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 be also expressed as a sum of vertex degrees over edges of G,

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

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 paper 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:

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

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 $\widetilde{\mathsf{T}}_{3k} \subset \mathsf{T}_{3k}$ family of trees G from T_{3k} such that for the unique vertex $w \in V(G)$ of degeree 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 veretex has degree 3 and all other vertices are pendant, while $\widetilde{\mathsf{T}}_{3k+1}$ denotes the family of trees G from T_{3k+1} such that for the unique vertex $w \in V(G)$ of degeree 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 $G \in \mathsf{T}_n$.

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 $G \in \widetilde{\mathsf{T}}_n$, or $n \equiv 2 \pmod 3$ and $G \in \mathsf{T}_n$.

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 degeree i. Then,

$$n_1 + n_2 + n_3 + n_4 = n \tag{1}$$

and from handshaking lemma

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

From (1) and (2) we conclude that

$$n_2 + 2n_3 + 3n_4 = n - 2. \tag{3}$$

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

$$M_1(G) = n_1 + 4n_2 + 9n_3 + 16n_4. \tag{4}$$

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

$$\begin{aligned} M_1(G_n) &= n_1 + 4n_2 + 9n_3 + 16n_4 \\ &= 4(n_2 + 2n_3 + 3n_4) + (n_1 + n_3 + n_4) + 3n_4 \\ &= 4(n-2) + n - n_2 + 3n_4 \\ &\leq 5n - 8 - n_2 + 3\left(\frac{n}{3} - 2\right) \\ &\leq 6n - 14. \end{aligned}$$

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 $G_n \in \mathrm{T}_n$.

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 $n_4 = k-1$, 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 no give the maximal M_1 index among chemical trees.

Similarly with the above discussion for $n \equiv 0 \pmod 3$, when $n_4 \le k-2$ we obtain that

$$\begin{aligned} M_1(G_n) &= 4(n-2)+n-n_2+3n_4 \\ &\le 5n-8-n_2+3\left(\frac{n-1}{3}-2\right) \\ &\le 6n-15. \end{aligned}$$

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

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

Similarly with the above discussion, for $n_4 = k$, 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, $n_4 \le k-1$ and we get:

$$\begin{aligned} M_1(G_n) &= 4(n-2)+n-n_2+3n_4 \\ &\le 5n-8-n_2+3\left(\frac{n-2}{3}-1\right) \\ &\le 6n-13. \end{aligned}$$

It follows that for $n \equiv 2 \pmod 3$, $n \ge 5$, if G_n is $n-$vertex chemical tree, then $M_1(G_n) \le 6n-10$ 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 $E(G_1) \cup E(G_2) \cup \{a_1 a_2\}$, 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 $a_1 a_2$. $G_1 > a_1 - a_2 < G_2$ 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 degeree 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, $i = \overline{1,3}$ its neighbours, respectively. Let $e_i = x_i x$ and $g_i = y_i y$ be appropriate edges for each $i = \overline{1,3}$. Without loss of generality, suppose that

$$d(x_1) + d(x_2) + d(x_3) \le d(y_1) + d(y_2) + d(y_3) \tag{5}$$

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 $G' = H_{x_3} > x_3 - y < H_x$ 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

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

and

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

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)

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

since $d(x_3) \ge 1$.

Now, suppose that the vertices x and y are neighbours. Then, the vertices x_1 and y_1 from the above construction are the vertices y and x, respectively, and the edges e_1 and g_1 are one and the same edge xy. Now, inequality (5) reduces to:

$$d(x_2) + d(x_3) \le d(y_2) + d(y_3), \tag{6}$$

and the next hold:

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

and

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

Due to (6)

$$\begin{aligned} M_2(G)-M_2(G') &= d(x_2)-d(x_3)+1-[d(y_2)+d(y_3)] \\ &\le d(x_2)-d(x_3)+1-[d(x_2)+d(x_3)] \\ &= 1-2d(x_3) \\ &< 0, \end{aligned}$$

since $d(x_3)\ge 1$.

■

Lemma 2. *If G is chemical tree with at least two vertices of degeree 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 loose of generality suppose that

$$d(x_1)+d(x_2)\le d(y_1)+d(y_2) \tag{7}$$

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,

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

and

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

Using the inequality (7),

$$\begin{aligned} M_2(G)-M_2(G') &= d(x_1)-d(x_2)-[d(y_1)+d(y_2)] \\ &\le d(x_1)-d(x_2)-[d(x_1)+d(x_2)] \\ &= -2d(x_2) \\ &< 0, \end{aligned}$$

since $d(x_2)\ge 1$.

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

$$d(x_2)\le d(y_2) \tag{8}$$

and we have that:

$$M_2(G) = \sum_{uv \notin S} d(u)d(v) + 2d(x_2) + 4 + 2d(y_2)$$

and

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

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 degeree 2 and at least one vertex of degeree 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 $G' = H_{x_2} > x_2 - y < H_x$ 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,

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

and

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

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:

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

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

and so

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

Since that degrees $d(x_2)$, $d(y_2)$ and $d(y_3)$ are at least 1, it follows that $M_2(G) - M_2(G') < 0$.

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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 degeree 2 and remaining have degrees 1 or 4;

(iii) *in $V(G)$ there is exactly one vertex of degeree 3 and remaining are of degerees 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 $n_2 + 2n_3 \equiv 0 \pmod 3$ 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 $n_2 + 2n_3 \equiv 2 \pmod 3$ 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

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

Hence,

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

i.e.

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

Finally, let $n = 3k,\ \ k \ge 2$. Similarly with the discussion from the above two cases we obtain that $n_2 = 1$, $n_3 = 0$, $n_1 = 2k$ and $n_4 = k-1$, that is $|A| = 2k$ and $|B| = k-1$. Let x be unique vertex of degree 2. It holds

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

and

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

So,

$$M_2(G_n) = \begin{cases} 24k-26, & x \text{ is incident with 1 pendant edge} \\ 24k-32, & x \text{ is not incident with pendant edges} \end{cases}$$

that is

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

Combining the above results we get that

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

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

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 verices 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*

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

The equality is attained if and only if $G \in \mathsf{T}_n$.

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

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

The equality is attained if and only if $n \equiv 0,1 \ (\text{mod } 3)$ and $G \in \widetilde{\mathsf{T}}_n$, or $n \equiv 2 \ (\text{mod } 3)$ and $G \in \mathsf{T}_n$.

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