Received: 23 July 2020 | Revised: 28 September 2020 | Accepted: 23 October 2020
DOI: 10.1002/qua.26547

FULL PAPER

International Journal of QUANTUM CHEMISTRY WILEY

On the first two extremum Zagreb indices and coindices of chemical trees

Zhibin Du[1] | Akbar Ali[2,3] | Rabbia Rafee[3] | Zahid Raza[4] | Muhammad Kamran Jamil[5]

[1]School of Software, South China Normal University, Foshan, Guangdong, China

[2]Department of Mathematics, Faculty of Science, University of Ha'il, Ha'il, Saudi Arabia

[3]Knowledge Unit of Science, University of Management and Technology, Sialkot, Pakistan

[4]Department of Mathematics, College of Sciences, University of Sharjah, Sharjah, United Arab Emirates

[5]Department of Mathematics, Riphah Institute of Computing and Applied Sciences, Riphah International University, Lahore, Pakistan

Correspondence
Akbar Ali, Department of Mathematics, Faculty of Science, University of Ha'il, Ha'il, Saudi Arabia.
Email: akbarali.maths@gmail.com

Funding information
National Natural Science Foundation of China, Grant/Award Number: 11701505; University of Sharjah, Grant/Award Number: 1802144068

Abstract

The first and second Zagreb indices are the molecular descriptors that were appeared within a study of molecular modeling more than four decades ago. The coindex versions of these Zagreb indices were introduced around one decade before. Finding trees with the first two extremum Zagreb indices/coindices from the class of all chemical trees of a fixed order is a chemical-graph-theoretic problem whose partial solution is known. This paper is devoted to reporting the complete solution of the aforementioned problem.

KEYWORDS

chemical graph theory, chemical tree, molecular descriptor, topological index, Zagreb indices and coindices

1 | INTRODUCTION

Graph theoretical tools have been (and are being) used in chemistry, or more precisely in quantitative structure–property relationship studies for predicting the physicochemical properties of molecules [1, 2] and for seeking combinatorial libraries to find molecular structures that are generally comparative to a target structure [3, 4]. This resulted in the discovery of a new interdisciplinary scientific field, which nowadays is referred to as the "chemical graph theory." In this interdisciplinary field, chemical compounds are usually represented by graphs, known as chemical graphs. In chemical graphs, vertices correspond to atoms of the considered chemical compound, and the edges correspond to the covalent bonds between atoms [5]. Graphs considered in this paper are hydrogen-depleted chemical graphs representing saturated hydrocarbons, and they contain neither loops nor multiple edges. Notation and terminology from (chemical) graph theory that are not defined in this paper can be found in the books [5–8].

Following Todeschini and Consonni [9], we define a *molecular structure descriptor* that is "the final result of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment." A molecular structure descriptor that is calculated from a molecular graph is usually known as a *topological index* [5]. In graph–theoretical notion, a topological index TI of a graph G is simply a graph invariant of G, that is the numerical quantity associated with G such that the equation $TI(G) = TI(G')$ holds for every graph G' isomorphic to G.

The first Zagreb index M_1, appeared within a formula derived in Gutman and Trinajstić [10], and the second Zagreb index M_2, introduced in Gutman et al. [11] within the study of molecular modeling, are among the most studied topological indices. For a graph G with vertex set $V(G)$ and edge set $E(G)$, these indices are defined as

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

where $d_u(G)$, $d_v(G)$ denote the degrees of the vertices $u, v \in V(G)$, respectively, and uv is the edge connecting u and v. The first Zagreb index can be rewritten (see exercise 10.30 in Lovász [12]) as

$$M_1(G) = \sum_{uv \in E(G)} (d_u(G) + d_v(G)).$$

The first and second Zagreb indices have been considered in various papers for their applications in chemistry, or more precisely, in quantitative structure–property relationships and quantitative structure–activity relationships. For example, see the recent papers [13, 14] for the chemical applications of the first and second Zagreb indices. Detail about the mathematical properties of these Zagreb indices can be found in the recent surveys [15, 16], recent papers [17–27] and related references mentioned therein.

The first Zagreb coindex $\bar{M}_1$ and the second Zagreb coindex $\bar{M}_2$ of a graph G are, respectively, defined [28] as

$$\bar{M}_1(G) = \sum_{uv \subseteq \bar{E}(G); u \neq v} (d_u(G) + d_v(G)) \text{ and } \bar{M}_2(G) = \sum_{uv \subseteq \bar{E}(G); u \neq v} d_u(G) d_v(G).$$

The first and second Zagreb coindices can be written [29] in terms of the first and/or second Zagreb indices:

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

$$\bar{M}_2(G) = 2m^2 - M_2(G) - \frac{M_1(G)}{2}, \tag{2}$$

where m and n are the size and order, respectively, of the graph G (a general form of the identity (1) is derived in Milovanović et al. [30]). Further detail about the Zagreb coindices can be found in Gutman et al. [31].

A chemical tree is a tree of maximum degree at most 4. Let us consider the following chemical-graph-theoretic problem.

Problem 1. Find trees with the first two extremum Zagreb indices/coindices from the class of all chemical trees of a fixed order $n \geq 5$.

Denote by $\mathbb{CT}_n$ the class of all chemical trees of a fixed order $n \geq 5$. Partial solution of Problem 1 is already known. Particularly, in Li and Zhao [32], the graphs having the first two minimum/maximum M_1 values from the class $\mathbb{CT}_n$ were obtained, and hence by using Equation (1) one obtains the graphs having the first two maximum/minimum $\bar{M}_1$ values from the aforementioned class. Also, from Equation (2) and the results established in References [32, 33], it follows that among all the members of $\mathbb{CT}_n$, the graphs having the first/second maximum $\bar{M}_2$ value are the same as those having the first/second minimum M_2 value given in theorem 2.1 of Li and Liu [33]. Moreover, in the class $\mathbb{CT}_n$, the graphs having the minimum $\bar{M}_2$ value or maximum M_2 value have already been determined in References [34, 35]. The main purpose of the present paper is to characterize the graphs with the second maximum M_2 value or second minimum $\bar{M}_2$ value from the class $\mathbb{CT}_n$ for $n \geq 7$. Thus, the results obtained in this paper complete the solution of Problem 1. Also, in the process of proving the main results of this paper, we revisit a result concerning the maximum second Zagreb index of chemical trees, proved in References [34, 35].

2 | MAIN RESULTS

Denote by $x_{i,j}(T)$ the number of those edges of a chemical tree T whose one end-vertex has degree i and the other end-vertex has degree j. Let $n_i(T)$ be the number of those vertices of T that having degree i. The symbol "(T)" will be omitted from the notations $d_u(T)$, $x_{i,j}(T)$ and $n_i(T)$ in the remaining part of this paper. In order to state and prove the main results of this paper, we need some lemmas first.

Lemma 1. [36] *Let T be a chemical tree of order $n \geq 6$. For every $i = 2,3,4$, it holds that*

$$x_{1,i} \le (i-1)n_i$$

with equality if and only if either $n_i = 0$ or every vertex of degree i is adjacent to exactly $i - 1$ vertices of degree 1.

The second Zagreb index M_2 for any chemical tree T can be rewritten as

$$M_2(T) = \sum_{1 \le i \le j \le 4} x_{ij} \cdot ij. \tag{3}$$

The following system of equations holds for any nontrivial chemical tree T of order n:

$$n_1 + n_2 + n_3 + n_4 = n, \tag{4}$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \tag{5}$$

$$x_{1,2} + x_{1,3} + x_{1,4} = n_1, \tag{6}$$

$$x_{1,2} + 2x_{2,2} + x_{2,3} + x_{2,4} = 2n_2, \tag{7}$$

$$x_{1,3} + x_{2,3} + 2x_{3,3} + x_{3,4} = 3n_3, \tag{8}$$

$$x_{1,4} + x_{2,4} + x_{3,4} + 2x_{4,4} = 4n_4. \tag{9}$$

From Equations (4) and (5), it follows that

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

and thus

$$n \equiv n_2 + 2n_3 + 2 \pmod 3. \tag{10}$$

Now, we solve the system of Equations (4)–(9) for the unknowns n_1, n_2, n_3, n_4, $x_{1,4}$, $x_{4,4}$. The expressions for the unknowns $x_{1,4}$ and $x_{4,4}$ are, respectively, given below (see also in References [37, 38]):

$$x_{1,4} = \frac{2n+2}{3} - \frac{4}{3}x_{1,2} - \frac{10}{9}x_{1,3} - \frac{2}{3}x_{2,2} - \frac{4}{9}x_{2,3} - \frac{1}{3}x_{2,4} - \frac{2}{9}x_{3,3} - \frac{1}{9}x_{3,4}$$

and

$$x_{4,4} = \frac{n-5}{3} + \frac{1}{3}x_{1,2} + \frac{1}{9}x_{1,3} - \frac{1}{3}x_{2,2} - \frac{5}{9}x_{2,3} - \frac{2}{3}x_{2,4} - \frac{7}{9}x_{3,3} - \frac{8}{9}x_{3,4}.$$

After substituting the expressions for the unknowns $x_{1,4}$ and $x_{4,4}$ into Equation (3), one has

$$M_2(T) = (8n-24) + 2x_{1,2} + \frac{1}{3}x_{1,3} - 4x_{2,2} - \frac{14}{3}x_{2,3} - 4x_{2,4} - \frac{13}{3}x_{3,3} - \frac{8}{3}x_{3,4}. \tag{11}$$

Consider

$$\Gamma_{M_2}(T) = 2x_{1,2} + \frac{1}{3}x_{1,3} - 4x_{2,2} - \frac{14}{3}x_{2,3} - 4x_{2,4} - \frac{13}{3}x_{3,3} - \frac{8}{3}x_{3,4}. \tag{12}$$

Then Equation (11) becomes

$$M_2(T) = (8n - 24) + \Gamma_{M_2}(T). \tag{13}$$

By using Equations (7) and (8) in (12), we have

$$\Gamma_{M_2}(T) = \frac{1}{3}(12(x_{1,2} - n_2) + 4(x_{1,3} - 2n_3) - n_3 - 5x_{2,3} - 6x_{2,4} - 7x_{3,3} - 5x_{3,4}). \tag{14}$$

It is worth mentioning that $x_{1,2} \le n_2$ and $x_{1,3} \le 2n_3$ from Lemma 1.

Next, we give some properties when $\Gamma_{M_2}(T) \ge -4$.

Lemma 2. *Let T be a chemical tree of order $n \ge 6$. If $\Gamma_{M_2}(T) \ge -4$, then $x_{2,2} = x_{2,3} = x_{3,3} = 0$, $x_{1,2} = x_{2,4}$, and $x_{1,3} = 2x_{3,4}$.*

Proof. We get our desired properties step by step, by using (14) repeatedly.

Claim 1. $x_{3,3} = 0$.

Recall that the inequalities $x_{1,2} \le n_2$ and $x_{1,3} \le 2n_3$ hold by Lemma 1, hence from Equation (14), it follows that $x_{3,3} \le 1$ because otherwise we have $\Gamma_{M_2}(T) < -4$, a contradiction. If $x_{3,3} = 1$, then $n_3 \ge 2$ and also by Lemma 1, it holds that $x_{1,3} < 2n_3$, which is equivalent to $x_{1,3} \le 2n_3 - 1$. Hence, from Equation (14), we get $\Gamma_{M_2}(T) < -4$, which is a contradiction.

Claim 2. $x_{2,3} = 0$.

Clearly, $x_{2,3} \le 2$ from Equation (14).

Suppose that $x_{2,3} = 2$. From Equation (14), we have $x_{2,4} = x_{3,4} = 0$ because $\Gamma_{M_2}(T) \ge -4$. On the other hand, from Lemma 1, it follows that either $x_{1,2} < n_2$ or $x_{1,3} < 2n_3$ (otherwise $n = 5$), in either case, we get $\Gamma_{M_2}(T) < -4$ from Equation (14).

Suppose that $x_{2,3} = 1$. Denote by u and v two adjacent vertices in T, where $d_u = 2$ and $d_v = 3$. From Equation (14), it follows that $x_{1,2} = n_2$, and thus the unique neighbor of u different from v is of degree 1. On the other hand, at least one neighbor of v different from u is of degree at least 2, otherwise $n = 5$. Moreover, recall that $x_{2,3} = 1$ and $x_{3,3} = 0$ (by Claim 1), it means that there must exist at least one neighbor of v which is of degree 4, that is, $x_{3,4} \ge 1$, which also implies that the vertex v can be adjacent to at most one vertex of degree 1, and hence by Lemma 1 it holds that $x_{1,3} < 2n_3$. So, we have $\Gamma_{M_2}(T) < -4$ from (14).

Claim 3. $x_{2,2} = 0$.

Contrarily suppose that $x_{2,2} \ge 1$. From Lemma 1, it follows that $x_{1,2} < n_2$, otherwise $n = 4$ which is a contradiction. Now, Equation (14) leads to $\Gamma_{M_2}(T) \le -4$, which together with the assumption that $\Gamma_{M_2}(T) \ge -4$, imply that $\Gamma_{M_2}(T) = -4$, and thus by using (14) again, we deduce that $x_{1,2} = n_2 - 1$, $x_{2,4} = 0$ and $n_3 = 0$.

By using Equation (7), we have $x_{1,2} + 2x_{2,2} = 2n_2$, which, together with $x_{1,2} = n_2 - 1$, imply that $n_2 + 1 = 2x_{2,2}$. Since $x_{2,3} = x_{2,4} = 0$, based on the edge whose end vertices are both of degree 2, we can see that every vertex in T can only be of degrees 1 or 2, that is, $T \cong P_n$. However, it is easy to see that a path P_n satisfying $n_2 + 1 = 2x_{2,2}$ can occur only when $n = 5$, which is a contradiction.

Claim 4. $x_{1,2} = x_{2,4}$.

Because of Claims 2 and 3, we have $x_{2,2} = x_{2,3} = 0$, which gives $x_{1,2} \le x_{2,4}$ and $x_{1,2} + x_{2,4} = 2n_2$ (from Equation 7). Suppose to the contrary that $x_{1,2} < x_{2,4}$, then $x_{1,2} < n_2$. Note that $x_{2,4} \ge 1$, and hence by using Equation (14), we have $\Gamma_{M_2}(T) < -4$, a contradiction.

Claim 5. $x_{1,3} = 2x_{3,4}$.

By Claims 1 and 2, we have $x_{2,3} = x_{3,3} = 0$, which yields $x_{1,3} \le 2x_{3,4}$ and $x_{1,3} + x_{3,4} = 3n_3$ (from Equation 8). Suppose to the contrary that $x_{1,3} < 2x_{3,4}$, then $x_{1,3} < 2n_3$. If $x_{3,4} \ge 2$, then from Equation (14), we have $\Gamma_{M_2}(T) < -4$, which is a contradiction. If $x_{3,4} = 1$, then $x_{1,3} = 0$ or 1 because $x_{1,3} < 2x_{3,4}$. However, from (8), we have $x_{1,3} = 3n_3 - 1 \ge 2$, again a contradiction.

The proof is completed.

The next lemma is a direct consequence of Equation (12).

Lemma 3. *Let T be an n-vertex chemical tree of order $n \geq 7$. If $x_{2,2} = x_{2,3} = x_{3,3} = 0$, $x_{1,2} = x_{2,4}$ and $x_{1,3} = 2x_{3,4}$, then*

$$\Gamma_{M_2}(T) = -2(x_{2,4} + x_{3,4}).$$

Now, we are prepared to state and prove one of the main results of this paper. While proving this result, that is concerned with the second maximum M_2 value of chemical trees, a result regarding the maximum M_2 value of chemical trees, given in [34, 35], is proved again.

Theorem 1. *Consider the class of all chemical trees of a fixed order $n \geq 5$.*

(1) *Suppose that $n \equiv 0$ (mod 3).*

(1.1) *The maximum M_2 value is $8n - 26$ for $n \geq 6$, which is attained only by those trees that contain a unique vertex of degree 2, that is, $n_2 = 1$, and no vertex of degree 3, that is, $n_3 = 0$, such that the unique vertex of degree 2 is adjacent to one vertex of degree 1 and one vertex of degree 4, that is, $x_{1,2} = x_{2,4} = 1$.*

(1.2) *The second maximum M_2 value is $8n - 28$ for $n \geq 9$, which is attained only by those trees that contain no vertex of degree 2, that is, $n_2 = 0$, and two vertices of degree 3, that is, $n_3 = 2$, such that each vertex of degree 3 is adjacent to two vertices of degree 1 and one vertex of degree 4, that is, $x_{1,3} = 4$, $x_{3,4} = 2$, and $x_{3,3} = 0$.*

(2) *Suppose that $n \equiv 1$ (mod 3).*

(2.1) *The maximum M_2 value is $8n - 26$ for $n \geq 7$, which is attained only by those trees that contain no vertex of degree 2, that is, $n_2 = 0$, and a unique vertex of degree 3, that is, $n_3 = 1$, such that the unique vertex of degree 3 is adjacent to two vertices of degree 1 and one vertex of degree 4, that is, $x_{1,3} = 2$ and $x_{3,4} = 1$.*

(2.2) *The second maximum M_2 value is $8n - 28$ for $n \geq 7$, which is attained only by those trees that contain two vertices of degree 2, that is, $n_2 = 2$, and no vertex of degree 3, that is, $n_3 = 0$, such that every vertex of degree 2 is adjacent to one vertex of degree 1 and one vertex of degree 4, that is, $x_{1,2} = x_{2,4} = 2$ and $x_{2,2} = 0$.*

(3) Suppose that $n \equiv 2$ (mod 3).

(3.1) *The maximum M_2 value is $8n - 24$ for $n \geq 5$, which is attained only by those trees that contain no vertices of degrees 2 or 3, that is, $n_2 = n_3 = 0$.*

(3.2) *The second maximum M_2 value is $8n - 28$ for $n \geq 8$, which is attained only by those trees that contain a unique vertex of degree 2, that is, $n_2 = 1$, and a unique vertex of degree 3, that is, $n_3 = 1$, such that the unique vertex of degree 2 is adjacent to one vertex of degree 1 and one vertex of degree 4, that is, $x_{1,2} = x_{2,4} = 1$ and $x_{2,3} = 0$, while the unique vertex of degree 3 is adjacent to two vertices of degree 1 and one vertex of degree 4, that is, $x_{1,3} = 2$ and $x_{3,4} = 1$.*

Corresponding to every part, a tree with the first/second maximum M_2 value is depicted in Figure 1.

Proof. It can be easily verified that the trees specified in each part of the theorem have M_2 value given in that part. Consequently, any tree having M_2 value less than $8n - 28$ (which is claimed to be the second maximum M_2 value) must have the ith maximum M_2 value for some $i \geq 3$, in

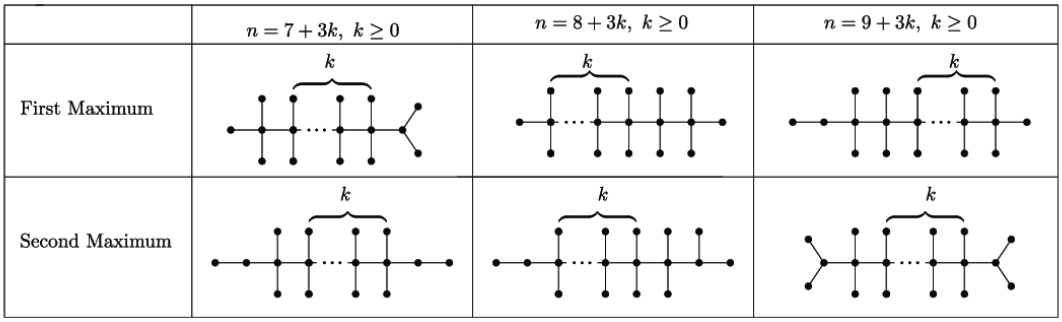

FIGURE 1 Examples of the trees, specified in Theorem 1, with the first two maximum M_2 values

the class of all chemical trees of a fixed order $n \geq 6$ (the result when $n = 5$ can be checked easily, since there are just three candidates). Hence, we have to find all those chemical trees of order $n \geq 6$ whose M_2 value is at least $8n - 28$, or equivalently, whose Γ_{M_2} value is at least -4.

Let T be a chemical tree of order $n \geq 6$. From Lemma 2, we assume that $x_{2,2} = x_{2,3} = x_{3,3} = 0$, $x_{1,2} = x_{2,4}$ and $x_{1,3} = 2x_{3,4}$. By using Equations (7) and (8), we have $x_{2,4} = n_2$ and $x_{3,4} = n_3$. Moreover, assume that $x_{2,4} + x_{3,4} \leq 2$, otherwise $\Gamma_{M_2}(T) < -4$ from Lemma 3.

Case 1. $n \equiv 0 \pmod 3$.

In this case, from Equation (10), it follows that $n_2 + 2n_3 \equiv 1 \pmod 3$, that is

$$x_{2,4} + 2x_{3,4} \equiv 1 \pmod 3.$$

If $x_{2,4} + x_{3,4} = 1$, then $x_{2,4} = 1$ and $x_{3,4} = 0$, that is, $n_2 = 1$ and $n_3 = 0$. By using Lemma 3, we have $\Gamma_{M_2}(T) = -2$.
If $x_{2,4} + x_{3,4} = 2$, then $x_{2,4} = 0$ and $x_{3,4} = 2$, which implies that $n_2 = 0$ and $n_3 = 2$. From Lemma 3, it follows that $\Gamma_{M_2}(T) = -4$.

Case 2. $n \equiv 1 \pmod 3$.

By using Equation (10), we have $n_2 + 2n_3 \equiv 2 \pmod 3$, that is

$$x_{2,4} + 2x_{3,4} \equiv 2 \pmod 3.$$

If $x_{2,4} + x_{3,4} = 1$, then $x_{2,4} = 0$ and $x_{3,4} = 1$, that is, $n_2 = 0$ and $n_3 = 1$. By Lemma 3, it holds that $\Gamma_{M_2}(T) = -2$.
If $x_{2,4} + x_{3,4} = 2$, then $x_{2,4} = 2$ and $x_{3,4} = 0$, which implies that $n_2 = 2$ and $n_3 = 0$. From Lemma 3, it follows that $\Gamma_{M_2}(T) = -4$.

Case 3. $n \equiv 2 \pmod 3$.

In this case, from Equation (10), $n_2 + 2n_3 \equiv 0 \pmod 3$, that is,

$$x_{2,4} + 2x_{3,4} \equiv 0 \pmod 3.$$

If $x_{2,4} + x_{3,4} = 0$, then $x_{2,4} = 0$ and $x_{3,4} = 0$, that is, $n_2 = 0$ and $n_3 = 0$, by Lemma 3, $\Gamma_{M_2}(T) = 0$.
If $x_{2,4} + x_{3,4} = 2$, then $x_{2,4} = 1$ and $x_{3,4} = 1$, that is, $n_2 = 1$ and $n_3 = 1$, by Lemma 3, $\Gamma_{M_2}(T) = -4$.

In Cases 1 and 2, the Γ_{M_2} values greater or equal to -4 are -2 and -4, which correspond to the trees specified in parts (1) and (2) having maximum and the second maximum M_2 values. In Case 3, the Γ_{M_2} values greater or equal to -4 are 0 and -4, which correspond to the trees specified in part (3) having maximum and the second maximum M_2 values.

From the class of all chemical trees of a fixed order $n \geq 5$, the graphs having the minimum value of the second Zagreb coindex $\bar{M}_2$ have already been determined in Vukićević and Popivoda [35]—in what follows, we will see that the graphs having the second minimum value of $\bar{M}_2$ in the aforementioned class of chemical trees are the same as those having the second maximum value of M_2 given in Theorem 1 when $n \equiv 0 \pmod 3$ or $n \equiv 2 \pmod 3$. To proceed, we need the following result.

Theorem 2. [32] *Consider the class of all chemical trees of a fixed order* $n \geq 5$.

(1) *Suppose that* $n \equiv 0$ *(mod 3).*
(1.1) *The maximum* M_1 *value is* $6n - 12$ *for* $n \geq 6$*, which is attained only by those trees that contain a unique vertex of degree* 2*, that is,* $n_2 = 1$*, and no vertex of degree* 3*, that is,* $n_3 = 0$.
(1.2) *The second maximum* M_1 *value is* $6n - 14$ *for* $n \geq 9$*, which is attained only by those trees that contain no vertex of degree* 2*, that is,* $n_2 = 0$*, and two vertices of degree* 3*, that is,* $n_3 = 2$.
(2) *Suppose that* $n \equiv 1$ *(mod 3).*
(2.1) *The maximum* M_1 *value is* $6n - 12$ *for* $n \geq 7$*, which is attained only by those trees that contain no vertex of degree* 2*, that is,* $n_2 = 0$*, and a unique vertex of degree* 3*, that is,* $n_3 = 1$.
(2.2) *The second maximum* M_1 *value is* $6n - 14$ *for* $n \geq 7$*, which is attained only by those trees that contain two vertices of degree* 2*, that is,* $n_2 = 2$*, and no vertex of degree* 3*, that is,* $n_3 = 0$.
(3) *Suppose that* $n \equiv 2$ *(mod 3).*

(3.1) *The maximum* M_1 *value is* $6n - 10$ *for* $n \geq 5$, *which is attained only by those trees that contain no vertices of degrees* 2 *or* 3, *that is,* $n_2 = n_3 = 0$.

(3.2) *The second maximum* M_1 *value is* $6n - 14$ *for* $n \geq 8$, *which is attained only by those trees that contain a unique vertex of degree* 2, *that is,* $n_2 = 1$, *and a unique vertex of degree* 3, *that is,* $n_3 = 1$.

From (2) and Theorems 1 and 2, the next result follows.

Theorem 3. *Consider the class of all chemical trees of a fixed order* $n \geq 5$.

(1) *Suppose that* $n \equiv 0$ *(mod 3).*

(1.1) *The minimum* $\bar{M}_2$ *value is* $2n^2 - 15n + 34$ *for* $n \geq 6$, *which is attained only by those trees that contain a unique vertex of degree* 2, *that is,* $n_2 = 1$, *and no vertex of degree* 3, *that is,* $n_3 = 0$, *such that the unique vertex of degree* 2 *is adjacent to one vertex of degree* 1 *and one vertex of degree* 4, *that is,* $x_{1,2} = x_{2,4} = 1$.

(1.2) *The second minimum* $\bar{M}_2$ *value is* $2n^2 - 15n + 37$ *for* $n \geq 9$, *which is attained only by those trees that contain no vertex of degree* 2, *that is,* $n_2 = 0$, *and two vertices of degree* 3, *that is,* $n_3 = 2$, *such that each vertex of degree* 3 *is adjacent to two vertices of degree* 1 *and one vertex of degree* 4, *that is,* $x_{1,3} = 4$, $x_{3,4} = 2$, *and* $x_{3,3} = 0$.

(2) *Suppose that* $n \equiv 1$ *(mod 3).*

(2.1) *The minimum* $\bar{M}_2$ *value is* $2n^2 - 15n + 34$ *for* $n \geq 7$, *which is attained only by those trees that contain no vertex of degree* 2, *that is,* $n_2 = 0$, *and a unique vertex of degree* 3, *that is,* $n_3 = 1$, *such that the unique vertex of degree* 3 *is adjacent to two vertices of degree* 1 *and one vertex of degree* 4, *that is,* $x_{1,3} = 2$ *and* $x_{3,4} = 1$.

(2.2) *The second minimum* $\bar{M}_2$ *value is* $2n^2 - 15n + 37$ *for* $n \geq 7$, *which is attained only by those trees that contain two vertices of degree* 2, *that is,* $n_2 = 2$, *and no vertex of degree* 3, *that is,* $n_3 = 0$, *such that every vertex of degree* 2 *is adjacent to one vertex of degree* 1 *and one vertex of degree* 4, *that is,* $x_{1,2} = x_{2,4} = 2$ *and* $x_{2,2} = 0$, *or those trees that contain no vertex of degree* 2, *that is,* $n_2 = 0$, *and a unique vertex of degree* 3, *that is,* $n_3 = 1$, *such that the unique vertex of degree* 3 *is adjacent to one vertex of degree* 1 *and two vertices of degree* 4, *that is,* $x_{1,3} = 1$ *and* $x_{3,4} = 2$.

(3) *Suppose that* $n \equiv 2$ *(mod 3).*

(3.1) *The minimum* $\bar{M}_2$ *value is* $2n^2 - 15n + 31$ *for* $n \geq 5$, *which is attained only by those trees that contain no vertices of degrees* 2 *or* 3, *that is,* $n_2 = n_3 = 0$.

(3.2) *The second minimum* $\bar{M}_2$ *value is* $2n^2 - 15n + 37$ *for* $n \geq 8$, *which is attained only by those trees that contain a unique vertex of degree* 2, *that is,* $n_2 = 1$, *and a unique vertex of degree* 3, *that is,* $n_3 = 1$, *such that the unique vertex of degree* 2 *is adjacent to one vertex of degree* 1 *and one vertex of degree* 4, *that is,* $x_{1,2} = x_{2,4} = 1$ *and* $x_{2,3} = 0$, *while the unique vertex of degree* 3 *is adjacent to two vertices of degree* 1 *and one vertex of degree* 4, *that is,* $x_{1,3} = 2$ *and* $x_{3,4} = 1$.

Proof. From Theorems 1 and 2, it follows that the n-vertex chemical trees having the maximum value of M_2 form a subclass of the class of n-vertex chemical trees having the maximum value of M_1. Hence, by (2), the n-vertex chemical trees having the minimum value of $\bar{M}_2$ are the same as those having the maximum value of M_2 given in Theorem 1.

Next, we discuss the second minimum value of $\bar{M}_2$. We discuss only the case when $n \equiv 0$ (mod 3) because the reasoning for the other two cases is similar. Assume that $n \equiv 0$ (mod 3). Let A be the class of chemical trees described in Theorem 2 (1.1) and A_1 be the class of chemical trees specified in Theorem 1 (1.1). It is obvious that $A_1 \subset A$. Take $A_2 = A \backslash A_1$.

We have known that the chemical trees in A_1 would attain the minimum value of $\bar{M}_2$. In what follows, assume that $T \in A_1$ is a chemical tree of order n.

First suppose that $T \in A$. Then, by using Theorem 2 (1.2), we have

$$M_1(T) \leq 6n - 14 \tag{15}$$

with equality if and only if T is a tree containing no vertex of degree 2, that is, $n_2 = 0$, and two vertices of degree 3, that is, $n_3 = 2$. Also, by using Theorem 1 (1.2), we get

$$M_2(T) \leq 8n - 28 \tag{16}$$

with equality if and only if T is a tree containing no vertex of degree 2, that is, $n_2 = 0$, and two vertices of degree 3, that is, $n_3 = 2$, such that each vertex of degree 3 is adjacent to two vertices of degree 1 and one vertex of degree 4, that is, $x_{1,3} = 4$, $x_{3,4} = 2$, and $x_{3,3} = 0$. From (2), (15) and (16), it follows that

$$\bar{M}_2(T) \geq 2(n-1)^2 - (8n-28) - \frac{6n-14}{2} = 2n^2 - 15n + 37$$

with equality if and only if T is a tree containing no vertex of degree 2, that is, $n_2 = 0$, and two vertices of degree 3, that is, $n_3 = 2$, such that each vertex of degree 3 is adjacent to two vertices of degree 1 and one vertex of degree 4, that is, $x_{1,3} = 4$, $x_{3,4} = 2$, and $x_{3,3} = 0$ (the same as those chemical trees depicted in Theorems 1 (1.2)).

Next suppose that $T \in A$, that is, $T \in A_2$. Recall that each chemical tree in A_1 satisfies $n_2 = 1$, $n_3 = 0$, and $x_{1,2} = x_{2,4} = 1$. So it is easy to see that the chemical trees in A_2 would satisfy $n_2 = 1$, $n_3 = 0$, $x_{1,2} = 0$ and $x_{2,4} = 2$. By direct calculations, the M_1 and M_2 values of such chemical trees are, respectively, $M_1(T) = 6n - 12$ and $M_2(T) = 8n - 32$, and thus

$$\bar{M}_2(T) = 2(n-1)^2 - (8n-32) - \frac{6n-12}{2} = 2n^2 - 15n + 40,$$

which is larger than the attainable lower bound $2n^2 - 15n + 37$ when $T \notin A$.

It needs to be remarked here that the n-vertex chemical trees with the first/second maximum M_2 value are the same as the n-vertex chemical trees with the first/second "modified first Zagreb connection index" (see Du et al. [39]), where $n \geq 9$. We end this paper with the following open question.

Question 1. *For $n \geq 9$, are the n-vertex chemical trees with the third maximum M_2 value the same as the n-vertex chemical trees with the third "modified first Zagreb connection index" (see Theorem 2 in Du et al. [39])?*

ACKNOWLEDGMENTS

The authors would like to express their sincere gratitude to three anonymous referees for their insightful comments and valuable suggestions, which led to a number of improvements in the earlier version of this manuscript. Zhibin Du was supported by the National Natural Science Foundation of China (Grant No. 11701505). Zahid Raza was funded by the University of Sharjah under the Project #1802144068 and MASEP Research Group.

AUTHOR CONTRIBUTIONS

Zhibin Du: Conceptualization; formal analysis; methodology; writing-original draft; writing-review and editing. **Akbar Ali:** Conceptualization; formal analysis; investigation; methodology; writing-original draft; writing-review and editing. **Rabbia Rafee:** Data curation; investigation; visualization; writing-original draft. **Zahid Raza:** Resources; validation; visualization; writing-review and editing. **Muhammad Kamran Jamil:** Resources; validation; visualization; writing-review and editing.

ORCID

Zhibin Du https://orcid.org/0000-0001-5795-3580
Akbar Ali https://orcid.org/0000-0001-8160-4196
Zahid Raza https://orcid.org/0000-0002-4910-2038

REFERENCES

[1] P. Gantzer, B. Creton, C. Nieto–Draghi, *Mol. Inf.* **2020**, *39*, 1900087.
[2] Y. Martínez-López, Y. Marrero-Ponce, S. J. Barigye, E. Teran, O. Martinez-Santiago, C. H. Zambrano, F. J. Torres, *Mol. Divers.* **2020**, *24*, 913.
[3] A. U. K. Danishuddin, *Drug Discov. Today* **2016**, *21*, 1291.
[4] J. C. Dearden, The use of topological indices in QSAR and QSPR modeling. in *Advances in QSAR Modeling* (Ed: K. Roy), Springer, Cham **2017**, p. 57.
[5] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL **1992**.
[6] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London **2008**.
[7] G. Chartrand, L. Lesniak, P. Zhang, *Graphs & Digraphs*, 6th ed., CRC Press, Boca Raton, FL **2016**.
[8] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, FL **2019**.
[9] R. Todeschini, V. Consomni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim **2000**.
[10] I. Gutman, N. Trinajstić, *Chem. Phys. Lett.* **1972**, *17*, 535.
[11] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *J. Chem. Phys.* **1975**, *62*, 3399.
[12] L. Lovász, *Combinatorial Problems and Exercises*, 2nd ed., North-Holland, Amsterdam **1993**.
[13] A. B. Zakharov, A. V. Dyachenko, V. V. Ivanov, *J. Chemom* **2019**, *33*, e3169.
[14] A. B. Zakharov, V. V. Ivanov, *Kharkov Univ. Bull. Chem. Ser* **2019**, *32*, 38.
[15] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, *MATCH Commun. Math. Comput. Chem.* **2018**, *80*, 5.

[16] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, *MATCH Commun. Math. Comput. Chem.* **2017**, *78*, 17.
[17] A. Ali, *Asian Eur. J. Math* **2018**, *11*, 1850064.
[18] A. Ali, K. C. Das, S. Akhter, *Miskolc Math. Notes* in press.
[19] A. R. Ashrafi, M. Eliasi, A. Ghalavand, *Linear Multilinear Algebra* **2019**, *67*, 1736.
[20] K. C. Das, A. Ali, *Discrete Math. Lett.* **2019**, *2*, 38.
[21] F. Javaid, M. K. Jamil, I. Tomescu, *Discrete Appl. Math.* **2019**, *270*, 153.
[22] M. Liu, K. Cheng, I. Tomescu, *Discrete Appl. Math.* **2020**, *284*, 616.
[23] S. Noureen, A. Ali, A. A. Bhatti, *MATCH Commun. Math. Comput. Chem.* **2020**, *84*, 513.
[24] H. M. A. Siddiqui, *Hacet. J. Math. Stat.* **2020**, *49*, 754.
[25] S. Wang, C. Wang, J. B. Liu, *Appl. Math. Comput.* **2018**, *332*, 338.
[26] F. Zhan, Y. Qiao, J. Cai, *MATCH Commun. Math. Comput. Chem.* **2019**, *81*, 383.
[27] E. H. Zogić, E. R. Glogić, *Sci. Pub. State Uni. Novi Pazar Ser. A: Appl. Math. Inform. Mech.* **2020**, *12*, 21.
[28] T. Došlić, *ARS Math. Contemp.* **2008**, *1*, 66.
[29] A. R. Ashrafi, T. Došlić, A. Hamzeh, *Discrete Appl. Math.* **2010**, *158*, 1571.
[30] I. Milovanović, M. Matejić, E. Milovanović, *Contrib. Math.* **2020**, *1*, 17.
[31] I. Gutman, B. Furtula, Z. K. Vukićević, G. Popivoda, *MATCH Commun. Math. Comput. Chem.* **2015**, *74*, 5.
[32] X. Li, H. Zhao, *MATCH Commun. Math. Comput. Chem.* **2004**, *50*, 57.
[33] B. Li, W. Liu, *Proc. Math. Sci.* **2013**, *123*, 167.
[34] Z. Raza, A. Ali, *Int. J. Quantum Chem.* **2020**, *120*, e26333.
[35] Z. K. Vukićević, G. Popivoda, *Iran. J. Math. Chem.* **2014**, *5*, 19.
[36] A. Ali, Z. Du, M. Ali, *Appl. Math. Comput.* **2018**, *335*, 231.
[37] G. Caporossi, I. Gutman, P. Hansen, *Comput. Chem* **1999**, *23*, 469.
[38] I. Gutman, O. Miljković, G. Caporossi, P. Hansen, *Chem. Phys. Lett.* **1999**, *306*, 366.
[39] Z. Du, A. Ali, N. Trinajstić, *Mol. Inf.* **2019**, *38*, 1800116.

How to cite this article: Du Z, Ali A, Rafee R, Raza Z, Jamil MK. On the first two extremum Zagreb indices and coindices of chemical trees. *Int J Quantum Chem*. 2021;121:e26547. https://doi.org/10.1002/qua.26547