**Chemical Trees with Extreme Values of Zagreb Indices and Coindices**

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**Abstract.** We give sharp upper bounds on the Zagreb indices and lower bounds on the Zagreb coindices of chemical trees and characterize the case of equality for each of these topological invariants.

**Keywords:** Zagreb index, Zagreb coindex, chemical tree.

1. **Introduction**

Let $G$ be chemical graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. For each $u, v \in V(G)$ the edge connecting $u$ and $v$ is denoted by $uv$ and $d_G(u)$ denotes the degree of $u$ in $G$. We will omit subscript $G$ when the graph is clear from the context. The Zagreb indices are defined as follows:

$$M_1(G) = \sum_{u \in V(G)} d(u)^2$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

Here, $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb index, respectively. The first Zagreb index can also be expressed as a sum of vertex degrees over edges of $G$,

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

The proof of this fact can be found in [8]. Many authors find this definition more useful than the original one. Nevertheless, in this paper we will use its original form.

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Zagreb indices belong to better researched topological invariants. Due to their chemical relevance, they have been studied for more than 30 years in numerous papers in chemical literature [3, 5, 6, 7, 8, 9]. Recently, Došlić ([4]) gave a generalisation of these numbers. He introduced two new graph invariants, the first and the second Zagreb coindices, defined as follows:

\[
\overline{M}_1(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)]
\]

and

\[
\overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u)d_G(v).
\]

Ashrafi, Došlić and Hamzeh in [1] determined the extremal graphs with respect to the Zagreb coindices. They wrote that it would be interesting to extend results presented in [1] to some other classes of graphs of chemical interest and emphasized that their "result leave open the question of the minimum values of Zagreb coindices over chemical trees". In this paper we give an answer to this question.

For \( n = 3k \geq 6 \) let \( T_{3k} \) be the family of chemical trees with \( n \) vertices such that: \( k - 1 \) vertices have degree 4, 1 vertex has degree 2 and remaining vertices are pendant. Denote by \( \overline{T}_{3k} \subset T_{3k} \) family of trees \( G \) from \( T_{3k} \) such that for the unique vertex \( w \in V(G) \) of degree 2 exactly one of its neighbours is pendant. For \( n = 3k + 1 \geq 7 \), denote by \( T_{3k+1} \) the family of chemical trees with \( n \) vertices such that: \( k - 1 \) vertices have degree 4, 1 vertex has degree 3 and all other vertices are pendant, while \( \overline{T}_{3k+1} \) denotes the family of trees \( G \) from \( T_{3k+1} \) such that for the unique vertex \( w \in V(G) \) of degree 3 exactly one of its neighbours is pendant. For \( n = 3k + 2 \geq 5 \), \( T_{3k+2} \) denotes the family of chemical trees with \( n \) vertices such that: \( k \) vertices have degree 4 and remaining are pendant.

Our main results are the next two theorems:

**Theorem 1.** Let \( G \) be chemical tree with \( n \geq 5 \) vertices. Then

\[
M_1(G) \leq \begin{cases} 
6n - 12, & n \equiv 0, 1 \pmod{3} \\
6n - 10, & n \equiv 2 \pmod{3}.
\end{cases}
\]

The equality is attained if and only if \( G \in T_n \).

**Theorem 2.** Let \( G \) be chemical tree with \( n \geq 5 \) vertices. Then

\[
M_2(G) \leq \begin{cases} 
8n - 26, & n \equiv 0, 1 \pmod{3} \\
8n - 24, & \text{otherwise}.
\end{cases}
\]

The equality is attained if and only if \( n \equiv 0, 1 \pmod{3} \) and \( G \in \overline{T}_n \), or \( n \equiv 2 \pmod{3} \) and \( G \in T_n \).
2. ON THE FIRST ZAGREB INDEX AMONG CHEMICAL TREES

In this section our goal is to obtain sharp upper bound on the first Zagreb index of chemical trees and, accordingly, to characterize the chemical trees with maximal values of the first Zagreb index.

Let $G$ be a chemical tree with $n$ vertices. For each $i \in \{1,2,3,4\}$ let $n_i$ denote the number of its vertices of degree $i$. Then,

$$n_1 + n_2 + n_3 + n_4 = n$$

and from handshaking lemma

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n - 1).$$

From (1) and (2) we conclude that

$$n_2 + 2n_3 + 3n_4 = n - 2.$$  

Using definition of the first Zagreb index we get that for any chemical tree $G$:

$$M_1(G) = n_1 + 4n_2 + 9n_3 + 16n_4.$$  

Let $G_n$ be $n$-vertex chemical tree such that $n = 3k$, $k \geq 2$. Then (3) reduces to

$$n_2 + 2n_3 + 3n_4 = 3k - 2$$

from which follows that $n_4 \leq k - 1$ and for $n_4 = k - 1$ hold $n_2 = 1$, $n_3 = 0$ and so, due to (1), $n_1 = 2k$. Hence, using Eq. (4)

$$M_1(G_n) = 6n - 12.$$  

Otherwise, $n_4 \leq k - 2$, that is $n_4 \leq \frac{n}{3} - 2$ and using equations (3) and (1) we get

$$M_1(G_n) = n_1 + 4n_2 + 9n_3 + 16n_4$$

$$= 4(n_2 + 2n_3 + 3n_4) + (n_1 + n_3 + n_4) + 3n_4$$

$$= 4(n - 2) + n - n_2 + 3n_4$$

$$\leq 5n - 8 - n_2 + 3\left(\frac{n}{3} - 2\right)$$

$$\leq 6n - 14.$$  

Therefore, for $n \equiv 0 \pmod{3}$, $n \geq 6$, if $G_n$ is $n$-vertex chemical tree $M_1(G_n) \leq 6n - 12$ and equality is attained if and only if in $V(G_n)$ there are $\frac{n}{3} - 1$ vertices of degree 4, 1 vertex of degree 2 and remaining vertices are pendant, that is $G_n \in \mathcal{T}_n$.

Now, let $G_n$ be $n$-vertex chemical tree such that $n = 3k + 1$, $k \geq 2$. Then (3) reduces to $n_2 + 2n_3 + 3n_4 = 3k - 1$ and, as in the previous case, follows that $n_4 \leq k - 1$.
For \( n_g = k - 1 \), we have the next two possibilities: \( n_2 = 0, n_3 = 1 \) or \( n_2 = 2, n_3 = 0 \). In the first case, \( M_1(G_n) = 6n - 12 \) and in the second one \( M_1(G_n) = 6n - 14 \). So, the second case can not give the maximal \( M_1 \) index among chemical trees.

Similarly with the above discussion for \( n \equiv 0 \pmod{3} \), when \( n_g \leq k - 2 \) we obtain that

\[
M_1(G_n) = 4(n - 2) + n - n_2 + 3n_4 \\
\leq 5n - 8 - n_2 + 3\left(\frac{n-1}{3} - 2\right) \\
\leq 6n - 15.
\]

Hence, for \( n \equiv 1 \pmod{3}, n \geq 7 \), if \( G_n \) is \( n \)-vertex chemical tree \( M_1(G_n) \leq 6n - 12 \) and equality is attained if and only if in \( V(G_n) \) there are \( \frac{n-1}{3} \) vertices of degree 4, 1 vertex of degree 3 and remaining vertices are pendant, i.e. \( G_n \in T_n \).

Finally, let \( G_n \) be chemical tree with \( n = 3k + 2, k \geq 1 \), vertices. Equality (3) reduces to \( n_2 + 2n_3 + 3n_4 = 3k \) and so \( n_g \leq k \).

Similarly with the above discussion, for \( n_g = k \), we have that \( n_2 = n_3 = 0 \) and the first Zagreb index on this class of trees takes value \( M_1(G_n) = 6n - 10 \).

Otherwise, \( n_g \leq k - 1 \) and we get:

\[
M_1(G_n) = 4(n - 2) + n - n_2 + 3n_4 \\
\leq 5n - 8 - n_2 + 3\left(\frac{n-2}{3} - 1\right) \\
\leq 6n - 13.
\]

It follows that for \( n \equiv 2 \pmod{3}, n \geq 5 \), if \( G_n \) is \( n \)-vertex chemical tree, then \( M_1(G_n) \leq 6n - 10 \) and equality is attained if and only if in \( V(G_n) \) there are \( \frac{n-2}{3} \) vertices of degree 4 and remaining vertices are pendant.

### 3. On the Second Zagreb Index Among Chemical Trees

Let \( G_1 \) and \( G_2 \) be vertex-disjoint graphs. Suppose that \( a_1 \in V(G_1) \) and \( a_2 \in V(G_2) \). We denote by \( G_1 > a_1 - a_2 < G_2 \) the graph with the vertex set \( V(G_1) \cup V(G_2) \) and the edge set \( E(G_1) \cup E(G_2) \cup \{a_1a_2\} \), that is the graph obtained from the union \( G_1 \cup G_2 \) connecting its two components \( G_1 \) and \( G_2 \) by an edge \( a_1a_2 \). \( G_1 > a_1 - a_2 < G_2 \) is edge-join of the graphs \( G_1 \) and \( G_2 \) across the vertices \( a_1 \) and \( a_2 \).
Lemma 1. If $G$ is chemical tree with at least two vertices of degree 3, then its second Zagreb index cannot be maximal.

Proof. Let $G$ be chemical tree and $x, y \in V(G)$ such that $d(x) = d(y) = 3$. Consider first in detail the case when the vertices $x$ and $y$ are not neighbours. Denote by $x_i$ and $y_i$, $i = 1, 3$ its neighbours, respectively. Let $e_i = x_i x$ and $g_i = y_i y$ be appropriate edges for each $i = 1, 3$. Without loss of generality, suppose that

$$d(x_1) + d(x_2) + d(x_3) \leq d(y_1) + d(y_2) + d(y_3) \quad (5)$$

and the unique path between $x$ and $y$ goes toward the vertices $x_1$ and $y_1$. Denote by $G - e_3$ the subgraph of $G$ obtained by deleting the edge $e_3$. The graph $G - e_3$ is forest with two components $H_{x_3}$ and $H_x$ such that $x_3 \in V(H_{x_3})$ and $x \in V(H_x)$. Let $G' = H_{x_3} \bigstar x - y < H_x$ be edge-join of the trees $H_{x_3}$ and $H_x$ across the edge $x_3 y$. We are going to prove that $M_2(G) < M_2(G')$. Let $S = \{e_1, e_2, e_3, g_1, g_2, g_3\}$. It holds

$$M_2(G) = \sum_{u \neq v \in S} d(u) d(v) + 3[d(x_1) + d(x_2) + d(x_3)] + 3[d(y_1) + d(y_2) + d(y_3)]$$

and

$$M_2(G') = \sum_{u \neq v \in S} d(u) d(v) + 2[d(x_1) + d(x_2)] + 4[d(y_1) + d(y_2) + d(y_3) + d(x_3)]$$

Therefore

$$M_2(G) - M_2(G') = d(x_1) + d(x_2) - d(x_3) - [d(y_1) + d(y_2) + d(y_3)]$$

and due to inequality (5)

$$M_2(G) - M_2(G') \leq d(x_1) + d(x_2) - d(x_3) - [d(x_1) + d(x_2) + d(x_3)] = -2d(x_3) < 0,$$

since $d(x_3) \geq 1$.

Now, suppose that the vertices $x$ and $y$ are neighbours. Then, the vertices $x_i$ and $y_i$ from the above construction are the vertices $y$ and $x$, respectively, and the edges $e_i$ and $g_i$ are one and the same edge $xy$. Now, inequality (5) reduces to:

$$d(x_1) + d(x_2) \leq d(y_1) + d(y_3), \quad (6)$$

and the next hold:

$$M_2(G) = \sum_{u \neq v \in S} d(u) d(v) + 3[d(x_2) + d(x_3)] + 9 + 3[d(y_2) + d(y_3)]$$

and

$$M_2(G') = \sum_{u \neq v \in S} d(u) d(v) + 2d(x_2) + 8 + 4[d(y_2) + d(y_3) + d(x_3)].$$

Due to (6)
\[ M_2(G) - M_2(G') = d(x_2) - d(x_3) + 1 - [d(y_2) + d(y_3)] \]
\[ \leq d(x_2) - d(x_3) + 1 - [d(x_2) + d(x_3)] \]
\[ = 1 - 2d(x_3) \]
\[ < 0, \]
since \( d(x_3) \geq 1. \)

**Lemma 2.** If \( G \) is chemical tree with at least two vertices of degree 2, then its second Zagreb index cannot be maximal.

**Proof.** Let \( G \) be chemical tree and \( x, y \in V(G) \) such that \( d(x) = d(y) = 2 \). Suppose that \( x \) and \( y \) are not neighbours and denote by \( x_1, x_2 \) and \( y_1, y_2 \) its neighbours, respectively. Let \( e_i = x_i x \), \( g_i = y_i y \) be appropriate edges for each \( i = 1, 2 \). Without loosen of generality suppose that

\[ d(x_1) + d(x_2) \leq d(y_1) + d(y_2) \quad (7) \]

and the unique \( x - y \) path goes toward the vertices \( x_1 \) and \( y_1 \). The graph \( G - e_2 \) is forest with two components \( H_{x_2} \) and \( H_x \) such that \( x_2 \in V(H_{x_2}) \) and \( x \in V(H_x) \). Let \( G' = H_{x_2} > x_2 - y < H_x \) be edge-join of the trees \( H_{x_2} \) and \( H_x \) across the edge \( x_2 y \). We are going to prove that \( M_2(G) < M_2(G') \). Let \( S = \{ e_1, e_2, g_1, g_2 \} \). Then,

\[ M_2(G) = \sum_{uv \in S} d(u)d(v) + 2[d(x_1) + d(x_2)] + 2[d(y_1) + d(y_2)] \]

and

\[ M_2(G') = \sum_{uv \in S} d(u)d(v) + d(x_1) + 3[d(y_1) + d(y_2) + d(x_2)] \]

Using the inequality (7),

\[ M_2(G) - M_2(G') = d(x_1) - d(x_2) - [d(y_1) + d(y_2)] \]
\[ \leq d(x_1) - d(x_2) - [d(x_1) + d(x_2)] \]
\[ = -2d(x_2) \]
\[ < 0, \]

since \( d(x_2) \geq 1. \)

When the vertices \( x \) and \( y \) are neighbours, the vertices \( x_1 \) and \( y_1 \) from the upper construction are the vertices \( y \) and \( x \), respectively, and the edges \( e_1 \) and \( g_1 \) are the one and the same edge \( xy \). Now, inequality (7) is equivalent with

\[ d(x_2) \leq d(y_2) \quad (8) \]

and we have that:
\[ M_2(G) = \sum_{u,v \in S} d(u)d(v) + 2d(x_2) + 4 + 2d(y_2) \]

and

\[ M_2(G') = \sum_{u,v \in S} d(u)d(v) + 3 + 3[d(y_2) + d(x_2)]. \]

Hence, due to \( d(x_2) \geq 1 \) and inequality (8)

\[ M_2(G) - M_2(G') = 1 - d(x_2) - d(y_2) \leq 1 - 2d(x_2) < 0. \]

Lemma 3. If \( G \) is chemical tree with at least one vertex of degree 2 and at least one vertex of degree 3, then its second Zagreb index cannot be maximal.

Proof. Let \( G \) be chemical tree and \( x, y \in V(G) \) such that \( d(x) = 2 \) and \( d(y) = 3 \). If \( x \) and \( y \) are not neighbours, denote by \( x_1, x_2 \) and \( y_1, y_2, y_3 \) its neighbours, respectively. Let \( e_1 = x_1x, e_2 = x_2x, g_1 = y_1y, g_2 = y_2y, \) and \( g_3 = y_3y \) and suppose that \( x - y \) path goes toward the vertices \( x_1 \) and \( y_1 \). The graph \( G - e_2 \) is forest with two components \( H_{x_2} \) and \( H_x \) such that \( x_2 \in V(H_{x_2}) \) and \( x \in V(H_x) \). Let \( G' = H_{x_2} \uplus H_x \) be edge–join of the trees \( H_{x_2} \) and \( H_x \) across the edge \( x_2y \). We are going to prove that \( M_2(G) < M_2(G') \).

Let \( S = \{e_1, e_2, g_1, g_2, g_3\} \). Then,

\[ M_2(G) = \sum_{u,v \notin S} d(u)d(v) + 2[d(x_1) + d(x_2)] + 3[d(y_1) + d(y_2) + d(y_3)] \]

and

\[ M_2(G') = \sum_{u,v \notin S} d(u)d(v) + d(x_1) + 4[d(y_1) + d(y_2) + d(y_3)] + d(x_2). \]

Therefore,

\[ M_2(G) - M_2(G') = d(x_1) - 2d(x_2) - [d(y_1) + d(y_2) + d(y_3)]. \]

Since \( d(x_2) \geq 1, d(y_1) \geq 2, d(y_2) \geq 1 \) and \( d(y_3) \geq 1 \), it follows that \( M_2(G) - M_2(G') < 0 \).

In the case when \( x \) and \( y \) are neighbours, that is \( x_1 \) is the same as \( y \) and \( y_1 \) is the same as \( x \), the next is true:

\[ M_2(G) = \sum_{u,v \notin S} d(u)d(v) + 2d(x_2) + 6 + 3[d(y_2) + d(y_3)], \]

\[ M_2(G') = \sum_{u,v \notin S} d(u)d(v) + 4 + 4[d(y_2) + d(y_3) + d(x_2)]. \]

and so

\[ M_2(G) - M_2(G') = 2 - 2d(x_1) - [d(y_2) + d(y_3)]. \]
Since that degrees \( d(x_2), d(y_2) \) and \( d(y_3) \) are at least 1, it follows that 
\[ M_2(G) - M_2(G') < 0. \]

From the upper three lemmas we make the next conclusion:

**Corollary 1.** If \( G \) is chemical tree such that
\[ M_2(G) = \max \{ M_2(T) \mid T \text{ is chemical tree} \}, \]
then \( G \) satisfies one of the next three conditions:

(i) all vertices of the graph \( G \) have degrees 1 or 4;

(ii) in \( V(G) \) there is exactly one vertex of degree 2 and remaining have degrees 1 or 4;

(iii) in \( V(G) \) there is exactly one vertex of degree 3 and remaining are of degrees 1 or 4.

Now, we are ready to prove Theorem 2.

**Proof of Theorem 2:** For edge \( e \) with end points \( u \) and \( v \) denote by \( w(e) \) the product \( d(u)d(v) \). Let \( A \) denotes the set of pendant edges in the graph \( G \) and \( B = E(G) - A \). Then,
\[ M_2(G) = \sum_{e \in A} w(e) + \sum_{e \in B} w(e) \]

First, consider the case \( n = 3k + 2, \ k \geq 1 \). From Eq. (3) we have that \( n_2 + 2n_3 \equiv 0 \) (mod 3) and so, from Corollary 1 we get \( n_2 = n_3 = 0 \). From (1) and (3) follows that \( n_4 = k \) and \( n_1 = 2k + 2 \), that is \( |A| = 2k + 2 \) and \( |B| = k - 1 \). Since
\[ w(e) = \begin{cases} 16, & e \in B \\ 4, & e \in A \end{cases} \]
we obtain that
\[ M_2(G_n) = \sum_{e \in A} w(e) + \sum_{e \in B} w(e) = 24k - 8 = 8n - 24. \]

Now, let \( n = 3k + 1, \ k \geq 2 \). From Eq. (3) we have that \( n_2 + 2n_3 \equiv 2 \) (mod 3) and so, from Corollary 1 we get \( n_2 = 0, \ n_3 = 1 \). Hence, \( n_4 = k - 1, \ n_1 = 2k + 1 \), that is \( |A| = 2k + 1 \) and \( |B| = k - 1 \). Let \( x \in V(G_n) \) be unique vertex of degree 3. Then,
\[ \sum_{e \in A} w(e) = \begin{cases} 8k + 2, & x \text{ is incident with 2 pendant edges} \\ 8k + 3, & x \text{ is incident with 1 pendant edge} \\ 8k + 4, & x \text{ is not incident with pendant edges} \end{cases} \]
and
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Consider the expression for the sum of weights of edges in a graph $G_n$:

$$\sum_{e \in B} w(e) = \begin{cases} 16k - 20, & \text{x is incident with 2 pendant edges} \\ 16k - 24, & \text{x is incident with 1 pendant edge} \\ 16k - 28, & \text{x is not incident with pendant edges}. \end{cases}$$

Hence,

$$M_2(G_n) = \begin{cases} 24k - 18, & \text{x is incident with 2 pendant edges} \\ 24k - 21, & \text{x is incident with 1 pendant edge} \\ 24k - 24, & \text{x is not incident with pendant edges}. \end{cases}$$

i.e.

$$M_2(G_n) = \begin{cases} 8n - 26, & \text{x is incident with 2 pendant edges} \\ 8n - 29, & \text{x is incident with 1 pendant edge} \\ 8n - 32, & \text{x is not incident with pendant edges}. \end{cases}$$

Finally, let $n = 3k$, $k \geq 2$. Similarly with the discussion from the above two cases we obtain that $n = 1$, $n = 0$, $n = 2k$ and $n = k - 1$, that is $|A| = 2k$ and $|B| = k - 1$. Let $x$ be unique vertex of degree 2. It holds

$$\sum_{e \in A} w(e) = \begin{cases} 8k - 2, & \text{x is incident with 1 pendant edge} \\ 8k, & \text{x is not incident with pendant edges} \end{cases}$$

and

$$\sum_{e \in B} w(e) = \begin{cases} 16k - 24, & \text{x is incident with 1 pendant edge} \\ 16k - 32, & \text{x is not incident with pendant edges}. \end{cases}$$

So,

$$M_2(G_n) = \begin{cases} 24k - 26, & \text{x is incident with 1 pendant edge} \\ 24k - 24, & \text{x is not incident with pendant edges} \end{cases}$$

that is

$$M_2(G_n) = \begin{cases} 8n - 26, & \text{x is incident with 1 pendant edge} \\ 8n - 32, & \text{x is not incident with pendant edges}. \end{cases}$$

Combining the above results we get that

$$M_2(G) \leq \begin{cases} 8n - 26, & n \equiv 0,1 \pmod{3} \\ 8n - 24, & \text{otherwise} \end{cases}$$

and equality is attained if and only if $n \equiv 0,1 \pmod{3}$ and $G \in \overline{T}_n$, or $n \equiv 2 \pmod{3}$ and $G \in T_n$. 

4. **ZAGREB COINDICES AMONG CHEMICAL TREES**

In [2] A. R. Ashrafi, T. Došlić and A. Hamzeh proved that for any connected graph $G$ with $n$ vertices and $m$ edges hold

$$
\overline{M}_1(G) = 2m(n-1) - M_1(G)
$$

and

$$
\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).
$$

The next two theorems are direct consequence of these equalities and theorems 1 and 2 proved in sections 2 and 3.

**Theorem 3.** Let $G$ be chemical tree with $n \geq 5$ vertices. Then

$$
\overline{M}_1(G) \geq \begin{cases} 
2n^2 - 10n + 14, & n \equiv 0,1 \pmod{3} \\
2n^2 - 10n + 12, & n \equiv 2 \pmod{3}.
\end{cases}
$$

The equality is attained if and only if $G \in T_n$.

**Theorem 4.** Let $G$ be chemical tree with $n \geq 5$ vertices. Then

$$
\overline{M}_2(G) \geq \begin{cases} 
2n^2 - 15n + 34, & n \equiv 0,1 \pmod{3} \\
2n^2 - 15n + 31, & \text{otherwise}.
\end{cases}
$$

The equality is attained if and only if $n \equiv 0,1 \pmod{3}$ and $G \in \overline{T}_n$, or $n \equiv 2 \pmod{3}$ and $G \in T_n$.

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