On the sharp lower bounds of Zagreb indices of graphs with given number of cut vertices

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Abstract

The first Zagreb index of a graph $G$ is the sum of the square of every vertex degree, while the second Zagreb index is the sum of the product of vertex degrees of each edge over all edges. In our work, we solve an open question about Zagreb indices of graphs with given number of cut vertices. The sharp lower bounds are obtained for these indices of graphs in $\mathcal{V}_{n,k}$, where $\mathcal{V}_{n,k}$ denotes the set of all $n$-vertex graphs with $k$ cut vertices and at least one cycle. As consequences, those graphs with the smallest Zagreb indices are characterized.

Keywords: Cut vertices; Extremal values; Zagreb indices.

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1 Introduction

A topological index is a constant which can be describing some properties of a molecular graph, that is, a finite graph represents the carbon-atom skeleton of an organic molecule of a hydrocarbon. During past few decades these have been used for the study of quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) and for the structural essence of biological and chemical compounds.

One of the most well-known topological indices is called Randić index, a molecular quantity of branching index \cite{1}. It is known as the classical Randić connectivity index, which is the most useful structural descriptor in QSPR and QSAR, see \cite{2,3,4,5}. Many mathematicians focus considerable interests in the structural and applied issues of Randić connectivity index, see \cite{6,7,8,9}. Based on these perfect considerations, Zagreb indices\cite{10} are introduced as expressing formulas for the total $\pi$-electron energy of conjugated molecules below.

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

where $G$ is a (molecular) graph, $uv$ is a bond between two atoms $u$ and $v$, and $d(u)$ (or $d(v)$, respectively) is the number of atoms that are connected with $u$ (or $v$, respectively).

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Zagreb indices are employing as molecular descriptors in QSPR and QSAR, see [11, 12]. In the interdisciplinary of mathematics, chemistry and physics, it is not surprising that there are numerous studies of properties of the Zagreb indices of molecular graphs [13, 14, 15, 16, 17, 18, 19, 20, 21]. In [22, 23], some bounds of (chemical) trees on Zagreb indices are studied and surveyed. Hou et al. [24] found sharp bounds for Zagreb indices of maximal outerplanar graphs. Li and Zhou [25] investigated the maximum and minimum Zagreb indices of graphs with connectivity at most $k$. The upper bounds on Zagreb indices of trees in terms of domination number is studied by Borovi´canin et al. [26]. In many mathematical literatures [27], the maximum and minimum Zagreb indices of trees with a given number of vertices of maximum degree are explored. Xu and Hua [28] provided a unified approach to extremal multiplicative Zagreb indices for trees, unicyclic and bicyclic graphs. Sharp upper and lower bounds of these indices about $k$-trees are introduced by Wang and Wei [29]. Liu and Zhang provided several sharp upper bounds for multiplicative Zagreb indices in terms of graph parameters such as the order, size and radius [30]. The bounds for the moments and the probability generating function of multiplicative Zagreb indices in a randomly chosen molecular graph with tree structure. Zhao and Li [31] investigated the upper bounds of Zagreb indices, and proposed an open question:

**Question 1.1** [31] How can we determine the lower bound for the first and the second Zagreb indices of $n$-vertex connected graphs with $k$ cut vertices? What is the characterization of the corresponding extremal graphs?

In the view of above results and open problem, we proceed to investigate Zagreb indices of graphs with given number of cut vertices in this paper. It is known that there are many results about Zagreb indices on the graph without cycles. We consider the set of all $n$-vertex graphs with $k$ cut vertices and at least one cycle, denoted by $\mathcal{V}_{n,k}$. In addition, the minimum values of $M_1(G)$ and $M_2(G)$ of graphs with given number of cut vertices are provided. Furthermore, we characterize graphs with the smallest Zagreb indices in $\mathcal{V}_{n,k}$.

## 2 Preliminary

In this section, we provide some important statements, and introduce several graph transformations. These are significant in the following section.

Let $G = (V, E)$ be a simple connected graph of $n$ vertices and $m$ edges, where $V = V(G)$ is a vertex set and $E = E(G)$ is an edge set. If $v \in V(G)$, then $N(v)$ is the neighborhood of $v$, that is, $N_G(v) = \{u \mid uv \in E(G)\}$ and the degree of $v$ is $d_G(v) = |N_G(v)|$. A pendent vertex is the vertex of degree 1 and a supporting vertex is the vertex adjacent to at least 1 pendent vertex. A pendent edge is incident to a supporting vertex and a pendent vertex. Given sets $S \subseteq V(G)$ and $F \subseteq E(G)$, denote by $G[S]$ the subgraph of $G$ induced by $S$, $G - S$ the subgraph induced by $V(G) - S$ and $G - F$ the subgraph of $G$ obtained by deleting $F$. A vertex $u$ (or an edge $e$, respectively) is said to be a cut vertex (or cut edge, respectively) of a connected graph $G$, if $G - v$ (or $G - e$) has at
least two components. A graph $G$ is called 2-connected if there does not exist a vertex whose removal disconnects the graph. A block is a connected graph which does not have any cut vertex. In particular, $K_2$ is a trivial block, and the endblock contains at most one cut vertex. Let $P_n$, $S_n$ and $C_n$ be a path, a star and a cycle on $n$ vertices, respectively. Let $T$ be a tree, and $C_m$ be a cycle of $G$. If $G$ contains $T$ as its subgraph via attaching some vertex of $T$ to some vertex of $C_m$, then we say tree $T$ is a pendent tree of $G$. Especially, replacing $T$ by $P_n|T|$ and choosing its pendent vertex to attach some vertex of $C_m$, we call path $P_n|T|$ a pendent path of $G$. In this exposition we may use the notations and terminology of (chemical) graph theory (see [32, 33]).

We start with an elementary lemma below.

**Lemma 2.1** Let $G$ be a graph. If $uv \in E(G)$, then $M_i(G - uv) < M_i(G)$ with $i = 1, 2$.

Besides the above lemma, we provide an useful tool about maximal 2-connected block on Zagreb indices.

**Lemma 2.2** Let $G \in V^k_n$ be a graph with the smallest Zagreb indices and $D$ a maximal 2-connected block of $G$ with $i = 1, 2$. If $|D| \geq 3$, then $D$ is a cycle.

**Proof.** If $|D| = 3$, then $D$ is a cycle. Otherwise, we prove the case of $|D| \geq 4$ by a contradiction. Assume that $D$ is a connected graph without cut vertices and $D$ is not a cycle. Then there exists an edge $uv$ in $D$ such that $D - uv$ has no cut vertices. Obviously, $G - uv \in V^k_n$. By Lemma 2.1 $M_i(G - uv) < M_i(G)$, which is contradicted to the choice of $G$.

The four crucial operations on graphs are given as follows.

**Operation I.** As shown in Fig.1, let $H_1$ be a connected graph with $d_{H_1(\mathbf{v})} \geq 3$ and $d_{H_1(v_1)} = 1$, and $u_1u_2$ belong to a cycle of $H_1$. If $H_2 = H_1 - \{u_1u_2,v_1v\} + \{u_1v_1,u_2v_1\}$, we say that $H_2$ is obtained from $H_1$ by **Operation I**.

![Fig.1 The graphs using in Operation I and Lemma 2.3](image)

Based on the above operation, we obtain a lemma below.

**Lemma 2.3** If $H_2$ is obtained from $H_1$ by **Operation I** as shown in Fig.1. Then $M_i(H_2) < M_i(H_1)$ for $i = 1, 2$.

**Proof.** Let $\mathbf{v}$ be a vertex of $H_1$ with $d_{H_1(\mathbf{v})} \geq 3$ and containing at least one pendent vertex $v_1$, and $u_1u_2$ be an edge of some cycle in $H_1$ with $d_{H_1(u_1)},d_{H_1(u_2)} \geq 2$. The neighbors of $\mathbf{v}$ are marked as $v_1, v_2, \ldots, v_\ell$ for $\ell \geq 3$ (see Fig.1).
If \( v \) doesn’t belong to any cycle of \( H_1 \). Then \( H_2 \) denotes the graph obtained from \( H_1 \) by deleting two edges \( vv_1, u_1w_2 \) and adding edges \( u_1v_1, u_2v_1 \). Note that the function \( f(x, y) \triangleq xy - x - y + 3 \), for \( (x, y) \in [2, +\infty) \times [2, +\infty) \), is more than zero. We now deduce that

\[
M_1(H_1) - M_1(H_2) = (d_{H_1}(v))^2 + (d_{H_1}(v_1))^2 - (d_{H_2}(v))^2 - (d_{H_2}(v_1))^2 \\
= (d_{H_1}(v) + d_{H_2}(v)) - (d_{H_1}(v_1) + d_{H_2}(v_1)) \\
\geq 5 - 3 = 2 > 0.
\]

In terms of the property of \( f(x, y) \), for \( M_2 \), we arrive at

\[
M_2(H_1) - M_2(H_2) \\
= \sum_{j=1}^{\ell} d_{H_1}(v) d_{H_1}(v_j) + d_{H_2}(u_j) d_{H_2}(u_2) \\
- \sum_{j=2}^{\ell} d_{H_2}(v) d_{H_2}(v_j) - d_{H_2}(u_1) d_{H_2}(v_1) - d_{H_2}(u_2) d_{H_2}(v_1) \\
= \sum_{j=2}^{\ell} d_{H_1}(v_j) + d_{H_1}(u_1) d_{H_1}(u_2) + d_{H_1}(v) - d_{H_2}(u_1) - d_{H_2}(u_2) \\
> d_{H_1}(u_1) d_{H_1}(u_2) - d_{H_1}(u_1) - d_{H_1}(u_2) + 3 \\
= f(d_{H_1}(u_1), d_{H_1}(u_2)) > 0.
\]

The special case \( v \) belongs to some cycles of \( H_1 \) should be discussed. If \( v_1 \) is the unique pendent vertex of \( H_1 \). Then there are nothing to do. If \( H_1 \) has another pendent vertex, marked as \( w_1 \), and \( H_2 = H_1 - vv_1 + v_1w_1 \). Then the conclusion is also verified. The proof precess of the case is similar with the above argument, so it is omitted.

Hence, the proof is finished.

**Operation II.** As shown in Fig. 2, let \( H_3 \) be a graph with \( d_{H_3}(v) \geq 3 \), and \( w_1w_2 \) be an edge included in some cycle of \( H_3 \). If \( H_4 = H_3 - \{vv_2, u_2v_2, w_1w_2\} + \{v_2w_1, v_2w_2, u_2w_1\} \) for some \( \ell \), we say that \( H_4 \) is obtained from \( H_3 \) by **Operation II**.

![](image1.png)

**Fig.2** The graphs using in Operation II and Lemma 2.4.

**Lemma 2.4** If \( H_4 \) is obtained from \( H_3 \) by **Operation II** as shown in Fig.2. Then \( M_i(H_4) < M_i(H_3) \) for \( i = 1, 2 \).

**Proof.** Let \( v \in V(H_3) \) with \( d_{H_3}(v) \geq 3 \) and \( w_1w_2 \) be an edge of some cycle in \( H_3 \). Its neighbors are labeled as \( v_1, v_2, \ldots, v_\ell (\ell \geq 3) \). If there is at least one pendent vertex of \( v \), then this case
Hence, the conclusion is verified.

Since $d_H(x, y)$ for $(x, y)$ has at least two pendent paths, e.g., $P_2(v_2u_21 \ldots u_2t_2) \times P_2(v_tu_t \ldots u_t)$ with $t_2, t_t \geq 1$. Let $H_4 = H_3 - \{v_2w, u_2v_2, w_1w_2\} \cup \{v_2w_1, v_2w_2, u_2v_{t_2}\}$. Observe that the function $g(x, y) = xy - 2x - 2y + 5$, for $(x, y) \in [2, +\infty) \times [2, +\infty)$, is more than zero. We now deduce that

$$M_1(H_3) - M_1(H_4) = (d_{H_3}(v)) - (d_{H_4}(v)) = (d_{H_3}(v) - d_{H_4}(v))$$

Hence, the conclusion is verified.

**Operation III.** As shown in Fig. 3, let $G_0$ be a connected graph with $|G_0| \geq 2$ and having two vertices $u$ and $w$, and $G_1$ be the graph which contains a cycle $C_1$. Let $H_5$ be a graph on order $n(\geq 6)$ obtained from $G_0$ by identifying some vertex of $C_1$ with vertex $u$ and some vertex of $C_2$ with vertex $v$, respectively. If $H_6$ denote the new graph from $H_5 - \{u_2w, v_0v_2, u_1u_2\} + \{u_1v_0, u_2v_1\}$, we say that $H_6$ is obtained from $H_5$ by **Operation III**.

![Fig.3 The graphs using in Operation III and Lemma 2.5](image_url)

**Lemma 2.5** If $H_6$ is obtained from $H_5$ by Operation III as shown in Fig. 3. Then $M_i(H_6) < M_i(H_5)$ for $i = 1, 2$.

**Proof.** Let $H_5$ be the graph shown in Fig. 3, $u$ and $w$ be two cut-vertex of $H_5$. $C_1$ and $C_2$ are its two cycles, where $C_2$ is an endblock. $v_1w, v_0v_2, v_2w \in E(C_2)$ and $u_1u_2 \in E(C_1)$ with with
Therefore, the proof is finished.

Similarly, for $M_2$, we can deduce that

$$
M_2(H_5) - M_2(H_6) = \sum_{j=1}^{t} d_{H_5}(w)d_{H_5}(v_j) + d_{H_5}(v_2)d_{H_5}(v_0) + d_{H_5}(u_1)d_{H_5}(u_2) \\
- \sum_{j=2}^{t} d_{H_6}(w)d_{H_6}(v_j) - d_{H_6}(u_1)d_{H_6}(v_0) - d_{H_6}(u_2)d_{H_6}(v_1) \\
= \sum_{j=3}^{t} d_{H_5}(v_j) + 3d_{H_5}(w) + d_{H_5}(u_1)d_{H_5}(u_2) - d_{H_5}(u_1) - d_{H_5}(u_2) \\
\geq d_{H_5}(u_1)d_{H_5}(u_2) - d_{H_5}(u_1) - d_{H_5}(u_2) + 11 \\
= f(d_{H_5}(u_1), d_{H_5}(u_2)) + 8 > 0.
$$

Therefore, the proof is finished.

**Operation IV.** As shown in Fig. 4, let $G_0$ be a connected graph having a vertex $v$, and $G_1$ be a graph which contains a cycle $C_1$. $H_7$ denotes the graph by attaching some vertex of $C_1$ and $C_2$ to the vertex $v$, respectively. Clearly, $C_2$ is an endblock of $H_7$. If $H_8 = H_7 - \{vv_2, v_0v_1\} + v_0v_2$, we say that $H_8$ is obtained from $H_7$ by **Operation IV**.

![Fig.4](image)

**Lemma 2.6** If $H_8$ is obtained from $H_7$ by Operation IV as shown in Fig.4. Then $M_i(H_8) < M_i(H_7)$ for $i = 1, 2$.

**Proof.** As shown in Fig.4, two cycles $C_1$ and $C_2$ of $H_7$ share a common vertex $v$ with $d_{H_7}(v) \geq 4$ whose neighbors are labeled as $v_1, v_2, \ldots, v_t$. Obviously, $t \geq 4$. In addition, $C_2$ is an endblock of $H_7$. Let $H_8$ denote the new graph obtained from $H_7$ by deleting edges $v_2v_0, v_0v_1$ and linking $v_2$ to $v_0$. We will deduce the relations of the two graphs $H_7$ and $H_8$ in terms of $M_1$ and $M_2$, respectively.

$$
M_1(H_7) - M_1(H_8) = (d_{H_7}(v))^2 + (d_{H_7}(v_1))^2 - (d_{H_8}(v))^2 - (d_{H_8}(v_1))^2 \\
= (d_{H_7}(v) + d_{H_7}(v_1)) + (d_{H_7}(v_1) + d_{H_8}(v_1)) \\
\geq 7 + 3 = 10 > 0,
$$

(1)
\[ M_2(H_7) - M_2(H_8) = \sum_{j=1}^{t} d_{H_7}(v) d_{H_7}(v_j) + d_{H_7}(v_0) d_{H_7}(v_1) \]
\[ - \sum_{j=3}^{t} d_{H_8}(v) d_{H_8}(v_j) - d_{H_8}(v) d_{H_8}(v_1) - d_{H_8}(v_0) d_{H_8}(v_2) \]
\[ = \sum_{j=3}^{t} d_{H_7}(v_j) + d_{H_7}(v) + (d_{H_7}(v) - 2)d_{H_7}(v_2) + 5 > 0. \]

Together Eq[1] with Eq[2] the conclusion is verified. \( \square \)

Let \( H \) be a connected graph with \( |E(H)| - |V(H)| \geq 0 \) and \( u, v \in V(H) \) contained in a cycle of \( H \). Denote by \( H(a, b) \) the graph formed from \( H \) by attaching two paths \( P_a \) and \( P_b \) to \( u \) and \( v \), respectively.

**Lemma 2.7** For \( d_{H(a, b)}(u), d_{H(a, b)}(v) \geq 3 \), we have \( M_i(H(a, b)) \geq M_i(H(1, a+b-1)) \) for \( i = 1, 2 \).

**Proof.** Since \( u, v \) belong to some cycle of \( H \), we have \( d_{H(a, b)}(u), d_{H(a, b)}(v) \geq 3 \). Without loss of generality, assume that \( d_{H(a, b)}(u) \geq d_{H(a, b)}(v) \). We now label all vertices of the two paths \( P_a \) and \( P_b \) as \( uu_1u_2\ldots u_{a-1} \) and \( vv_1v_2\ldots v_{b-1} \), respectively. Suppose that, besides \( u_1 \), the other neighbors of \( u \) are \( w_1, w_2, \ldots, w_t \) with \( t \geq 2 \). \( H(1, a+b-1) \) is the graph formed from \( H(a, b) \) by deleting edge \( uu_1 \) and connecting \( u_1 \) with \( v_{b-1} \). For short, we mark \( H(a, b) \) and \( H(1, a+b-1) \) as \( H_0 \) and \( H_0' \), respectively. We first consider \( M_1 \) and deduce that
\[ M_1(H_0) - M_1(H_0') = (d_{H_0}(u))^2 + (d_{H_0}(v_{b-1}))^2 - (d_{H_0'}(u))^2 - (d_{H_0'}(v_{b-1}))^2 \]
\[ = d_{H_0}(u) + d_{H_0'}(u) + 3 > 0. \]

Similarly, for \( M_2 \), we get that
\[ M_2(H_0) - M_2(H_0') \]
\[ = \sum_{j=1}^{t} d_{H_0}(u)d_{H_0}(w_j) + d_{H_0}(u)d_{H_0}(u_1) + d_{H_0}(v_{b-2})d_{H_0}(v_{b-1}) \]
\[ - \sum_{j=1}^{t} d_{H_0'}(u)d_{H_0'}(w_j) - d_{H_0'}(v_{b-2})d_{H_0'}(v_{b-1}) - d_{H_0'}(v_{b-1})d_{H_0'}(u_1) \]
\[ = \sum_{j=1}^{t} d_{H_0}(w_j) + d_{H_0}(u_1)(d_{H_0}(u) - d_{H_0'}(v_{b-1})) - d_{H_0}(v_{b-2}) \]
\[ \geq d_{H_0}(u) + d_{H_0}(u_1) - d_{H_0}(v) > 0. \]

Therefore, we complete the proof. \( \square \)

Especially, the two vertices \( u \) and \( v \) are identified in \( H(a, b) \). Then, use the similar way of Lemma 2.7 we also got a new graph \( H(2, a+b-2) \) such that \( M_i(H(a, b)) \geq M_i(H(a', b')) \) with \( a' = 2, b' = a+b-2 \) for \( i = 1, 2 \). Obviously, \( P_{a'} = uu_1 \) and \( u_1 \) is a pendant. Hence, from Lemma 2.3 we deduce
that there exists $H′$ with $|H'| = |H| + 1.$ (It is obtained from $H$ by subdividing its one edge $w_1w_2$ included in some cycle and marking the vertex as $u_1$.) such that $M_i(H(a, b)) \geq M_i(H'(1, a + b - 2))$ for $i = 1, 2.$ We list the result as follows.

**Corollary 2.8** If two vertices $u$ and $v$ are identified in $H(a, b).$ Then there exists a graph $H'$ on order $|H| + 1$ such that $M_i(H(a, b)) \geq M_i(H'(1, a + b - 2))$ for $i = 1, 2.$

### 3 Main results

In this section, we provide the lowest bounds on Zagreb indices of graphs in $\mathbb{V}_k^n.$ The corresponding graphs are characterized as well.

**Theorem 3.1** Let $G$ be a graph in $\mathbb{V}_k^n.$ Then

$(i)$ $M_1(G) \geq 4n + 2,$ the equality holds if and only if $G \cong C_{n,k},$

$(ii)$ $M_2(G) \geq 4n + 4,$ the equality holds if and only if $G \cong C_{n,k}.$

**Proof.** Choose a graph $G \in \mathbb{V}_k^n$ such that $G$ has the minimal value of $M_i$ with $i = 1, 2$ in all connected graphs possessing $k$ cut vertices. We claim that $G$ includes at least a pendent tree. If not, we will get a new graph $G'$ from $G$, and by Lemma 2.5, Lemma 2.6 and $M_i(G')$ is less than $M_i(G).$ We get a contradiction. In addition, every pendent tree of $G$ must be a path. If not, from Lemma 2.4, there exists a new graph $G''$ such that $M_i(G'') < M_i(G),$ which contradicts with the choice of $G.$ If $G$ includes at least two pendent paths. By means of Lemma 2.7 and Corollary 2.8, there is a graph $G_1$ for which $M_i(G_1) < M_i(G).$ This is a contradiction. Note that the number $|B|$ is not changed during these operations. Thus, we complete the proof of this claim.

According to Lemma 2.7 and Claim 1, we know that $G$ is a block graph and its blocks consists of cycle and $K_2,$ and $G$ has a unique pendent path, marked as $X(P).$ If $G$ just contains one cycle, then there is nothing to do. We now suppose that $G$ possesses at least two cycles.

We now claim that all endblocks of $G$ are cycles except for $K_2$ of $X(P).$ Otherwise, $G$ has no less than two pendent paths which contradicts with Claim 1.

**Case 1.** $G$ just includes two endblocks.

According the above argument, we can deduce that the two endblocks of $G$ are one cycle $C_1$ and $K_2.$ From the assumption, $G$ contains another cycle $C_2.$ In terms of Lemma 2.4 and Lemma 2.6, there is a graph $G'$ for which $M_i(G') < M_i(G)$ for $i = 1, 2.$

**Case 2.** The number of endblocks in $G$ is more than two.
By means of the assumption, $G$ includes at least two cycles endblocks, e.g., $C_3$ and $C_4$. We will get a new graph $G''$ obtained from $G$ such that $M_i(G'') < M_i(G)$ for $i = 1, 2$ through Lemma 2.5 and Lemma 2.6.

By combining Case 1 and Case 2, we deduce a contradiction with the choice of $G$. Hence, $G$ just possesses unique cycle $C_5$. Since $G$ belongs to $V^k_n$, we can deduce that $C_5 \cong C_{n-k}$ and $X(P) \cong P_{k+2}$. Therefore, $G \cong C_{n,k}$. By direct calculation, We arrive at $M_1(C_{n,k}) = 4n + 2$, $M_2(C_{n,k}) = 4n + 4$. We hence complete the proof.

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