Further Properties of the Second Zagreb Index[1]

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Abstract

We determine the maximum value of the second Zagreb index among graphs
with given numbers of vertices, edges, minimum and maximum vertex degrees. As
the extremal graphs may happen to be multigraphs, we, in addition, determine trees
with the maximum value of the second Zagreb index among all trees with given num-
ber of vertices and maximum vertex degree. As an application of the latter result,
we answer the question of Ashrafi, Došlić and Hamzeh [*MATCH Commun. Math.
Comput. Chem.* **65** (2011), 85–92] on the minimum values of Zagreb coindices over
chemical trees.

1 Introduction

Let $G = (V, E)$ be a graph with the vertex set V, $n = |V|$, and the edge set E, $m = |E|$.
For a vertex $u \in V$, let d_u be its degree. The first and the second Zagreb indices, defined
as

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

$$M_2 = M_2(G) = \sum_{uv \in E} d_u d_v,$$

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are widely studied degree-based topological indices, that were introduced by Gutman and Trinajstić [1] in 1972. Gutman provides an overview of recent developments among degree-based topological indices in [2], while further mathematical properties of M_1 and M_2 are surveyed in [3, 4]. Although the first Zagreb index has attracted considerable attention in literature, the second Zagreb index has been much less studied, with some of the earliest general properties of M_2 reported only in 2004 in [5].

Zhou and Gutman [6] presented an upper bound for M_1 in terms of n, m, the minimum vertex degree δ and the maximum vertex degree Δ:

Theorem 1 ([6]) *Let G be a graph with n vertices, m edges, the minimum vertex degree $\delta \geq 1$, and the maximum vertex degree $\Delta > \delta$. Then*

$$M_1(G) \leq 2m(\delta + \Delta) - n\delta\Delta + (\delta - k)(\Delta - k) \tag{1}$$

where k is the integer defined via

$$k - \delta \equiv 2m - n\delta \pmod{\Delta - \delta}, \qquad \delta \leq k \leq \Delta - 1,$$

i.e.,

$$k = 2m - \delta(n - 1) - (\Delta - \delta) \left\lfloor \frac{2m - n\delta}{\Delta - \delta} \right\rfloor.$$

Equality in (1) is attained if and only if at most one vertex of G has degree different from Δ and δ.

Our main goal here is to provide an analogous bound for M_2 in terms of n, m, δ and Δ. This new bound is proved and discussed in Section 2. As the extremal graphs may happen to be multigraphs, as pointed out in Subsection 2.1, we, in addition, determine trees with the maximum value of M_2 among trees with given n and Δ in Subsection 2.2. As an application of these results, we resolve a question of Ashrafi, Došlić and Hamzeh [7] on the minimum values of Zagreb coindices over chemical trees in Section 3.

2   Upper bound for the second Zagreb index

Here we prove the following upper bound on M_2 for general values of n, m, δ and Δ.

Theorem 2 *Let G be a graph with n vertices, m edges, the minimum vertex degree $\delta \geq 1$ and the maximum vertex degree $\Delta > \delta + 1$. Then*

$$M_2 \leq \frac{(2m - k)\left(\Delta^2 + \Delta\delta + \delta^2\right) - (n-1)\Delta\delta(\Delta + \delta)}{2} + \begin{cases} k\delta\left(k - \frac{\delta}{2}\right) & \text{if } k \leq (\Delta + \delta)/2, \\ k\Delta\left(k - \frac{\Delta}{2}\right) & \text{if } k > (\Delta + \delta)/2, \end{cases} \tag{2}$$

where k is the integer defined via

$$2m - n\delta \equiv k - \delta \pmod{\Delta - \delta}, \qquad \delta \leq k \leq \Delta - 1,$$

i.e.,

$$k = 2m - \delta(n-1) - (\Delta - \delta)\left\lfloor \frac{2m - n\delta}{\Delta - \delta} \right\rfloor. \tag{3}$$

A graph G attains equality in Eq. (2) if and only if G does not contain an edge connecting a vertex of degree Δ to a vertex of degree δ and it contains at most one vertex of degree $k \neq \Delta, \delta$ such that:

(i) the vertex of degree k is adjacent to vertices of degree δ only, when $k < (\Delta + \delta)/2$;

(iii) the vertex of degree k is adjacent to vertices of degree Δ only, when $k > (\Delta + \delta)/2$.

The proof of this theorem will rely on the use of edge rotations to increase the value of M_2. For a vertex $u \in V$, let $N_u = \{v : uv \in E\}$ and $m_u = \sum_{v \in N_u} d_v$ denote the neighborhood of u and the sum of degrees of the neighbors of u, respectively. Further, for vertices $u, a, b \in V$ such that $ua \in E$, an *edge rotation* from a to b around u, shortly denoted as $ua \to ub$, is a transformation in which the edge ua is deleted and a new edge ub is added to a graph. In other words, after an edge rotation the transformed graph becomes $G' = G - ua + ub$. Edge rotation decreases the degree of a by 1 and increases the degree of b by 1, leaving all other vertex degrees unchanged. The difference between $M_2(G')$ and $M_2(G)$ is then due to: deletion of edge ua from G, addition of edge ub to G', decrease in contributions of edges va, $v \neq u$, to M_2, increase in contributions of edges wb, $w \neq u$, and, provided that a and b are adjacent, the change in contribution of edge ab. Hence,

$$M_2(G') - M_2(G) = \begin{cases} d_u(d_b - d_a + 2) + (m_b - m_a), & ab \notin E, \\ d_u(d_b - d_a + 2) + (m_b - m_a) - 1, & ab \in E. \end{cases} \tag{4}$$

In case the edge rotation was applied in the other direction, so that edge ub is deleted from G and edge ua is added to obtain G'', then

$$M_2(G'') - M_2(G) = \begin{cases} d_u(d_a - d_b + 2) + (m_a - m_b), & ab \notin E, \\ d_u(d_a - d_b + 2) + (m_a - m_b) - 1, & ab \in E. \end{cases} \tag{5}$$

The following lemma is the main ingredient of the proof of Theorem 2.

Lemma 3 *If G contains at least two vertices whose degrees are different from δ and Δ, then there exists an edge rotation that strictly increases the value of $M_2(G)$.*

Proof Suppose, on the contrary, that G contains two vertices a and b such that $\delta + 1 \leq d_a, d_b \leq \Delta - 1$ and that no edge rotation (either of the form $ua \to ub$ or $vb \to va$) strictly increases the value of M_2. Suppose first that a and b are not adjacent. Then for each $u \in N_a$

$$d_u(d_b - d_a + 2) + (m_b - m_a) \leq 0$$

and for each $v \in N_b$

$$d_v(d_a - d_b + 2) + (m_a - m_b) \leq 0.$$

Summing up the above inequalities for all $u \in N_a$ and $v \in N_b$ separately, we obtain

$$\sum_{u \in N_a} [d_u(d_b - d_a + 2) + (m_b - m_a)] \leq 0,$$
$$\sum_{v \in N_b} [d_v(d_a - d_b + 2) + (m_a - m_b)] \leq 0,$$

which yields

$$m_a(d_b - d_a + 2) + d_a(m_b - m_a) \leq 0,$$
$$m_b(d_a - d_b + 2) + d_b(m_a - m_b) \leq 0.$$

Adding these two inequalities together and rearranging the terms we get

$$m_a + m_b \leq (m_a - m_b)(d_a - d_b).$$

Since $m_a + m_b > 0$, this implies that the differences $m_a - m_b$ and $d_a - d_b$ are of the same sign. If $m_a - m_b$ and $d_a - d_b$ are both negative, then a rotation $ua \to ub$ around any $u \in N_a$ increases M_2 by (4). If $m_a - m_b$ and $d_a - d_b$ are both positive, then a rotation $vb \to va$ around any $v \in N_b$ increases M_2 by (5). In both cases we obtain a contradiction to the starting assumption that no edge rotation increases M_2.

An analogous argument applies in case that a and b are adjacent. If for each $u \in N_a$

$$d_u(d_b - d_a + 2) + (m_b - m_a) - 1 \leq 0$$

and for each $v \in N_b$

$$d_v(d_a - d_b + 2) + (m_a - m_b) - 1 \leq 0,$$

then summing up these inequalities for all $u \in N_a$ and $v \in N_b$ we get, after rearranging the terms,

$$m_a + m_b - \frac{d_a + d_b}{2} \leq (m_a - m_b)(d_a - d_b).$$

Since $m_a \geq \delta d_a \geq d_a$ and $m_b \geq \delta d_b \geq d_b$, the left-hand side $m_a + m_b - \frac{d_a + d_b}{2} \geq \frac{d_a + d_b}{2}$ is positive and the differences $m_a - m_b$ and $d_a - d_b$ are, therefore, of the same sign. This shows that either an edge rotation $ua \to ub$ or an edge rotation $vb \to va$ increases M_2, once again giving a contradiction to the starting assumption that no edge rotation increases M_2. ∎

Proof of Theorem 2 Starting with an arbitrary graph with n vertices, m edges, the minimum vertex degree δ and the maximum vertex degree Δ, we see that we can strictly increase the value of M_2 by repeated application of Lemma 3 as long as graph contains at least two vertices with degrees different from Δ, δ. Since the subsequent values of M_2 are integers and bounded from above (say, by the trivial bound $m\Delta^2$), Lemma 3 can be applied finitely many times only. This means that as a result of repeated application of Lemma 3 we arrive at a graph that contains at most one vertex with degree different from Δ and δ. The degree of such vertex, if it exists, can be obtained by considering the numbers n_Δ of vertices of degree Δ and n_δ of vertices of degree δ. Namely, if all vertices have degree either Δ or δ, then n_Δ and n_δ satisfy the system

$$
\begin{aligned}
n &= n_\Delta + n_\delta, \\
2m &= \Delta n_\Delta + \delta n_\delta,
\end{aligned}
$$

which has an integer solution if and only if $\Delta - \delta | 2m - n\delta$. Otherwise, if there exists a vertex of degree k, $\delta < k < \Delta$, then

$$
\begin{aligned}
n &= n_\Delta + n_\delta + 1, \\
2m &= \Delta n_\Delta + \delta n_\delta + k,
\end{aligned}
$$

wherefrom

$$
k - \delta \equiv 2m - n\delta \pmod{\Delta - \delta}
$$

and

$$
n_\Delta = \frac{(2m - n\delta) - (k - \delta)}{\Delta - \delta}, \tag{6}
$$

$$
n_\delta = \frac{(n\Delta - 2m) - (\Delta - k)}{\Delta - \delta}. \tag{7}
$$

In order to find the maximum value of M_2 among all graphs having vertices of degree Δ, δ and at most one vertex of degree k, satisfying (3), we need to classify the edges of a graph according to degrees of their end vertices:

- $m_{\Delta,\Delta}$ is the number of edges having both end vertices of degree Δ;

- $m_{\Delta,\delta}$ is the number of edges joining a vertex of degree Δ with a vertex of degree δ;

- $m_{\delta,\delta}$ is the number of edges having both end vertices of degree δ;

- $m_{k,\Delta}$ is the number of edges between a vertex of degree k and vertices of degree Δ;

- $m_{k,\delta}$ is the number of edges between a vertex of degree k and vertices of degree δ.

Counting the numbers of edges having an end vertex of a given degree (Δ, δ or k) in two ways, we get the following system

$$
\begin{aligned}
\Delta n_\Delta &= 2m_{\Delta,\Delta} + m_{\Delta,\delta} + m_{k,\Delta}, \\
\delta n_\delta &= m_{\Delta,\delta} + 2m_{\delta,\delta} + m_{k,\delta}, \\
k &= m_{k,\Delta} + m_{k,\delta}.
\end{aligned}
$$

Assuming $m_{\Delta,\delta}$ and $m_{k,\Delta}$ to be free variables, we can express $m_{\Delta,\Delta}$, $m_{\delta,\delta}$ and $m_{k,\delta}$:

$$
\begin{aligned}
m_{\Delta,\Delta} &= \frac{\Delta n_\Delta - m_{\Delta,\delta} - m_{k,\Delta}}{2}, \\
m_{\delta,\delta} &= \frac{\delta n_\delta - m_{\Delta,\delta} + m_{k,\Delta} - k}{2}, \\
m_{k,\delta} &= k - m_{k,\Delta}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
M_2 &= \Delta^2 m_{\Delta,\Delta} + \Delta\delta m_{\Delta,\delta} + \delta^2 m_{\delta,\delta} + k\Delta m_{k,\Delta} + k\delta m_{k,\delta} \\
&= \frac{\Delta^3 n_\Delta + \delta^3 n_\delta}{2} + k\delta\left(k - \frac{\delta}{2}\right) - \frac{m_{\Delta,\delta}}{2}(\Delta - \delta)^2 - m_{k,\Delta}(\Delta - \delta)\left(\frac{\Delta + \delta}{2} - k\right). \quad (8)
\end{aligned}
$$

The maximal possible value of M_2 is obtained for $m_{\Delta,\delta} = 0$ and

- if $k < (\Delta + \delta)/2$, for $m_{k,\Delta} = 0$ and $m_{k,\delta} = k$;

- if $k = (\Delta + \delta)/2$, for arbitrary nonnegative $m_{k,\Delta} + m_{k,\delta} = k$, and

- if $k > (\Delta + \delta)/2$, for $m_{k,\Delta} = k$ and $m_{k,\delta} = 0$.

Hence,

$$
M_2 \leq \frac{\Delta^3 n_\Delta + \delta^3 n_\delta}{2} + \begin{cases} k\delta\left(k - \frac{\delta}{2}\right) & \text{if } k \leq (\Delta + \delta)/2, \\ k\Delta\left(k - \frac{\Delta}{2}\right) & \text{if } k > (\Delta + \delta)/2. \end{cases}
$$

Finally, after substituting n_Δ and n_δ from Eqs. (6) and (7) we get

$$M_2 \leq \frac{(2m - k)\left(\Delta^2 + \Delta\delta + \delta^2\right) - (n - 1)\Delta\delta(\Delta + \delta)}{2} + \begin{cases} k\delta\left(k - \frac{\delta}{2}\right) & \text{if } k \leq (\Delta + \delta)/2, \\ k\Delta\left(k - \frac{\Delta}{2}\right) & \text{if } k > (\Delta + \delta)/2. \end{cases}$$

In order for equality to be attained in Eq. (2), the graph G has to have at most one vertex of degree k different from Δ and δ (so that Lemma 3 cannot be applied). The degree of vertex k satisfies (3) and then Eq. (8) holds for G. The upper bound in Eq. (8) is equal to the one in Eq. (2) if and only if $m_{\Delta,\delta} = 0$ and $m_{k,\Delta} = 0$ if $k < (\Delta + \delta)/2$, while $m_{k,\delta} = 0$ if $k > (\Delta + \delta)/2$. ■

2.1 Extremal graphs may be disconnected multigraphs

From the case of equality in Eq. (2) it is evident that, if $k \neq (\Delta + \delta)/2$, then the graph with the maximum value of M_2 for given n, m, Δ and δ is necessarily disconnected: if $k < (\Delta + \delta)/2$, then the vertices of degree Δ are adjacent only to other vertices of degree Δ, while if $k > (\Delta + \delta)/2$, the vertices of degree δ are adjacent only to other vertices of degree δ. Only when $k = (\Delta + \delta)/2$, an M_2-maximal graph may be connected, as then the vertex of degree k may be adjacent both to vertices of degree Δ and to vertices of degree δ.

Further, as the argument applied in the proof of Theorem 2 does not allow us to impose restrictions on edge rotations, it is possible that an M_2-maximal graph is no longer a simple graph, but a multigraph containing parallel edges and/or loops. Consider, for example, the case of $m = n$, $\Delta = n - 1$, $\delta = 1$, and arbitrary $n > 3$. There exists exactly one simple graph with these parameters — a star S_n with an additional edge joining two of its leaves — which contains two vertices (say, a and b) of degree two. Regardless of how we apply an edge rotation $ua \rightarrow ub$ we have to end up with one of multigraphs depicted in Fig. 1 — edge rotation around one of a or b produces a loop, while edge rotation around the central vertex produces two parallel edges.

The same situation of implicit appearance of multigraphs is present in Zhou and Gutman's Theorem 1 as well. Namely, their argument within the proof of Theorem 1 in [6] that there exists a graph with n vertices and m edges, possessing a unique vertex of degree k different from δ and Δ, starts with a graph with n vertices and all degrees equal to δ (except, possibly, one vertex with degree 0 if both n and δ are odd), and involves the process of adding edges to this graph in order to increase the vertex degrees up to Δ and k, without ensuring that the resulting graph is either simple or connected. In particular,
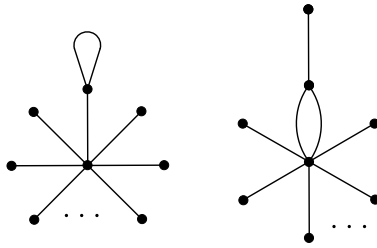
Figure 1: Multigraphs with maximal M_2 for $m = n, \Delta = n - 1$ and $\delta = 1$.

for the special case $m = n = 8$, $\Delta = 7$ and $\delta = 1$ this argument starts with four disjoint edges and then adds new edges as long as it does not reach one of multigraphs depicted in Fig. 1.

Note that all this is not, by any means, a mistake — it simply means that graphs attaining the maximum value of the first or the second Zagreb index may happen to be disconnected multigraphs.

2.2 Trees with the maximum second Zagreb index

The appearance of disconnected multigraphs as extremal graphs for the second Zagreb index may be avoided in the case of trees. Namely, we have

Theorem 4 *Let T be a tree with n vertices and the maximum vertex degree $\Delta \geq 2$. Then*

$$M_2(T) \leq \Delta(2n - \Delta - 1 - k) + k(k - 1), \tag{9}$$

where k is the integer defined via

$$k \equiv n - 1 \pmod{\Delta - 1}, \qquad 1 \leq k \leq \Delta - 1,$$

i.e.,

$$k = n - 1 - (\Delta - 1)\left\lfloor \frac{n - 2}{\Delta - 1} \right\rfloor.$$

Equality is attained in Eq. (9) if and only if T has at most one vertex of degree k that is adjacent to a single vertex of degree Δ, and all other vertices of T have degree either Δ or 1.

The proof of this theorem will be analogous to that of Theorem 2, with the distinction that we have to forbid rotation of an edge ua to ub if $T - ua + ub$ is not a tree. Let P be

the unique path between vertices a and b in T. If u is a neighbor of a that does not belong to P, then $T - ua + ub$ contains P and, consequently, $T - ua + ub$ remains connected: if ua has appeared in a walk between any two vertices of T, then it may be replaced by the edge ub followed by the path P from b to a (moreover, $T - ua + ub$ contains no loop or parallel edge in this case). On the other hand, if u belongs to P, then $T - ua + ub$ no longer contains P and a and b necessarily belong to distinct components of $T - ua + ub$. Hence, we only need to forbid rotation of edge ua to ub if u is the neighbor of a belonging to the unique path between a and b. Now we can prove the following variant of Lemma 3.

Lemma 5 *If a tree T contains two vertices whose degrees are different from Δ and 1, then there exists an edge rotation that from T produces a tree T' with $M_2(T) < M_2(T')$.*

Proof   Suppose first that T contains two adjacent vertices a and b such that $2 \le d_a, d_b \le \Delta - 1$. Choose arbitrarily $u \in N_a \setminus \{b\}$ and $v \in N_b \setminus \{a\}$. If neither of edge rotations $ua \to ub$ and $vb \to va$ increases M_2, then from Eqs. (4) and (5) we have

$$d_u(d_b - d_a + 2) + m_b - m_a - 1 \le 0,$$
$$d_v(d_a - d_b + 2) + m_a - m_b - 1 \le 0.$$

Adding these two inequalities together and rearranging the terms yields

$$2(d_u + d_v - 1) \le (d_v - d_u)(d_b - d_a). \tag{10}$$

Since the left-hand side of (10) is positive, we see that the case $d_a = d_b$ is impossible.

Suppose therefore that $d_a < d_b$. Then also $d_u < d_v$ has to hold, as otherwise the right-hand side of (10) would be nonpositive. Since u and b were arbitrarily chosen, we conclude that $d_u < d_v$ holds for each $u \in N_a \setminus \{b\}$ and each $v \in N_b \setminus \{a\}$. Let a' have the largest degree among the vertices in $N_a \setminus \{b\}$ and let b' have the smallest degree among the vertices in $N_b \setminus \{a\}$. Then

$$m_a - d_b = \sum_{u \in N_a \setminus \{b\}} d_u \le (d_a - 1)d_{a'} < (d_a - 1)d_{b'} < (d_b - 1)d_{b'} \le \sum_{v \in N_b \setminus \{a\}} d_v = m_b - d_a.$$

However, this yields a contradiction with the assumption that edge rotation $ua \to ub$ does not increase M_2:

$$0 \ge d_u(d_b - d_a + 2) + m_b - m_a - 1 \ge d_b - d_a + 2 + m_b - m_a - 1 > 1.$$

A contradiction is obtained similarly in the case $d_a > d_b$.

Hence, we conclude that if T contains two adjacent vertices a and b with $2 \leq d_a, d_b \leq \Delta - 1$, then one of edge rotations $ua \rightarrow ub$ and $vb \rightarrow va$, $u \in N_a \setminus \{b\}$, $v \in N_b \setminus \{a\}$, produces a tree T' with $M_2(T) < M_2(T')$.

Suppose, therefore, that no two vertices whose degrees are different from Δ and 1 are adjacent in T. Choose arbitrarily vertices a and b with $2 \leq d_a, d_b \leq \Delta - 1$. Let P be the unique path between a and b in T, and denote by a^* and b^* the neighbors of a and b on path P, respectively. Since no two vertices whose degrees are different from Δ and 1 are adjacent in T, and $d_{a^*}, d_{b^*} \geq 2$ (as a^* and b^* belong to the path P), we conclude that $d_{a^*} = d_{b^*} = \Delta$.

Now, if none of edge rotations $ua \rightarrow ub$, $u \in N_a \setminus \{a^*\}$, and $vb \rightarrow va$, $v \in N_b \setminus \{b^*\}$, increases M_2, then from Eqs. (4) and (5) we have

$$d_u(d_b - d_a + 2) + m_b - m_a \leq 0,$$
$$d_v(d_a - d_b + 2) + m_a - m_b \leq 0.$$

Summing up these inequalities for all $u \in N_a \setminus \{a^*\}$ and $v \in N_b \setminus \{b^*\}$, and rearranging the terms, we obtain

$$m_a + m_b - 2\Delta \leq (m_b - m_a)(d_b - d_a). \tag{11}$$

Note that $m_a, m_b > \Delta$, as both a and b have a neighbor of degree Δ (equal to a^* and b^*, respectively) and at least one more neighbor due to $d_a, d_b \geq 2$. Therefore, the left-hand side of (11) is positive, implying that the differences $m_b - m_a$ and $d_b - d_a$ are of the same sign. If $m_b - m_a$ and $d_b - d_a$ are both positive, then a rotation $ua \rightarrow ub$ around any $u \in N_a \setminus \{a^*\}$ increases M_2 by (4). If $m_b - m_a$ and $d_b - d_a$ are both negative, then a rotation $vb \rightarrow va$ around any $v \in N_b \setminus \{b^*\}$ increases M_2 by (5). In both cases, we arrive at a contradiction with the starting assumption that none of edge rotations increases M_2.
∎

Proof of Theorem 4 Starting with an arbitrary tree with n vertices and the maximum vertex degree Δ, we see that we can strictly increase the value of M_2 by repeated application of Lemma 5 if the tree contains at least two vertices with degrees different from Δ and 1.

Hence, the maximum value of M_2 is obtained by some tree that has at most one vertex a of degree different from Δ and 1. The degree k of vertex a, as in the proof of Theorem 2, satisfies (3), which for $m = n - 1$ and $\delta = 1$ reads $k = n - 1 - (\Delta - 1) \left\lfloor \frac{n-2}{\Delta-1} \right\rfloor$. In

addition, the numbers n_Δ and n_1 of vertices of T of degree Δ and 1, respectively, satisfy Eqs. (6) and (7).

Let $t \geq 1$ be the number of neighbors of a of degree Δ. The tree T then has $k - t$ edges with end-degrees k and 1, $n_1 - k + t$ edges with end-degrees 1 and Δ, and $n - n_1 - t - 1$ edges with both end-degrees Δ, so that

$$
\begin{aligned}
M_2(T) &= tk\Delta + (k - t)k + (n_1 - k + t)\Delta + (n - n_1 - t - 1)\Delta^2 \\
&= -t(\Delta - 1)(\Delta - k) + \left[(n - n_1 - 1)\Delta^2 + (n_1 - k)\Delta + k^2\right].
\end{aligned}
$$

Since the summand in the brackets above is constant and $(\Delta - 1)(\Delta - k)$ is positive, we conclude that the maximum value of $M_2(T)$ is obtained for $t = 1$, which yields (9) after replacing n_1 from (7).

At the end, it is visible from above that if equality is attained in (9), then T has to have at most one vertex of degree different from Δ and 1 (as otherwise Lemma 5 could be applied to T to increase M_2), and that vertex has to be adjacent to a single vertex of degree Δ (as otherwise $t \geq 2$). ∎

3 Zagreb coindices of chemical trees and benzenoid chains

Thanks to Theorems 1 and 4, we are now in position to resolve open questions of Ashrafi, Došlić and Hamzeh [7] on the minimum values of Zagreb coindices over chemical trees.

The Zagreb coindices, opposites of the Zagreb indices, were introduced in [8]:

$$
\begin{aligned}
\overline{M}_1(G) &= \sum_{uv \notin E} (d_u + d_v), \\
\overline{M}_2(G) &= \sum_{uv \notin E} d_u d_v.
\end{aligned}
$$

The Zagreb coindices turn out to be closely related to the Zagreb indices via the following formulas, obtained in [9]:

$$
\overline{M}_1(G) = 2m(n - 1) - M_1(G), \tag{12}
$$

$$
\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G). \tag{13}
$$

3.1 The first Zagreb coindex of chemical trees

Recall that a tree is a connected graph with exactly $m = n - 1$ edges. From Eq. (12) it is then apparent that the sum $M_1(T) + \overline{M}_1(T) = 2(n - 1)^2$ is constant for fixed n, so

that the task of determining the minimum first Zagreb coindex translates to the task of determining the maximum first Zagreb index. The latter problem has been studied in many papers, and the case of chemical trees has been resolved in [6], where Theorem 1 is proved. For chemical trees, in which $\delta = 1$ and $\Delta = 4$, this theorem yields

Corollary 6 *For a chemical tree T with $n \geq 2$ vertices*

$$M_1(T) \leq \begin{cases} 6n - 10 & \text{if } n \equiv 2 \pmod 3, \\ 6n - 12 & \text{otherwise,} \end{cases}$$

with equality if and only if either (i) every vertex of T is of degree 1 or 4 (in which case $n \equiv 2 \pmod 3$), or (ii) one vertex of T has degree 2 or 3, and all other vertices are of degree 1 or 4.

Therefore, for the first Zagreb coindex of a chemical tree T

$$\overline{M}_1(T) \geq 2(n-1)^2 - \begin{cases} 6n - 10 & \text{if } n \equiv 2 \pmod 3, \\ 6n - 12 & \text{otherwise,} \end{cases}$$

with equality as stated in Corollary 6.

3.2   The second Zagreb coindex of chemical trees

From Eq. (13) we see that a tree T has the minimum second Zagreb coindex if and only if it has the maximum value of $M_2(T) + \frac{1}{2}M_1(T)$. Since the trees with the maximum value of M_2 among trees with given n and Δ have, at the same time, also the maximum value of M_1 (but not necessarily vice versa), we see that the maximum value of $M_2(T) + \frac{1}{2}M_1(T)$ is obtained exactly for trees attaining equality in (9). Note that for chemical trees with $\Delta = 4$, Theorem 4 yields

Corollary 7 *For a chemical tree T with $n \geq 2$ vertices*

$$M_2(T) \leq \begin{cases} 8n - 24 & \text{if } n \equiv 2 \pmod 3, \\ 8n - 26 & \text{otherwise,} \end{cases}$$

with equality if and only if either (i) every vertex of T is of degree 1 or 4 (in which case $n \equiv 2 \pmod 3$), or (ii) one vertex of T has degree 2 or 3 and it is adjacent to a single vertex of degree 4, while all other vertices are of degree 1 or 4.

Therefore, for the second Zagreb coindex of a chemical tree T

$$\overline{M}_2(T) \geq 2(n-1)^2 - \begin{cases} 11n - 29 & \text{if } n \equiv 2 \pmod 3, \\ 11n - 32 & \text{otherwise,} \end{cases}$$

with equality as stated in Corollary 7.

3.3 The Zagreb coindices of benzenoid chains

Ashrafi, Došlić and Hamzeh [7] have also posed the question of the minimum values of Zagreb coindices of benzenoid chains. This question is, however, implicitly resolved in a later paper of Došlić [10]. For the sake of completeness, let us explain this briefly.

As in [10], a hexagonal system is a collection of congruent regular hexagons arranged in a plane in such a way that two hexagons are either disjoint or have a common edge. The hexagonal system whose interior is 1-connected is called the benzenoid system. To each benzenoid system corresponds a benzenoid graph, obtained by taking the vertices of hexagons as the vertices of the graph, and the sides of hexagons as graph edges. The resulting graph is simple, planar, with all bounded faces being hexagons. The vertices of a benzenoid graph belonging to the unbounded face are called external, while the remaining vertices are called internal. A benzenoid graph without internal vertices is called catacondensed. It follows by a simple counting argument that a catacondensed benzenoid with h hexagons has $4h+2$ vertices and $5h+1$ edges [11]. Its h hexagons belong to one of the four possible types, depending on the number and the relative position of the edges they share with other hexagons. If a hexagon shares one edge with another hexagon, it is called *terminal*. If it shares three edges, no two of which are incident to the same vertex, it is called *branching*. If two shared edges are parallel, the hexagon is called *straight*, and if they are not parallel, it is called *kinky*.

Došlić [10] has proved that for a catacondensed benzenoid graph with h hexagons

$$M_1 = 26h - 2,$$
$$M_2 = 34h - 11 + B - S,$$

where B and S are the number of branching and straight hexagons, respectively. From Eqs. (12) and (13) follows

$$\overline{M}_1 = 40h^2 - 8h + 4,$$
$$\overline{M}_2 = 50h^2 - 27h + 14 - B + S.$$

Thus, all catacondensed benzenoids with h hexagons have constant first Zagreb coindex, while the minimum value of the second Zagreb coindex is obtained for catacondensed benzenoids having the maximum number of branching hexagons and minimum number of straight hexagons ($S = 0$). In particular, if a catacondensed benzenoid is a benzenoid chain, as asked by Ashrafi, Došlić and Hamzeh in [7], then it contains no branching

hexagons ($B = 0$) and the minimum value $50h^2 - 27h + 14$ of the second Zagreb coindex is achieved for benzenoid chains consisting of kinky hexagons only (and two terminal hexagons).

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