in which the Randić connectivity index was used in QSAR appeared soon after the original publication, also in [35]. Mathematicians also exhibited considerable interest in the properties of the Randić connectivity index; see [6, 7, 23, 24, 38, 42, 43, 54, 56]. The Randić connectivity index has also evolved into several variants [20, 36, 37, 55, 58, 59, 67].

The Randić connectivity index has been extended as the *general Randić connectivity index* and *general zeroth-order Randić connectivity index*, and then the *Zagreb indices* appear to be the special cases of them [13, 14, 29, 43]. The Zagreb indices have been introduced in 1972 in the report of Gutman and Trinajstić on the topological basis of the π-electron energy [25]—-two terms appeared in the topological formula for the total π-energy of alternant hydrocarbons, which were in 1975 used by Gutman et al. [26] as branching indices, denoted by M_1 and M_2, and later employed as molecular descriptors in QSPR and QSAR; see [3, 4]. The name Zagreb indices instead of the term branching indices was first used by Balaban et al. [1].

There are three groups of closed related problems which have attracted the attention of researchers for a long time:

- How $M_1(G)$ (respectively, $M_2(G)$) depends on the structure of G.
- Given a set of molecular graph $\mathscr{G}$, find upper and lower bounds for $M_1(G)$ and $M_2(G)$ of graphs in $\mathscr{G}$ and characterize the graphs in which the maximal (respectively, minimal) M_1-, M_2-value is attained, respectively.

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• How $M_1(G)$ and $M_2(G)$ can be efficiently calculated, especially without the aid of a computer.

In view of these problems, it is not surprising that in the chemical literature there are numerous studies of properties of the Zagreb indices of molecular graphs. In fact, investigation of the above problems mainly deal with graphs whose cyclomatic number is at most 2 as the sole objects [15, 18, 31, 40, 48, 56, 62, 66]; Mathematical and computational properties of Zagreb indices have also been considered [17, 27, 28, 53, 69, 70]. The reformulation of Zagreb indices are also attract more and more researchers' attention [22, 61]. Other direction of investigation include studies of relation between $M_1(G)$ (respectively, $M_2(G)$) and the corresponding invariant of elements of the graph G (vertices, pendants, cut-edges, diameter, maximum degree, girth, perfect matching, connectivity and cut-vertices); see [11, 15, 16, 19, 31, 39–41, 46, 47, 62, 69, 70]. For the applications of the Zagreb indices and their variants to modelling properties of molecules, one may refer to [9, 30, 49–51, 65].

In addition to the myriad applications of the Zagreb indices in chemistry there are many situations in communication, facility location, cryptology, etc., that are effectively modeled by a connected graph G satisfying certain restriction. In light of the information available for M_1 and M_2 of trees, unicyclic graphs, bicyclic graphs, et al., it is natural to consider other classes of graphs, and the n-vertex cactus graph with k pendant vertices is a reasonable starting point for such an investigation. The cactus graph has been considered in mathematical literature [2, 8, 12, 21, 32, 45, 71], whereas to our best knowledge, the Zagreb indices of n-vertex cacti with k pendant vertices were, so far, not considered in the chemical literature. On the other hand, cacti represent important class of molecules [44, 45].

In this paper, we determine the n-vertex cacti with k pendant vertices having extremal (maximal and minimal) values of M_1 and M_2. As a consequence, we determine the n-vertex cacti having the maximal Zagreb indices, as well we determine the n-vertex cacti with a perfect matching having the maximal Zagreb indices. In our exposition we will use the terminology and apparatus of (chemical) graph theory (see [5, 10, 64]).

2. Preliminaries

Let $G = (V_G, E_G)$ be a simple graph with vertex set $V_G = \{v_1, v_2, \dots, v_n\}$ and edge set E_G. $n = |G|$ $(= |V_G|)$ is the order of G. Throughout the paper we denote by P_n and C_n the n-vertex graph equals to the path and cycle, respectively. $G - v$, $G - uv$ denote the graph obtained from G by deleting a vertex $v \in V_G$, or an edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex, or edge, is deleted). Similarly, $G + v$ and $G + uv$ are obtained from G by adding a vertex $v \notin V_G$, or an edge $uv \notin E_G$, respectively (note, if a vertex v is added to G, then its neighbours in G should be specified somehow). For a vertex x of the graph G, we denote the neighborhood and the degree of x by $N_G(x)$ and $d_G(x)$ (or $N(x)$ and $d(x)$ for short), respectively. In particular, let $N[x] = N(x) \cup \{x\}$. For $u, v \in V_G$, let $d(u, v)$ denote the distance between u and v in G. In the whole of our context denote by $\mathscr{C}_{n,k}$ the set of all connected cacti on n vertices with k pendants. The *Randić connectivity index* [57] $R = R(G)$ of G is defined as

$$R = R(G) = \sum_{uv \in E_G} (d_G(u)d_G(v))^{-1/2}.$$

The *zeroth order Randić connectivity index* [42, 43] $R' = R'(G)$ is defined as

$$R' = R'(G) = \sum_{u \in V_G} (d_G(u))^{-1/2}.$$

The *first Zagreb index* $M_1 = M_1(G)$ and the *second Zagreb index* $M_2 = M_2(G)$ [17, 25–27, 53] of the graph G are given by

$$M_1 = M_1(G) = \sum_{u \in V_G} d_G(u)^2, \quad M_2 = M_2(G) = \sum_{uv \in E_G} d_G(u)d_G(v).$$

Further on we will need the following lemmas.

Lemma 2.1. *Let u, v be two distinct vertices of a connected graph G. Suppose that $\{v_1, v_2, \dots, v_s\} \subseteq N(v) \setminus N[u]$, where $1 \leqslant s \leqslant d_G(v)$. Let $G^* = G - \{vv_1, vv_2, \dots, vv_s\} + \{uv_1, uv_2, \dots, uv_s\}$. If $d_G(u) + s > d_G(v)$, then $M_1(G^*) > M_1(G)$.*

Proof. Note that $d_{G^*}(u) = d_G(u) + s$, $d_{G^*}(v) = d_G(v) - s$ and $d_{G^*}(x) = d_G(x)$ for any $x \in V_G \setminus \{u, v\}$. Hence, by the definition of the first Zagreb index we have

$$M_1(G^*) - M_1(G) = d_{G^*}(u)^2 + d_{G^*}(v)^2 - d(u)^2 - d(v)^2 = 2s^2 + 2s(d(u) - d(v)) = 2s(d(u) + s - d(v)) > 0,$$

where the last inequality follows by $s \geqslant 1$ and $d_G(u) + s > d_G(v)$. Hence, we have $M_1(G^*) > M_1(G)$. $\square$

Lemma 2.2. *Let u, v be two distinct vertices of a connected graph G with $d_G(u) \geqslant d_G(v)$. Suppose that $N(v) \setminus N[u] = \{v_1, v_2, \ldots, v_s, v_{s+1}, \ldots, v_j\}$, $1 \leqslant j \leqslant d(v)$, $N(u) \setminus N[v] = \{u_1, u_2, \ldots, u_t\}$ with $\sum_{i=1}^{t} d_G(u_i) \geqslant \sum_{i=s+1}^{j} d_G(v_i)$. Let $G^* = G - \{vv_1, vv_2, \ldots, vv_s\} + \{uv_1, uv_2, \ldots, uv_s\}$.*

(i) *If $uv \notin E_G$, then $M_2(G^*) > M_2(G)$.*
(ii) *If $uv \in E_G$, then $M_2(G^*) \geqslant M_2(G)$.*

Proof. For convenience, suppose that $N(v) \bigcap N(u) = \{v_{j+1}, v_{j+2}, \ldots, v_{d(v)}\}$. Note that $d_{G^*}(u) = d_G(u) + s$, $d_{G^*}(v) = d_G(v) - s$ and $d_{G^*}(x) = d_G(x)$ for any $x \in V_G \setminus \{u, v\}$. For convenience, let $d(u) = d_G(u)$ for any $u \in V_G$.

(i) Note that $uv \notin E_G$, hence by the definition of the second Zagreb index we have

$$\begin{aligned}
M_2(G^*) - M_2(G) &= d_{G^*}(v) \sum_{i=s+1}^{d(v)} d(v_i) + d_{G^*}(u) \sum_{i=j+1}^{d(v)} d(v_i) + d_{G^*}(u) \sum_{i=1}^{s} d(v_i) + d_{G^*}(u) \sum_{i=1}^{t} d(u_i) \\
&\quad - d(u) \sum_{i=1}^{t} d(u_i) - d(u) \sum_{i=j+1}^{d(v)} d(v_i) - d(v) \sum_{i=1}^{d(v)} d(v_i) \\
&= (d_{G^*}(u) - d(v)) \sum_{i=1}^{s} d(v_i) + (d_{G^*}(v) - d(v)) \sum_{i=j+1}^{d(v)} d(v_i) + (d_{G^*}(u) - d(u)) \sum_{i=1}^{t} d(u_i) \\
&\quad + (d_{G^*}(u) - d(u)) \sum_{i=j+1}^{d(v)} d(v_i) + (d_{G^*}(v) - d(v)) \sum_{i=s+1}^{j} d(v_i) \\
&= (d_{G^*}(u) - d(v)) \sum_{i=1}^{s} d(v_i) - s \sum_{i=j+1}^{d(v)} d(v_i) + s \sum_{i=1}^{t} d(u_i) + s \sum_{i=j+1}^{d(v)} d(v_i) - s \sum_{i=s+1}^{j} d(v_i) \\
&= (d_{G^*}(u) - d(v)) \sum_{i=1}^{s} d(v_i) + s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) \\
&> (d(u) - d(v)) \sum_{i=1}^{s} d(v_i) + s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) \\
&\geq 0.
\end{aligned}$$

The last second inequality follows by $d_{G^*}(u) > d(u)$; whereas the last inequality follows by $\sum_{i=1}^{t} d(u_i) \geqslant \sum_{i=s+1}^{j} d(v_i)$ and $d(u) \geqslant d(v)$. Hence, $M_2(G^*) > M_2(G)$.

(ii) Note that $uv \in E_G$, hence by direct computing we have

$$\begin{aligned}
M_2(G^*) - M_2(G) &= (d_{G^*}(u) - d(v)) \sum_{i=1}^{s} d(v_i) + s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) + d_{G^*}(u) d_{G^*}(v) - d(u)d(v) \\
&= (t + s - j) \sum_{i=1}^{s} d(v_i) + s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) + (d(u) + s)(d(v) - s) - d(u)d(v) \\
&= (t + s - j) \sum_{i=1}^{s} d(v_i) + s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) + s(d(v) - d(u)) - s^2 \\
&\geqslant (t + s - j)s + s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) + s(j - t) - s^2 \\
&= s(\sum_{i=1}^{t} d(u_i) - \sum_{i=s+1}^{j} d(v_i)) \\
&\geqslant 0.
\end{aligned}$$

The last inequality follows by $\sum_{i=1}^{t} d_G(u_i) \geqslant \sum_{i=s+1}^{j} d_G(v_i)$. Hence, $M_2(G^*) \geqslant M_2(G)$.

This completes the proof. □

Remark 1. *The proof of Lemma 2.2* (ii) *implies that if there exists a vertex v_i with $d(v_i) \geq 2$, $i \in \{1, 2, \ldots, s\}$, or $\sum_{i=1}^{t} d(u_i) > \sum_{i=s+1}^{j} d(v_i)$, then we can obtain $M_2(G^*) > M_2(G)$.*

The following result follows directly by the definition of the first and second Zagreb indices.

Lemma 2.3. *Let G be a connected graph and G' is a proper subgraph of G. Then $M_i(G) > M_i(G')$ for $i = 1, 2$.*

Let G_1(resp. G_2) be the graph with n vertices and k pendant vertices which, as shown in Fig. 1, is obtained from a connected subgraph H by attaching a path P_{m+1} (resp. a path P_{m-1} and a cycle C_3) to a vertex u_0 of H; H_1 (resp. H_2) be the graph with n vertices and k pendant vertices which, as shown in Fig. 1, is obtained from a connected subgraph H by attaching $\frac{m-1}{2}$ C_3's and a path P_2 (resp. $\frac{m-2}{2}$ C_3's and a P_3) to u_0 when m is odd (resp. even), where $|V_H| \geqslant 3$ and $m \geqslant 3$.

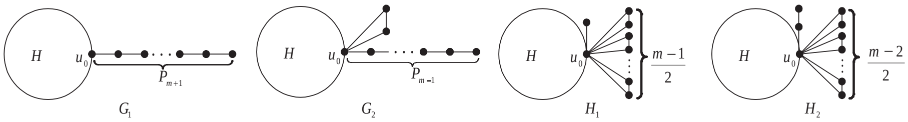

Figure 1: Graphs G_1, G_2, H_1 and H_2.

Lemma 2.4. *Let G_1, G_2, H_1 and H_2 be the graphs as depicted in Fig. 1. Then, for $i = 1, 2$, we have*

(i) $M_i(G_1) < M_i(G_2)$;
(ii) $M_i(G_1) < M_i(H_1)$ *if m is odd, otherwise* $M_i(G_1) < M_i(H_2)$.

Proof. (i) In G_1 denote the path P_{m+1} by $u_0u_1 \ldots u_m$. Let $G' = G_1 - u_2u_3 + u_0u_3$. Note that $d(u_0) > d(u_2)$, hence by Lemmas 2.1 and 2.2, we get $M_1(G_1) < M_1(G')$ and $M_2(G_1) < M_2(G')$. Note that G' is a proper subgraph of G_2, hence by Lemma 2.3 $M_i(G') < M_i(G_2)$ for $i = 1$, 2. This completes the proof of (i).

(ii) From (i) we know that our result holds for $m = 3$, 4. So in what follows we consider the case $m \geqslant 5$. By repeated using the similar discussion as in (i) on G_2, we finally get the graph H_1 if m is odd or, the graph H_2 if m is even. So, $M_i(G_1) < M_i(H_1)$ if m is odd, otherwise $M_i(G_1) < M_i(H_2)$ for $i = 1, 2$. This completes the proof of (ii). □

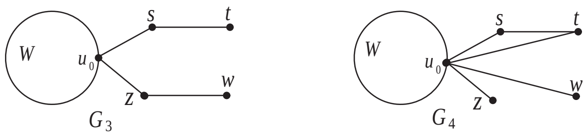

Figure 2: Graphs G_3 and G_4.

Let W be a connected $(n-4)$-vertex graph with $k-2$ pendant vertices. Let G_3 be the graph obtained from W by attaching two paths of length 2 to a vertex, say u_0, of W; see Fig. 2. Set $G_4 = G_3 - zw + \{u_0w, u_0t\}$ (see Fig. 2). It is easy to see that G_3 (resp. G_4) is an n-vertex graph with k pendant vertices.

Lemma 2.5. *Let G_3 and G_4 be the graphs with n vertices and k pendant vertices as shown in Fig. 2. Then $M_1(G_3) < M_1(G_4)$ and $M_2(G_3) < M_2(G_4)$.*

Proof. Let $G' = G_3 - \{st, zw\} + \{u_0t, u_0w\}$, by Lemmas 2.1 and 2.2 we obtain that $M_1(G_3) < M_1(G')$ and $M_2(G_3) \leqslant M_2(G')$. Note that G' is a proper subgraph of G_4. By Lemma 2.3, we get $M_1(G') < M_1(G_4)$ and $M_2(G') < M_2(G_4)$. Hence, $M_i(G_3) < M_i(G_4)$ for $i = 1$, 2. □

Let Y be a connected $(n-m+1)$-vertex graph with k pendants and $u_0 \in V_Y$. Let G_5 (resp. G_6) be an n-vertex graph obtained from Y by attaching C_m (resp. C_{m-2} and C_3) to u_0 (see Fig. 3); G_7 (resp. G_8) be an n-vertex graph obtained from Y by attaching $\frac{m-1}{2}$ C_3's (resp. $\frac{m-4}{2}$ C_3's and a C_4) to u_0 when m is odd (resp. even), where $m \geqslant 5$. Graphs G_7 and G_8 are depicted in Fig. 3.

Lemma 2.6. *Let G_5, G_6, G_7 and G_8 be the graphs defined as above (see Fig. 3). Then, for $i = 1, 2$, we have*

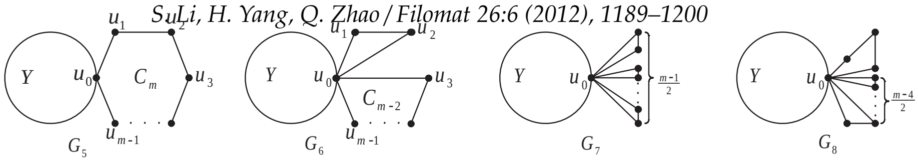

Figure 3: Graphs G_5, G_6, G_7 and G_8.

(i) $M_i(G_5) < M_i(G_6)$;
(ii) $M_i(G_5) < M_i(G_7)$ *if m is odd; otherwise* $M_i(G_5) < M_i(G_8)$.

Proof. (i) Denote by $C_m = u_0u_1u_2 \dots u_{m-1}u_0$. Let $G' = G_5 - u_2u_3 + u_0u_2$. Note that $d(u_0) \geq d(u_3)$, hence by Lemmas 2.1 and 2.2, we get $M_1(G_5) < M_1(G')$ and $M_2(G_5) < M_2(G')$. Notice that G' is a proper subgraph of G_6, hence by Lemma 2.3, we have $M_i(G') < M_i(G_6)$. Thus, we get $M_i(G_5) < M_i(G_6)$ for $i = 1, 2$.

(ii) From (i) we know that our result holds for $m = 5$, 6, so in what follows we consider the case for $m \geqslant 7$. In this case, by repeated using the similar discussion as in (i) on G_6, we, finally, get the graph G_7 if m is odd or, the graph G_8 if m is even. Hence, $M_i(G_5) < M_i(G_7)$ if m is odd; otherwise, $M_i(G_5) < M_i(G_8)$ for $i = 1$, 2. □

Figure 4: Graphs H_3 and H_4.

Lemma 2.7. *Let H_3 and H_4 be the graphs as depicted in Fig. 4, where U is a connected $(n-6)$-vertex graph with k pendants. Then, $M_i(H_3) < M_i(H_4)$ for $i = 1$, 2.*

Proof. Let $H' = H_3 - u_2u_3 + u_0u_2$. Note that $d_{H_3}(u_0) \geq d_{H_3}(u_3)$, hence by Lemmas 2.1 and 2.2, we have $M_1(H_3) < M_1(H')$ and $M_2(H_3) \leqslant M_2(H')$. Furthermore, let $H'' = H' - u_5u_6 + u_0u_5$, by Lemmas 2.1 and 2.2, we have $M_1(H_3) < M_1(H'')$ and $M_2(H_3) \leqslant M_2(H'')$. Note that H'' is a proper subgraph of H_4, by Lemma 2.3, we have $M_i(H'') < M_i(H_4)$ for $i = 1$, 2. This completes the proof. □

Lemma 2.8. *Let H_5 and H_6 be the graphs with n vertices and k pendant vertices as shown in Fig. 5. Then $M_1(H_5) < M_1(H_6)$ and $M_2(H_5) < M_2(H_6)$.*

Figure 5: Graphs H_5 and H_6.

Proof. Let $H' = H_5 - u_2u_3 + u_0u_2$. Note that $d_{H_5}(u_0) \geq d_{H_5}(u_3)$, hence by Lemmas 2.1 and 2.2, we have $M_1(H_5) < M_1(H')$ and $M_2(H_5) \leqslant M_2(H')$. Since H' is a proper subgraph of H_6, by Lemma 2.3, $M_1(H') < M_1(H_6)$ and $M_2(H') < M_2(H_6)$. Hence, $M_i(H_5) < M_i(H_6)$ for $i = 1$, 2. □

Lemma 2.9. *Let H_7 and H_8 be the n-vertex graphs as shown in Fig. 6, where Z is a connected subgraph with $k-1$ pendants. Then, $M_1(H_7) = M_1(H_8)$ and $M_2(H_7) < M_2(H_8)$.*

Figure 6: Graphs H_7 and H_8.

Proof. Note that $d_{H_7}(z) = d_{H_8}(z)$ for any $z \in V_Z$, hence by the definition of the first and second Zagreb indices we have

$$M_1(H_8) - M_1(H_7) = 0,$$
$$M_2(H_8) - M_2(H_7) = d_{H_7}(u_0) - 2 > 0.$$

Hence, we have $M_1(H_7) = M_1(H_8)$ and $M_2(H_7) < M_2(H_8)$. □

Lemma 2.10. *Let C be a cycle of graph $G \in \mathscr{C}_{n,k}$ with $u, v \in V_C$ satisfying $\min\{d_G(u), d_G(v)\} > 2$. Then there exists a graph $G^* \in \mathscr{C}_{n,k}$ such that $M_2(G) < M_2(G^*)$.*

Proof. Note that $u, v \in V_C$, hence there exist two paths, say P and P', connecting u and v. For convenience, let $P = u_1u_2 \dots u_p$ and $P' = u_1v_1 \dots u_p$ with $|E_P| \leqslant |E_{P'}|$. We distinguish the following three possible cases to prove our result.

Case 1. $|E_C| = 3$, i.e. $P = u_1u_2$ and $P' = u_1v_1u_2$. Assume, without loss of generality, that $d_G(u_1) \leqslant d_G(u_2)$. Let $G' = G - \{u_1y | y \in N(u_1) \setminus \{v_1, u_2\}\} + \{u_2y | y \in N(u_1) \setminus \{v_1, u_2\}\}$. Then $G' \in \mathscr{C}_{n,k}$. By Lemma 2.2 and Remark 1, we get $M_2(G) < M_2(G')$, as desired.

Case 2. $|E_C| = 4$. In this case, if $P = u_1u_2u_3$ and $P' = u_1v_1u_3$, then assume, without loss of generality, that $d_G(u_1) \leqslant d_G(u_3)$, then let $G' = G - \{u_1y | y \in N(u_1) \setminus \{v_1, u_2\}\} + \{u_3y | y \in N(u_1) \setminus \{v_1, u_2\}\}$. It is easy to see that $G' \in \mathscr{C}_{n,k}$ and by Lemma 2.2, we get $M_2(G) < M_2(G')$, a contradiction. In order to complete the proof of this case, it suffices to consider that $P = u_1u_2$ and $P' = u_1v_1v_2u_2$.

• $d_G(v_1) = d_G(v_2) = 2$. Let w be a pendant vertex of G. Set $G^* = G - \{v_1v_2, v_2u_2\} + \{v_1u_2, wv_2\}$. By direct computing, we obtain $M_2(G) \leqslant M_2(G^*)$. By Case 1, there exists a cactus $G_0 \in \mathscr{C}_{n,k}$ such that $M_2(G^*) < M_2(G_0)$. Hence, we obtain $M_2(G) < M_2(G_0)$, as required.

• $\max\{d_G(v_1), d_G(v_2)\} > 2$. Assume, without loss of generality, that $d_G(v_1) \geqslant 3$. If $d_G(v_1) \leqslant d_G(u_2)$, then let $G' = G - \{v_1y | y \in N(v_1) \setminus \{u_1, v_2\}\} + \{u_2y | y \in N(v_1) \setminus \{u_1, v_2\}\}$; otherwise let $G'' = G - \{u_2y | y \in N(u_2) \setminus \{u_1, v_2\}\} + \{v_1y | y \in N(u_2) \setminus \{u_1, v_2\}\}$. It is easy to see that $G', G'' \in \mathscr{C}_{n,k}$ and by Lemma 2.2, we get $M_2(G) < M_2(G')$ or, $M_2(G) < M_2(G'')$, as required.

Case 3. $|E_C| \geqslant 5$. In this case, if $d_G(v_2) \leqslant d_G(u_1)$, then let $G^* = G - \{v_2y | y \in N_G(v_2) \setminus \{v_1\}\} + \{u_1y | y \in N_G(v_2) \setminus \{v_1\}\}$; otherwise let $G^{**} = G - \{u_1y | y \in N_G(u_1) \setminus \{v_1\}\} + \{v_2y | y \in N_G(u_1) \setminus \{v_1\}\}$. It is straightforward to check that $G^* + v_2u_1$ (resp. $G^{**} + u_1v_2$) is in $\mathscr{C}_{n,k}$ and by Lemmas 2.2 and 2.3 we get $M_2(G) < M_2(G^*)$ or, $M_2(G) < M_2(G^{**})$, as required.

This completes the proof. □

3. Characterization of graphs in $\mathscr{C}_{n,k}$ with maximal Zagreb indices

We call G a *cactus* if it is connected and any two of its cycles have at most one common vertex. If all cycles of the cactus G have exactly one common vertex, we say that they form a bundle. In the following, we determine the graphs with the largest M_1-, M_2-values in the class $\mathscr{C}_{n,k}$, respectively.

Theorem 3.1. *Let G be a graph in $\mathscr{C}_{n,k}$.*

(i) *If $n - k \equiv 1 \pmod 2$, then $M_1(G) \leqslant n^2 + 2n - 3k - 3$, with equality if and only if $G \cong C^1(n, k)$, where $C^1(n, k)$ is depicted in Fig. 7.*
(ii) *If $n - k \equiv 0 \pmod 2$, then $M_1(G) \leqslant n^2 - 3k$, with equality if and only if $G \cong C^2(n, k)$ or, $C^3(n, k)$, where $C^2(n, k)$ and $C^3(n, k)$ are depicted in Fig. 7.*

Proof. Choose $G \in \mathscr{C}_{n,k}$ such that its M_1-value is as large as possible. First we prove that all the cycles contained in G forms a bundle.

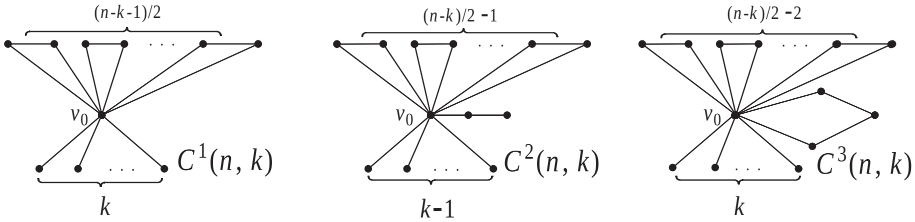

Figure 7: Graphs $C^1(n,k)$, $C^2(n,k)$ and $C^3(n,k)$.

Claim 3.2. *Any two cycles of graph G have one common vertex.*

Proof. Assume, on the contrary, that there are two disjoint cycles contained in G. We can choose two such cycles, say C^1 and C^2, such that the path P connecting C^1 and C^2 is as short as possible. For convenience, let $P = u_1u_2\ldots u_p$ with $V_P \cap V_{C^1} = \{u_1\}$ and $V_P \cap V_{C^2} = \{u_p\}$. In what follows, we consider two possible cases to prove our result.

Case 1. The path P (connecting C^1 and C^2) has no common edge with any other cycle(s) contained in G.

Assume, without loss of generality, that $d_G(u_1) \geqslant d_G(u_p)$. Let y be a neighbor of u_p which belongs to C^2. Set $G' = G - \{u_py\} + \{u_1y\}$. It is easy to see that $G' \in \mathscr{C}_{n,k}$. By Lemma 2.1, we have $M_1(G') > M_1(G)$, a contradiction.

Case 2. The path P (connecting C^1 and C^2) has common edge(s) with some other cycle, say C^3, contained in G. Note that, from the choice of C^1 and C^2, it suffices to consider that u_1 is just the common vertex of C^3 and C^1, whereas u_p is the only common vertex of C^3 and C^2. Assume that $V_{C^3} \cap N(u_p) = \{u_{p-1}, y\}$, then let $G' = G - \{u_px | x \in N(u_p) \setminus \{u_{p-1}, y\}\} + \{u_1x | x \in N(u_p) \setminus \{u_{p-1}, y\}\}$. By Lemma 2.1, we get $M_1(G) < M_1(G')$, a contradiction.

This completes the proof. □

Claim 3.3. *Any three cycles contained in G have exactly one common vertex.*

Proof. In the opposite case the graph G is not a cactus, because there exist cycles which have at least one common edge. □

By Claim 1 and Claim 2, all cycles of the graph G have exactly one common vertex, i.e. they form a bundle. Let us denote by v_0 the common vertex of all cycles in this bundle.

Next we show that if G contains a tree T attached to a cycle at a vertex v (we call v the *root* of T), then the root of T is v_0.

Claim 3.4. *Any pendant tree T contained in G is attached to the common vertex v_0 of all cycles of the bundle.*

Proof. In the opposite case there exists a tree T attached to a vertex u ($u \neq v_0$) on a cycle C of G. Let $y_1, y_2, \ldots, y_t$ be the neighbors of vertex u in T. If $d(v_0) \geqslant d(u)$, let $G' = G - \{uy_1, uy_2, \ldots, uy_t\} + \{v_0y_1, v_0y_2, \ldots, v_0y_t\}$; otherwise, let $G' = G - \{v_0y | y \in N(v_0) \setminus V_C\} + \{uy | y \in N(v_0) \setminus V_C\}$. In either case, we have $G' \in \mathscr{C}_{n,k}$. By Lemma 2.1, we have $M_1(G) < M_1(G')$, a contradiction. □

Claim 3.5. *Let T be the tree attached to the common vertex v_0 of all cycles of the bundle G, then $d_G(v) \leqslant 2$ for $v \in V_T \setminus \{v_0\}$.*

Proof. In the opposite case, assume that $u \in V_T \setminus \{v_0\}$ is of degree $r \geq 3$ furthest from the root v_0. If $d(v_0) \geq d(u)$, let $y_1, y_2, \ldots, y_{r-2}$ be $r-2$ neighbors in T and each y_i is further from v_0 than u, and $G' = G - \{uy_1, uy_2, \ldots, uy_{r-2}\} + \{v_0y_1, v_0y_2, \ldots, v_0y_{r-2}\}$. If $d(v_0) < d(u)$, let y be a neighbor of v_0 which belongs to a cycle and $G' = G - \{v_0y\} + \{uy\}$. Then, in either case, $G' \in \mathscr{C}_{n,k}$, and by Lemma 2.1, we have $M_1(G) < M_1(G')$, a contradiction. □

By Lemmas 2.4 and 2.5, the length of all paths attached to the common vertex v_0 are 1 or 2, and at most one of them has length 2. By Lemma 2.6 and 2.7, the length of all cycles in G are 3 or 4, and at most one of them has length 4. By Lemma 2.8, G can not have both a cycle with length 4 and a path attached to v_0 with length 2. Hence, if $n - k \equiv 1 \pmod 2$, then $G \cong C^1(n,k)$; otherwise, $G \cong C^2(n,k)$ or, $C^3(n,k)$. By Lemma 2.9, we know that $M_1(C^2(n,k)) = M_1(C^3(n,k))$. Hence, if $n - k \equiv 0 \pmod 2$, then $G \cong C^2(n,k)$ or, $C^3(n,k)$. By direct computing, we have

$$M_1(C^1(n,k)) = n^2 + 2n - 3k - 3, \quad M_1(C^2(n,k)) = M_1(C^3(n,k)) = n^2 - 3k.$$

This completes the proof. □

Theorem 3.6. *Let G be a graph in $\mathscr{C}_{n,k}$.*

(i) *If $n-k \equiv 1 \pmod 2$, then $M_2(G) \leqslant 2n^2-(k+2)n-k$, with equality if and only if $G \cong C^1(n,k)$, where $C^1(n,k)$ is depicted in Fig. 7.*

(ii) *If $n-k \equiv 0 \pmod 2$, then $M_2(G) \leqslant 2n^2-(k+5)n+4$, with equality if and only if $G \cong C^2(n,k)$, where $C^2(n,k)$ is depicted in Fig. 7.*

Proof. Choose $G \in \mathscr{C}_{n,k}$ such that its M_2-value is as large as possible. First we prove that all the cycles contained in G forms a bundle.

Fact 1. *Any two cycles of the graph G have one common vertex.*

Proof. Assume, on the contrary, that there are two disjoint cycles contained in G. We can choose two such cycles, say C^1 and C^2, so that the path P connecting C^1 and C^2 is as short as possible. For convenience, let $P = u_1u_2 \dots u_p$ with $V_P \cap V_{C^1} = \{u_1\}$ and $V_P \cap V_{C^2} = \{u_p\}$. In what follows, we consider two possible cases to prove our result.

Case 1. The path P (connecting C^1 and C^2) has no common edge with any other cycle(s) contained in G.

In this case, it is easy to see that if the length of P is at least 2, then let $G' = G + u_1u_p$. We get $G' \in \mathscr{C}_{n,k}$ and by Lemma 2.3, we have $M_2(G) < M_2(G')$, a contradiction. Hence, we only consider that P is of length 1, i.e., $P = u_1u_2$. Assume, without loss of generality, that $d_G(u_1) \geqslant d_G(u_2)$.

For convenience, let $C^2 = u_2v_1v_2 \dots u_2$. By Lemma 2.10, we have $d_G(v_1) = 2$. Let $G' = G - \{u_2y | y \in N(u_2) \backslash \{u_1, v_1\}\} + \{u_1y | y \in N(u_2) \backslash \{u_1, v_1\}\}$. Then, $G' \in \mathscr{C}_{n,k}$. By Lemma 2.2 and Remark 1, we have $M_2(G) < M_2(G')$, a contradiction.

Case 2. The path P (connecting C^1 and C^2) has common edge(s) with some other cycle, say C^3, contained in G. By the choice of C^1 and C^2, it suffices to consider that u_1 is just the common vertex of C^3 and C^1, whereas u_p is the only common vertex of C^3 and C^2. It is easy to see that $d_G(u_1), d_G(u_p) \geqslant 3$, hence by Lemma 2.10, there exists a graph $G' \in \mathscr{C}_{n,k}$ such that $M_2(G) < M_2(G')$, a contradiction.

By Cases 1 and 2, we complete the proof of Fact 1. □

Fact 2. *Any three cycles have exactly one common vertex.*

Proof. In the opposite case the graph G is not a cactus, because there exist cycles which have at least one common edge. □

By Facts 1 and 2, all cycles contained in G have exactly one common vertex, i.e. they form a bundle. Denote by v_0 the common vertex of all cycles in this bundle.

Next we show that if G contains a tree T attached to a cycle at a vertex v, then the root of T is v_0. That is:

Fact 3. *Any tree T of the graph G is attached to the common vertex v_0 of all cycles of the bundle.*

Proof. In the opposite case there exists a tree T attached to a vertex u ($u \neq v_0$) on a cycle C_m of G. Note that u, v_0 are on C_m with $d_G(u), d_G(v_0) \geqslant 3$, hence by Lemma 2.10 there exists a graph $G' \in \mathscr{C}_{n,k}$ such that $M_2(G) < M_2(G')$, a contradiction. □

Fact 4. *Let T be the tree attached to the common vertex v_0 of all cycles of the bundle G, then $d_G(v) \leqslant 2$ for $v \in V_T \setminus \{v_0\}$.*

Proof. In the opposite case, assume that $u \in V_T \backslash \{v_0\}$ is of degree $r \geqslant 3$ furthest from the root v_0. If $d(u, v_0) \geqslant 2$, then let $G' = G + uv_0$. Then $G' \in \mathscr{C}_{n,k}$ and by Lemma 2.3 we have $M_2(G) < M_2(G')$, a contradiction. Then $d(u, v_0) = 1$. Let $y_0, y_1, y_2, \dots, y_{r-2}$ be $r-1$ neighbors of u in T and each y_i is further from v_0 than u. By Lemmas 2.4 and 2.5, there exists at most one vertex, say y_0, in $\{y_0, y_1, y_2, \dots, y_{r-2}\}$ such that $d(y_0) = 2$. Here, it is easy to see that there does not exist such y_0; otherwise let $G'' = G + v_0y_0$. Then $G'' \in \mathscr{C}_{n,k}$ and by Lemma 2.3 we have $M_2(G) < M_2(G'')$, a contradiction. If $d_G(v_0) \geqslant d_G(u)$, then let $G^* = G - \{uy_1, uy_2, \dots, uy_{r-2}\} + \{v_0y_1, v_0y_2, \dots, v_0y_{r-2}\}$; otherwise choose a neighbor, say w, of v_0 on a cycle of G and let $G^{**} = G - \{v_0x | x \in N(v_0) \setminus \{w, u\}\} + \{ux | x \in N(v_0) \setminus \{w, u\}\}$. Then $G^*, G^{**} \in \mathscr{C}_{n,k}$. By Lemma 2.2 and Remark 1, we have $M_2(G) < M_2(G^*)$ or, $M_2(G) < M_2(G^{**})$, a contradiction. □

Finally, by Lemmas 2.4 and 2.5, the length of all paths attached to the common vertex v_0 are 1 or 2, and at most one of them has length 2. By Lemmas 2.6 and 2.7, the length of all cycles in G are 3 or 4, and at most one of them has length 4. By Lemma 2.8, G can not have both a cycle with length 4 and a path attached to v_0 with length 2. So, G is $C^1(n,k)$ when the parities of n and k are different; G is one of $C^2(n,k)$ and $C^3(n,k)$ when the parities of n and k are same, where $C^1(n,k), C^2(n,k)$ and $C^3(n,k)$ are depicted in Fig. 7. By Lemma 2.9,

$M_2(C^2(n,k)) > M_2(C^3(n,k))$. Hence, $G \cong C^1(n,k)$ if $n-k \equiv 1 \pmod 2$; otherwise, $G \cong C^2(n,k)$. By an elementary calculation, we have

$$M_2(C^1(n,k)) = 2n^2 - (k+2)n - k,\ \ M_2(C^2(n,k)) = 2n^2 - (5+k)n + 4.$$

This completes the proof of Theorem 3.2. □

Denote by $\mathscr{C}_n$ the set of all connected cacti with n vertices. Let C_n^1, C_n^2, C_n^3 and C_n^4 be the cacti with n vertices depicted in Fig. 8.

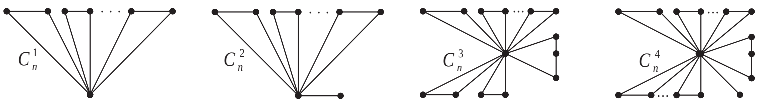

Figure 8: Graphs C_n^1, C_n^2, C_n^3 and C_n^4.

Note that $C^3(n,k)$ is a spanning subgraph of C_n^3 or, C_n^4, hence by Lemma 2.3, if n is even, then $M_1(C^3(n,k)) < M_1(C_n^3)$ and $M_1(C^3(n,k)) < M_1(C_n^4)$ otherwise. Denote the unique 4-cycle in C_n^3 by $v_0v_1v_2v_3v_0$. Then $C_n^2 \cong C_n^3 - v_1v_2 + v_0v_2$. By Lemma 2.1, we get $M_1(C_n^2) > M_1(C^3(n))$. Similarly, in C_n^4 let $C_4 = v_0u_1u_2u_3v_0$ be the unique cycle, u_4 be the unique pendant vertex. Set $C_n^{4*} = C_n^4 - u_1u_2 + v_0u_2$. By Lemma 2.1, $M_1(C_n^{4*}) > M_1(C_n^4)$. Note that $C_n^1 \cong C_n^{4*} + u_1u_4$, hence by Lemma 2.3, we have $M_1(C_n^1) > M_1(C_n^4)$. So we have the following result.

Corollary 3.7. *Let G be a graph in $\mathscr{C}_n$. Then*

(i) $M_1(G) \leqslant n^2 + 2n - 3$ *for odd n, and the equality holds if and only if* $G \cong C_n^1$;
(ii) $M_1(G) \leqslant n^2 + 2n - 6$ *for even n, and the equality holds if and only if* $G \cong C_n^2$.

If n is odd, then $C^1(n,k)$ (resp. $C^2(n,k)$) is a spanning subgraph of C_n^1; if n is even, then $C^1(n,k)$ (resp. $C^2(n,k)$) is a spanning subgraph of C_n^2. By Lemma 2.3, $M_2(C^1(n,k)) < M_2(C_n^1)$ and $M_2(C^2(n,k)) < M_2(C_n^2)$. Hence, we have the following result.

Corollary 3.8. *Let G be a graph in $\mathscr{C}_n$. Then,*

(i) $M_2(G) \leqslant 2n^2 - 2n$ *for odd n, and the equality holds if and only if* $G \cong C_n^1$.
(ii) $M_2(G) \leqslant 2n^2 - 3n - 1$ *for even n, and the equality holds if and only if* $G \cong C_n^2$.

At last, based on the results obtained as above, we determine the sharp upper bound, respectively, for Zagreb indices of cacti with a perfect matching. Let $\widetilde{\mathscr{C}_{2k}}$ be the set of all $2k$-vertex cacti with a perfect matching.

Based on Corollaries 3.3 and 3.4, we get

Corollary 3.9. *Let G be a graph in $\widetilde{\mathscr{C}_{2k}}$. Then,* $M_i(G) \leqslant M_i(C_{2k}^2)$ *for* $i = 1, 2$, *and the equality holds if and only if* $G \cong C_{2k}^2$.

4. Characterization of graphs in $\mathscr{C}_{n,k}$ with minimal Zagreb indices

In this section, we determine sharp lower bounds for M_1- and M_2-values of graphs in $\mathscr{C}_{n,k}$. Here we assume that for all G in $\mathscr{C}_{n,k}$, G contains at lease one cycle. Recall that unicyclic graphs are connected graphs with n vertices and n edges. For convenience, denote

$\mathscr{U}_{n,k} = \{G : G$ is a unicyclic graph with n vertices and k pendant vertices$\}$.

$\mathscr{U}_{n,k}^* = \{G \in \mathscr{U}_{n,k} : \Delta(G) \le 3$ and the number of vertices with degree 3 is equal to the number of pendant vertices $k\}$.

$\mathscr{U}_{n,k}^+ = \{G \in \mathscr{U}_{n,k} : \Delta(G) \le 3$, each pendant vertices of G is adjacent to another vertex of degree 3 and every pair of vertices of degree 3 are nonadjacent$\}$.

Proposition 4.1. *Let* $G \in \mathscr{U}_{n,k}$, $0 \le k \le n-3$, *then* $M_1(G) \ge 4n + 2k$. *Equality holds if and only if* $n \ge 2k$ *and* $G \in \mathscr{U}_{n,k}^*$.

Proof. Since G is a unicyclic graph with k pendant vertices, then we have

$$2n = \sum_{v \in V_G} d(v) = k + \sum_{i=1}^{n-k}(2 + x_i)$$

where $d(v_i) = 2 + x_i$, v_i is non-pendant vertex and x_i is a nonnegative integer, $i = 1, 2, \ldots, n-k$.

Then we get $\sum_{i=1}^{n-k} x_i = k$. Hence, $\sum_{i=1}^{n-k} x_i^2 \geq k$ and

$$\begin{aligned} M_1(G) &= \sum_{v \in V_G} d(v)^2 = k \cdot 1^2 + \sum_{i=1}^{n-k}(2 + x_i)^2 \\ &= k + 4(n-k) + 4\sum_{i=1}^{n-k} x_i + \sum_{i=1}^{n-k} x_i^2 \\ &\geq k + 4(n-k) + 4k + k \qquad (4.1) \\ &= 4n + 2k. \end{aligned}$$

Equality in (4.1) holds if and only if $\sum_{i=1}^{n-k} x_i^2 = k$ which implies $n \geq 2k$ and $x_1 = x_2 = \cdots = x_k = 1, x_{k+1} = x_{k+2} = \cdots = x_{n-k} = 0$. That is $G \in \mathscr{U}_{n,k}^*$. □

The following result characterize the unicyclic graph with k pendant vertices having the minimal second Zagreb index (see [66]).

Proposition 4.2. *Let $G \in \mathscr{U}_{n,k}$, $0 \leq k \leq n-3$. Then*

$$M_2(G) \geq 4n + 3k.$$

Equality holds if and only if $n \geq 3k$ and $G \in \mathscr{U}_{n,k}^+$.

Theorem 4.3. *Let $G \in \mathscr{C}_{n,k}$, $0 \leq k \leq n-3$. Then*

$$M_1(G) \geq 4n + 2k.$$

Equality holds if and only if $n \geq 2k$ and $G \in \mathscr{U}_{n,k}^*$.

Proof. Since $G \in \mathscr{C}_{n,k}$, we assume that $C_1, C_2, \ldots, C_s$ are cycles in G and $e_1, e_2, \ldots, e_s$ are edges of theirs, respectively. Let G^* be the unicyclic graph obtained from G by deleting $e_2, e_3, \ldots, e_s$, then we have $G^* \in \mathscr{U}_{n,m} \subset \mathscr{C}_{n,m}$ where $m \geq k$. By Lemma 2.3 and Proposition 4.1, we have

$$M_1(G) \geq M_1(G^*) \geq 4n + 2m \geq 4n + 2k.$$

Hence, $M_1(G) = 4n + 2k$ holds if and only if $n \geq 2m = 2k$ and $G \cong G^* \in \mathscr{U}_{n,k}^*$. And by direct computing, we have, for any $G^* \in \mathscr{U}_{n,k}^*$, $M_1(G^*) = 4n + 2k$.

This completes the proof. □

Similarly, we get the following theorem.

Theorem 4.4. *Let $G \in \mathscr{C}_{n,k}$, $0 \leq k \leq n-3$. Then*

$$M_2(G) \geq 4n + 3k.$$

Equality holds if and only if $n \geq 3k$ and $G \in \mathscr{U}_{n,k}^+$.

References

[1] A.T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topological indices for structure-activity correlations, Topics Curr. Chem. 114 (1983) 21-55.
[2] K. Balasubramanian, Recent developments in tree-pruning methods and polynomials for cactus graphs and trees. Methods of mathematical chemistry (Galveston, TX, 1989), J. Math. Chem. 4 (1-4) (1990) 89-102.
[3] S.C. Basak, G.D. Grunwald, G.J. Niemi, Use of graph-theoretic geometric molecular descriptors in structure-activity relationships, in From Chemical Topology to Three-Dimensional Geometry, ed. by A.T. Balaban (Plenum Press, New York, 1997), pp. 73-116.
[4] S.C. Basak, B.D. Gute, G.D. Grunwald, A hierarchical approach to the development of QSAR models using topological, geometrical and quantum chemical parameters, in Topological Indices and Related Descriptors in QSAR and QSPR, ed. by J. Devillers, A.T. Balaban (Gordon & Breach, Amsterdam, 1999), pp. 675-696.
[5] B. Bollobás, Modern Graph Theory (Springer-Verlag, 1998).
[6] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars Comb. 50 (1998) 225-233.
[7] B. Bollobás, P. Erdös, A. Sarkar, Extremal graphs for weights, Discrete Math. 200(1999) 5-19.
[8] M. Bona, M. Bousquet, G. Labelle, and P. Leroux, Enumeration of m-ary cacti, Adv. Appl. Math. 24 (2000) 22-56.
[9] D. Bonćhev, N. Trinajstić, Overall molecular descriptors. 3. Overall Zagreb indices, Sar Qsar Environ. Res. 12 (2001) 213-236.
[10] J.A. Bondy and U.S. Murty, Graph Theory and its Applications (The Macmillan Press, London, 1976).
[11] D.de Caen, An upper bound on the sum of squares of degrees in a graph, Discrete Math. 185 (1998) 245-248.
[12] C.Y. Chao, E.G. Whitehead Jr, On chromatic equivalence of graphs, in Theory and Applications of Graphs (Proceedings of the International Conference, Western Michigan University, Kalamazoo, Michigan, 1976), Y. Alavi and D.R. Lick, eds., Springer-Verlag, Berlin, (1978) 121-131.
[13] S. Chen, H. Deng, Extremal $(n, n + 1)$-graphs with respected to zeroth-order general Randić index, J. Math. Chem. 42 (2007) 555-564.
[14] S.M. Cioabǎs, Sum of powers of the degrees of a graph, Discrete Math. 306 (2006) 1959-1964.
[15] D. Vukičević, S.M. Rajtmajer and N. Trinajstić, Trees with maximal second Zagreb index and prescribed number of vertices of the given degree, MATCH Commun. Math. Comput. Chem. 60 (2008) 65-70.
[16] K. Das, Maximizing the sum of the squares of degrees of a graph, Discrete Math. 257 (2004) 57-66.
[17] K. Das, I. Gutman, Some properties of the second Zagreb index, MATCH Commun. Math. Comput. Chem. 52 (2004) 103-112.
[18] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, MATCH Commun. Math. Comput. Chem. 57 (2007) 597-616.
[19] Y. Feng, X. Hu, S. Li, On the extremal Zagreb indices of graphs with cut edges, Acta Appl. Math. 110 (2010) 667-684.
[20] R. Garcia-Domenech, J. Galvez, J.V. de Julian-Ortiz, L. Pogliani, Some new trends in chemical graph theory, Chem. Rev. 108 (2008) 1127-1169.
[21] D. Geller, B. Manvel, Reconstruction of cacti, Canad. J. Math. 21 (1969) 1354-1360.
[22] M. Ghorbani, M.A. Hosseinzadeh, A new version of Zagreb indices, Filomat 26 (1) (2012) 93-100.
[23] I. Gutman, Chemical graph theory—The mathematical connection, in Advances in Quantum Chemistry, vol. 51, ed. by J.R. Sabin, E.J. Brädas (Elsevier, Amsterdam, 2006), pp. 125-138.
[24] I. Gutman, B. Furtula (eds.), Recent Results in the Theory of Randić Index (University of Kragujevac, Kragujevac, 2008)
[25] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.
[26] I. Gutman, B. Ruščić, N. Trinajstić, C.F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, J. Chem. Phys. 62 (1975) 3399-3405.
[27] I. Gutman, K. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83-92.
[28] A.L. Hou, S.C. Li, L.Z. Song, B. Wei, Sharp bounds for Zagreb indices of maximal outerplanar graphs, J. Comb. Optim. 22 (2011) 252-269.
[29] D. Ismailescu, D. Stefanica, Minimizer graphs for a class of extremal problems, J. Grpah Theory, 39 (2002) 230-240.
[30] D. Janezić, A. Milićević, S. Nikolić, N. Trinajstić and D. Vukičević, Zagreb indices: extension to weighted graphs representing molecules ontaining heteroatoms, Croat. Chem. Act 80 (2007) 541-545.
[31] Y. Jiang and M. Lu, On the connectivity index of trees, J. Math. Chem. 43 (2008) 955-965.
[32] N. Khan, A. Pal, M. Pal, Edge colouring of cactus graphs, Adv. Model. Optim. 11 (4) (2009) 407-421.
[33] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research (Academic Press, New York, 1976)
[34] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure-Activity Analysis (Research Studies Press/Wiley, Letchworth/New York, 1986)
[35] L.B. Kier, L.H. Hall, W.J. Murray, M. Randić, Molecular-connectivity I: Relationship to nonspecific local anesthesia, J. Pharm. Sci. 64 (1975) 1971-1974.
[36] S.C. Li, L.X. Yan, Sums of powers of the degrees of graphs with k cut edges, Graphs Combin. 27 (5) (2011) 727-740.
[37] S.C. Li, M.J. Zhang, Sharp bounds on the zeroth-order general Randić indices of conjugated bicyclic graphs, Math. Comput. Modelling. 53 (2011) 1990-2004.
[38] S.C. Li, M.J. Zhang, Sharp bounds for the Zagreb indices of bipartite graphs with a given diameter, Appl. Math. Lett. 24 (2011) 131-137.
[39] S.C. Li, Q. Zhao, Sharp upper bounds on Zagreb indices of bicyclic graphs with a given matching number, Math. Comput. Modelling. 54 (2011) 2869-2879.
[40] S.C. Li, Q. Zhao, On acyclic and unicyclic conjugated graphs with maximum Zagreb indices, Util. Math. 86 (2011) 115-128.
[41] S.C. Li, H. Zhou, On the maximum and minimum Zagreb indices of graphs with connectivity at most k, Appl. Math. Lett. 23 (2010) 128-132.

[42] X. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors (University of Kragujevac, Kragujevac, 2006)
[43] X. Li, Y. Shi, A survey on the Randić index, MATCH Commun. Math. Comput. Chem. 59(2008) 127-156.
[44] A.H. Lin, R. Luo, X.Y. Zha, A sharp lower bound of the Randić index of cacti with r pendants, Discrete Appl. Math. 156 (10) (2008) 1725-1735.
[45] H.Q. Liu, M. Lu, A unified approach to extremal cacti for different indices. MATCH Commun. Math. Comput. Chem. 58 (1) (2007) 183-194.
[46] B. Liu, Some estimations of Zagreb indices, Util. Math. 74 (2007) 239-245.
[47] B. Liu, I. Gutman, Upper bounds for Zagreb indices of connected graphs, MATCH Commun. Math. Comput. Chem. 55 (2006) 439-446.
[48] H. Liu, M. Lu, F. Tian, Tree of extremal connectivity index, Discrete Appl. Math. 154 (2006) 106-119.
[49] A. Milićević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, Molecular Diversity 8 (2004) 393-399.
[50] S. Nikolić, A. Milićević, N. Trinajstić and A. Jurić, On the use of the variable Zagreb M_2 index in QSPR: boiling points of benzenoid hydrocarbons, Molecules 9 (2004) 1208-1221.
[51] S. Nikolić, I.M. Tolic, N. Trinajstić and I. Baucic, On the Zagreb indices as complexity indices, Croat. Chem. Act 73, 909-921 (2000).
[52] S. Nikolić, N. Trinajstić, I. Baučić, Comparison between the vertex- and edge-connectivity indices for benzenoid hydrocarbons, J. Chem. Inform. Comput. Sci. 38(1998) 42-46.
[53] S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta. 76 (2003) 113-124.
[54] R. Pepper, D.J. Klein, Some theorems about the Randić connectivity index, MATCH Commun. Math. Comput. Chem. 58(2007) 359-364
[55] L. Pogliani, From molecular connectivity indices to semiempirical connectivity terms: Recent trends in graph theoretical descriptors, Chem. Rev. 100(2000) 3827-3858.
[56] J. Rada, C. Uzcátegui, Randić ordering of chemical trees, Discrete. Appl. Math. 150(2005) 232-250.
[57] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609-6615.
[58] M. Randić, On history of the Randić index and emerging hostility toward chemical graph theory, MATCH Commun. Math. Comput. Chem. 59(2008) 5-124.
[59] M. Randić, The connectivity index 25 years after, J. Mol. Graph. Modell. 20(2001) 19-35.
[60] d.H. Rouvray, The search for useful topological indices in chemistry, American Scientist, 61(1973) 729-735.
[61] G.F. Su, L.M. Xiong, L. Xu, B.B. Ma, On the maximum and minimum first reformulated Zagreb index of graphs with connectivity at most k, Filomat 25 (4) (2011) 75-83.
[62] L.L. Sun, R.S. Chen, The second Zagreb index of acyclic conjugated molecules, MATCH Commun. Math. Comput. Chem. 60 (2008)57-64.
[63] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
[64] N. Trinajstić, Chemical Graph Theory, CRC Press,1992.
[65] D. Vukičević, N. Trinajstić, Modified Zagreb index M_2- comparison with the Randić connectivity index for benzenoid systems, Croat. Chem. Act 76 (2003) 183-187.
[66] Z. Yan, H. Liu, H. Liu, Sharp bounds for the second Zagreb index of unicyclic graphs, J. Math. Chem. 42 (2007) 565-574.
[67] M.J. Zhang, S.C. Li, On the zeroth-order general Randić index, J. Math. Chem. 49 (2011) 325-327
[68] Q. Zhao, S. Li, On the maximum Zagreb indices of graphs with k cut vertices, Acta Appl. Math. 111 (2010) 93-106.
[69] B. Zhou, I. Gutman, Further properties of Zagreb indices, MATCH Commun. Math. Comput. Chem. 54 (2005) 233-239.
[70] B. Zhou, Zagreb indices, MATCH Commun. Math. Comput. Chem. 52 (2004) 113-118.
[71] B. Zmazek, J. Žerovnik, The obnoxious center problem on weighted cactus graphs. The 1st Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW 2001), Discrete Appl. Math. 136 (2-3) (2004) 377-386.