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Research article

Extremal values of the first reformulated Zagreb index for molecular trees with application to octane isomers

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Abstract: A connected acyclic graph in which the degree of every vertex is at most four is called a molecular tree. A number associated with a molecular tree that can help to approximate the physical or chemical properties of the corresponding molecule is called a topological index. It is of great importance to investigate the relation between the structure and the thermodynamic properties of those molecules. In this paper, we investigated the extreme value of the first reformulated Zagreb index with a given order and degree of a graph. Further, we investigated the molecular trees that attain the maximum and minimum values. As an application, we presented the regression models to predict the acentric factor and entropy of octane isomers. Our extremal graphs give the minimum and the maximum acentric factor and entropy, which satisfied the experimental values.

Keywords: molecular tree; first reformulated Zagreb index; extremal trees; entropy; isomers
Mathematics Subject Classification: 05C92, 05C90

1. Introduction

A graph is defined as $\mathcal{J} = (\mathcal{V}_\alpha, \mathcal{E}_\alpha)$, where $\mathcal{V}_\alpha$ is the graph's vertex set and $\mathcal{E}_\alpha$ is its edge set, respectively. Structures of chemical compounds are represented by chemical bonds. One type of these bonds is a covalent bond in which the sharing of electrons takes place, and this sharing is indicated by lines called edges in chemical graphs and atoms as vertices. An edge between two vertices u_α and v_α is denoted by $u_\alpha v_\alpha$. The vertex degree denoted by $\rho_{\mathfrak{J}}(u_\alpha)$ of a vertex u_α is measured by the total count of links connected with u_α. The maximum degree in a graph is denoted as $\triangle(\mathcal{J})$, or simply $\triangle$. A

single-component graph having no cycle with $\triangle = 4$ is known as a molecular tree. The structures of acyclic molecules can be modeled by using molecular trees.

For a molecular graph, a topological descriptor is a numeral linked with this graph. This value can help to analyze some physical or chemical properties of the corresponding molecular structure. The family of Zagreb indices is an important family of topological indices, which contains various versions of the Zagreb indices. In 1972, the first and the second Zagreb indices were introduced [1, 2].

The above two indices for $\mathcal{J}$ are defined as:

$$M_1(\mathcal{J}) = \sum_{u_\alpha \in \mathcal{V}(\mathcal{J})} \rho(u_\alpha)^2,$$
$$M_2(\mathcal{J}) = \sum_{u_\alpha v_\alpha \in \mathcal{E}(\mathcal{G})} \rho(u_\alpha)\rho(v_\alpha).$$

Miličević et al. [3] formulated the first and second Zagreb indices based on the edge degree. For the edge $e = u_\alpha v_\alpha$, the degree of e is $\rho(e) = \rho(u_\alpha) + \rho(v_\alpha) - 2$ and the reformulated Zagreb descriptor is formulated by:

$$EM_1(\mathcal{J}) = \sum_{e \in \mathcal{E}(\mathcal{J})} \rho(e)^2 = \sum_{u_\alpha v_\alpha \in \mathcal{E}(\mathcal{J})} (\rho(u_\alpha) + \rho(v_\alpha) - 2)^2,$$
$$EM_2(\mathcal{J}) = \sum_{e_1 \sim e_2} \rho(e_1)\rho(e_2).$$

Extreme values of first and lower bounds for second reformulated Zagreb indices are calculated in [4]. A relation between a graph and its line graph is used to determine a relationship among original and reformulated Zagreb indices in [5]. In article [6], the authors discussed the maximum and minimum values of trees for $EM_1(\mathcal{J})$ and $EM_2(\mathcal{J})$. In [7, 8], authors investigated the first, second, and third maximum Randić indices of molecular trees.

Ji et al. [9] investigated the extermal trees, unicyclic and bicyclic graphs with given order for the first reformulated Zagreb indices. Some important results for dendrimers, related to the above two indices are presented in [10]. In [11], authors found the extremal tricyclic graphs for the index. In [12, 13], the extremal values of molecular trees are calculated for Sombor indices. Bounds on $EM_1(\mathcal{J})$ were observed by Milovanović et al. in [14], in terms of some graph parameters. The dependency of energy on cube of degree of vertices is shown in [15]. Neighborhood of Zagreb index on product of graphs is discussed in [16]. Su et al. [17] studied with given connectivity and determined the extremal graphs for the same index. The exact expressions for the same index as the first reformulated Zagreb index are presented in [18] for some familiar graph operations. For the general Randić index, the extremal molecular trees with the given number of pendant vertices are discussed in [19–21]. Liu and Li explored further properties of the molecular trees for the harmonic index in [22], and they also gave the extremal values of the harmonic descriptor of trees with $\triangle = 4$. Husin et al. [23] extended the results and determined the fourth maximum Randić index for the same class. Hundreds of topological indices have been introduced up to the date for history and latest results on this topic, we suggest [24–29].

In this paper we extended the work on the molecular trees for the first reformulated Zagreb index and determined the molecular trees, which give the extremal values of the index.

2. Main results

In this section, we presented some auxiliary lemmas and our main results. In the following for $1 \leq i, j \leq 4$, the count of atoms having degree i is represented by n_i, while the count of bonds with one end atom having degree i and the other end atom containing degree j is represented by ζ_{ij}.

For a molecular tree T we have the following information:

$$n_1 + n_2 + n_3 + n_4 = n, \tag{2.1}$$
$$\zeta_{12} + \zeta_{13} + \zeta_{14} = n_1, \tag{2.2}$$
$$\zeta_{21} + 2\zeta_{22} + \zeta_{23} + \zeta_{24} = 2n_2, \tag{2.3}$$
$$\zeta_{31} + \zeta_{32} + 2\zeta_{33} + \zeta_{34} = 3n_3, \tag{2.4}$$
$$\zeta_{41} + \zeta_{42} + \zeta_{43} + 2\zeta_{44} = 4n_4, \tag{2.5}$$
$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1). \tag{2.6}$$

Applying the definition of $EM_1(T)$,

$$\begin{aligned} EM_1(T) &= \sum_{u_\alpha v_\alpha \in \mathcal{E}(T)} (\rho(u_\alpha) + \rho(v_\alpha) - 2)^2 \\ &= \zeta_{12} + 4\zeta_{13} + 9\zeta_{14} + 4\zeta_{22} + 9\zeta_{23} + 16\zeta_{24} + 16\zeta_{33} + 25\zeta_{34} + 36\zeta_{44}. \end{aligned} \tag{2.7}$$

From Eqs (2.1) and (2.6), we have

$$3n_1 + 2n_2 + n_3 = 2(1+n). \tag{2.8}$$

Using Eqs (2.2)–(2.4) in (2.8), we get

$$\zeta_{14} = \frac{2n+2}{3} - \frac{4}{3}\zeta_{12} - \frac{10}{9}\zeta_{13} - \frac{2}{3}\zeta_{22} - \frac{4}{9}\zeta_{23} - \frac{1}{3}\zeta_{24} - \frac{2}{9}\zeta_{33} - \frac{1}{9}\zeta_{34}.$$

Solving Eqs (2.1) and (2.6), we have

$$n_2 + 2n_3 + 3n_4 = n - 2. \tag{2.9}$$

Using Eqs (2.3)–(2.5) in (2.9), we get

$$\frac{1}{2}(\zeta_{21} + 2\zeta_{22} + \zeta_{23} + \zeta_{24}) + \frac{2}{3}(\zeta_{31} + \zeta_{32} + 2\zeta_{33} + \zeta_{34}) + \frac{3}{4}(\zeta_{41} + \zeta_{42} + \zeta_{43} + 2\zeta_{44}) = (n-2)$$
$$\zeta_{44} = \frac{n-5}{3} + \frac{1}{3}\zeta_{21} - \frac{1}{3}\zeta_{22} - \frac{5}{9}\zeta_{23} - \frac{2}{3}\zeta_{24} + \frac{1}{9}\zeta_{13} - \frac{7}{9}\zeta_{33} - \frac{8}{9}\zeta_{34}.$$

Substituting the values of ζ_{14} and ζ_{44} in Eq (2.7), we have

$$EM_1(T) = \zeta_{12} - 2\zeta_{13} - 14\zeta_{22} - 15\zeta_{23} - 11\zeta_{24} - 14\zeta_{33} - 8\zeta_{34} + 18n - 54. \tag{2.10}$$

The following result provides information about the maximum value of $EM_1(T)$ for the molecular trees and the proof is given after some auxiliary lemmas.

Theorem 2.1. *Let T be a molecular tree of order $n \geq 5$, then the maximum value of the first reformulated Zagreb index is*

$$EM_1(T) \leq \begin{cases} 18n - 64, n \equiv 0(mod\ 3), \\ 18n - 72, n \equiv 1(mod\ 3), \\ 18n - 54, n \equiv 2(mod\ 3), \end{cases}$$

and the maximum first reformulated Zagreb index is achieved if, and only if, one of the following conditions is satisfied:

- *T has exactly one edge of degree one and one edge of degree sixteen,*
- *two edges are of degree four and degree of one edge is twenty five,*
- *degree of all the edges are either nine or thirty six.*

Now we present some lemmas.

Lemma 2.2. *Let a molecular tree T has at least two vertices of degree three, then T cannot attain the maximal first reformulated Zagreb Index.*

Proof. Suppose we have a molecular tree T with at least two vertices of degree three, and u_α and v_α are three degree vertices, i.e., $\rho(u_\alpha) = \rho(v_\alpha) = 3$. Based on adjacency of u_α and v_α, we have the following two cases.

Case I. When $u_\alpha v_\alpha \notin \mathcal{E}(T)$.

Suppose $u_{\alpha_1}, u_{\alpha_2}, u_{\alpha_3}$ are the neighbors of u_α in T and $e_i = u_\alpha u_{\alpha_i}$ for $1 \leq i \leq 3$, and $v_{\alpha_1}, v_{\alpha_2}, v_{\alpha_3}$ are the neighbors of v_α in T and $f_i = v_\alpha v_{\alpha_i}$ for $1 \leq i \leq 3$.

Further, suppose that $\rho(u_{\alpha_1}) + \rho(u_{\alpha_2}) + \rho(u_{\alpha_3}) \leq \rho(v_{\alpha_1}) + \rho(v_{\alpha_2}) + \rho(v_{\alpha_3})$.

Now, we construct a new graph $T' = T - u_\alpha u_{\alpha_2} + v_\alpha u_{\alpha_2}$, and in T' we have $d_{T'}(u_\alpha) = 2$ and $d_{T'}(v_\alpha) = 4$.

Suppose $A = \{e_1, e_2, e_3, f_1, f_2, f_3\}$. Now, from the definition of T we have:

$$\begin{aligned} EM_1(T) - EM_1(T') = &\{1 + \rho(u_{\alpha_1})\}^2 + \{1 + \rho(u_{\alpha_2})\}^2 + \{1 + \rho(u_{\alpha_3})\}^2 + \{1 + \rho(v_{\alpha_1})\}^2 + \\ &\{1 + \rho(v_{\alpha_2})\}^2 + \{1 + \rho(v_{\alpha_3})\}^2 - \{\rho(u_{\alpha_1})\}^2 - \{\rho(u_{\alpha_3})\}^2 - \{2 + \rho(u_{\alpha_2})\}^2 - \{2 + \rho(v_{\alpha_1})\}^2 - \\ &\{\rho(v_{\alpha_2}) + 2\}^2 - \{\rho(v_{\alpha_3}) + 2\} < 0. \end{aligned}$$

Case II. When $u_\alpha v_\alpha \in \mathcal{E}(T)$.

Here, we suppose that $u_{\alpha_1} = u_\alpha$, $v_{\alpha_1} = v_\alpha$ and $e_1 = u_\alpha v_\alpha = f_1$. Without loss of generality, take $\rho(u_{\alpha_2}) + \rho(u_{\alpha_3}) \leq \rho(v_{\alpha_2}) + \rho(v_{\alpha_3})$. We construct a new tree $T' = T - u_\alpha u_{\alpha_3} + v_\alpha u_{\alpha_3}$. Let $A = \{e_2, e_3, f_2, f_3\}$, then

$$\begin{aligned} EM_1(T) - EM_1(T') = &\{1 + \rho(u_{\alpha_2})\}^2 + \{1 + \rho(u_{\alpha_3})\}^2 + \{1 + \rho(v_{\alpha_2})\}^2 + \{1 + \rho(v_{\alpha_3})\}^2 \\ &- \{\rho(u_{\alpha_2})\}^2 - \{1 + \rho(v_{\alpha_2})\}^2 - \{2 + \rho(v_{\alpha_3})\}^2 - \{2 + \rho(u_{\alpha_3})\}^2 < 0, \end{aligned}$$

which is a contradiction. □

Lemma 2.3. *If a molecular tree has at least two vertices of degree two, then it cannot attain the maximum reformulated Zagreb index.*

Proof. Suppose we have a molecular tree T with at least two vertices of degree two. Let u_α and v_α have degree two. There are two possibilities either $u_\alpha v_\alpha \notin \mathcal{E}(T)$ or $u_\alpha v_\alpha \in \mathcal{E}(T)$, and we discuss both the cases separately.

Case I. When $u_\alpha v_\alpha \notin \mathcal{E}(T)$.

Since $\rho(u_\alpha) = 2 = \rho(v_\alpha)$, let $e_1 = u_\alpha u_{\alpha_1}, e_2 = u_\alpha u_{\alpha_2}, f_1 = v_\alpha v_{\alpha_1}$ and $f_2 = v_\alpha v_{\alpha_2}$. Without loss of generality, suppose that $\rho(u_{\alpha_1}) + \rho(u_{\alpha_2}) \leq \rho(v_{\alpha_1}) + \rho(v_{\alpha_2})$.

We construct a new molecular tree from T as $T' = T - u_\alpha u_{\alpha_2} + v_\alpha u_{\alpha_2}$, then

$$EM_1(T) - EM_1(T') = \rho(u_{\alpha_1})^2 + \rho(u_{\alpha_2})^2 + d(v_{\alpha_1})^2 + \rho(v_{\alpha_2})^2 - \{\rho(u_{\alpha_1}) - 1\}^2 - \{1 + \rho(u_{\alpha_2})\}^2 - \{1 + \rho(v_{\alpha_1})\}^2 - \{1 + \rho(v_{\alpha_2})\}^2 < 0.$$

Case II. When $u_\alpha v_\alpha \in \mathcal{E}(T)$.

Since the degree of u_α and v_α is two, suppose u_{α_2} and v_{α_2} are their other neighbors. The new molecular graph is constructed from T as $T' = T - u_\alpha u_{\alpha_2} + v_\alpha u_{\alpha_2}$. In this new graph, the degree of u_α is one and the degree of v_α is three.

$$EM_1(T) - EM_1(T') = \rho(u_{\alpha_2})^2 + \rho(v_{\alpha_2})^2 - \{1 + \rho(u_{\alpha_2})\}^2 - \{1 + \rho(v_{\alpha_2})\}^2 < 0.$$
$$EM_1(T) < EM_1(T').$$

In both cases we get a contradiction as we supposed T gives the maximum first reformulated Zagreb index. □

Lemma 2.4. *Let T be a molecular tree with at least one vertex of degree two, and at least one vertex of degree three, then T cannot attain the maximum first reformulated Zagreb index.*

Proof. Let T be a molecular tree with a vertex u_α of degree two and a vertex v_α of degree three.

Case I. Vertices u_α and v_α are not adjacent.

Since the degrees of u_α and v_α are two and three, respectively, let $e_1 = u_\alpha u_{\alpha_1}, e_2 = u_\alpha u_{\alpha_2}, f_1 = v_\alpha v_{\alpha_1}, f_2 = v_\alpha v_{\alpha_2}$ and $f_3 = v_\alpha v_{\alpha_3}$. By deleting edge $u_\alpha u_{\alpha_2}$ and adding an edge $v_\alpha u_{\alpha_2}$ from T, we get another molecular graph T'.

$$EM_1(T) - EM_1(T') = \rho(u_{\alpha_1})^2 + \rho(u_{\alpha_2})^2 + \{1 + \rho(v_{\alpha_1})\}^2 + \{1 + \rho(v_{\alpha_2})\}^2 + \{1 + \rho(v_{\alpha_3})\}^2 - \{\rho(u_{\alpha_1}) - 1\}^2 - \{2 + \rho(v_{\alpha_1})\}^2 - \{2 + \rho(v_{\alpha_2})\}^2 - \{2 + \rho(v_{\alpha_3})\}^2 \{2 + \rho(u_{\alpha_2})\}^2 < 0.$$

Case II. Vertices u_α and v_α are adjacent.

Let the vertex u_{α_2} be different from v_α as adjacent to u_α, and vertices v_{α_1} and v_{α_2} different from u_α are adjacent the vertex v_α. The new molecular graph T' is constructed from T by deleting the edge $u_\alpha u_{\alpha_2}$ and adding an edge $v_\alpha u_{\alpha_2}$. When u_α and v_α are neighbors of each other, then u_{α_1} and v_{α_1} are actually vertices u_α and v_α. Graph T' is obtained by deleting edge $u_\alpha u_{\alpha_2}$ and adding edge $v_\alpha u_{\alpha_2}$.

$$EM_1(T) - EM_1(T') = \{\rho(u_{\alpha_2})\}^2 + \{1 + \rho(v_{\alpha_2})\}^2 + \{\rho(v_{\alpha_3}) + 1\}^2 - \{\rho(v_{\alpha_2}) + 2\}^2 - \{\rho(v_{\alpha_3}) + 2\}^2 - \{\rho(u_{\alpha_2}) + 2\}^2 < 0.$$

□

From the above three Lemmas, we draw following conclusion.

2.1. Conclusion

If T is a molecular tree with the maximum first reformulated Zagreb index, then T must satisfy one of the following three conditions.

- all vertices of T have a degree of either one or four,
- exactly one vertex of the graph is of degree two and remaining vertices are of degree one or four,
- exactly one vertex of the graph is of degree three and remaining vertices are of degree one or four.

2.2. Proof of Theorem 2.1

Proof. For any molecular tree T, we have the following formula for the first reformulated Zagreb index derived in Eq (2.10)

$$EM_1(T) = 18n - 54 + \zeta_{12} - 2\zeta_{13} - 14\zeta_{22} - 15\zeta_{23} - 11\zeta_{24} - 14\zeta_{33} - 8\zeta_{34}.$$

Let T be a molecular tree with the maximum value of the first reformulated Zagreb index. Based on the order of T, we have the three cases given as:
Case I. When $n \equiv 0 \mod (3)$.
Let $n = 3\hbar$ and $\hbar \geq 2$. From Eq (2.9), we get

$$n_2 + 2n_3 + 3n_4 = 3\hbar - 2. \tag{2.11}$$

Since T has the maximal first reformulated Zagreb index, then by Lemmas 2.2–2.4, the solution of the Eq (2.11) exists if, and only if, $n_4 = \hbar - 1$, $n_3 = 0$ and $n_2 = 1$. Putting these values in Eq (2.10), we have,

$$EM_1(T) = 18n - 54 + \zeta_{12} - 11\zeta_{24}.$$

Moreover,

$$EM_1(T) = \begin{cases} 18n - 76, & if\ \zeta_{12} = 0, \zeta_{24} = 2, \\ 18n - 64, & if \zeta_{12} = 1 = \zeta_{24}. \end{cases}$$

However,

$$EM_1(T) \leq 18n - 64,$$

gives the maximum value and the equality holds if, and only if, T has exactly one edge of degree one and one vertex edge of degree sixteen.
Case II. When $n \equiv 1 \mod (3)$.
Let $n = 3\hbar + 1$, and $\hbar \geq 2$, then Eq (2.9) becomes

$$n_2 + 2n_3 + 3n_4 = 3\hbar - 1. \tag{2.12}$$

From Lemmas 2.2–2.4, the solution of Eq (2.12) exists if, and only if, $n_4 = \hbar - 1$, $n_2 = 0$ and $n_3 = 1$. In the case of all $\zeta_{ij} = 0$, if any of $i = 2$ or $j = 2$, then ζ_{33}=0. Thus Eq (2.10) reduces to,

$$EM_1(T) = 18n - 54 - 2\zeta_{13} - 8\zeta_{34}.$$

Moreover,

$$EM_1(T) = \begin{cases} 18n - 78, & if \zeta_{34} = 3, \zeta_{13} = 0, \\ 18n - 66, & if\ \zeta_{13} = 2, \zeta_{34} = 1. \end{cases}$$

Hence,

$$EM_1(T) \leq 18n - 66,$$

and the equality holds if, and only if, the degree of two edges of the molecular tree are four and the degree of one edge is twenty five.

Case III. When $n \equiv 2 \mod (3)$.

Let $n = 3\hbar + 2$ for $\hbar \geq 2$, and from Eq (2.9) we have $n_2 + 2n_3 + 3n_4 = 3\hbar$. As in previous cases, the solution of the equation exists if, and only if, $n_4 = \hbar$, $n_3 = 0$ and $n_2 = 0$, then $\zeta_{ij} = 0$, for $i = 2, 3$ or $j = 2, 3$. Hence, the first reformulated Zagreb index is

$$EM_1(T) = 18n - 54,$$

and the above is attained if, and only if, the degree of all the edges are either nine or thirty six, which completes the proof. □

3. Minimum value of the reformulated Zagreb index

In the following, we will work on the minimal first reformulated Zagreb index of molecular trees for $2 \leq \Delta \leq 4$.

Lemma 3.1. *Let T be a molecular tree with $\triangle = 3$ and with two vertices of degree three, then T cannot attain the minimal first reformulated Zagreb index.*

Proof. Let T be a molecular tree on n vertices and $\triangle = 3$ with two vertices of degree three, i.e., $\rho(u_\alpha) = \rho(v_\alpha) = 3$ and with the minimal first reformulated Zagreb index. Suppose that there is a vertex w_α such that $\rho(w_\alpha) = 1$. Let $u_{\alpha 1}, u_{\alpha 2}, u_{\alpha 3}$ be neighbors of u_α and $w_{\alpha 1}$ is the neighbor of w_α in T. Let's construct a new graph T' as, $T' = T - u_\alpha u_{\alpha_1} + w_\alpha u_{\alpha_1}$. Further we have,

$$EM_1(T) - EM_1(T') = 2(\rho(u_{\alpha_1}) + \rho(u_{\alpha_2}) + \rho(u_{\alpha_3})) - 2\rho(w_{\alpha_1}) + 4 > 0.$$

This result shows that the molecular tree is not minimal for two vertices of degree three. □

Following lemmas can be proved similarly.

Lemma 3.2. *Let T be a molecular tree with maximum degree four and two vertices of degree four, then the first reformulated Zagreb index of T is not minimum.*

Lemma 3.3. *Let T be a molecular tree of order n having a maximum degree four with one vertex of degree four and one vertex of degree three, then the first reformulated Zagreb descriptor cannot be minimum for T.*

Proof. Let T be a tree with $\triangle = 3$ and $\rho(u_\alpha) = 3$ and $\rho(w_\alpha) = 4$. Suppose that u_α has neighbors $u_{\alpha_1}, u_{\alpha_2}$ and u_{α_3} and w_α has neighbor w_{α_1}. Now, construct T' such that $T' = T - u_\alpha u_{\alpha_1} + w_\alpha u_{\alpha_1}$, then $EM_1(T) - EM_1(T') > 0$. □

Theorem 3.4. *Let a molecular tree with n number of vertices such that $n \geq 5$ and $2 \leq \Delta \leq 4$, then the minimal value of the first reformulated Zagreb index is given as*

$$EM_1(T) \geq \begin{cases} n-10 \; for \; \triangle = 2, \; \textit{equality holds when } T \textit{ is a path}, \\ 4n-2 \; for \; \triangle = 3, \; \textit{equality holds when } T \textit{ contains two edges of degree four}, \\ 4n+20 \; for \; \triangle = 4, \; \textit{equality holds when } T \textit{ contains three edges of degree nine}. \end{cases}$$

Proof. • If $\Delta = 2$, then clearly tree is a path graph and we have $EM_1(T) = 4n - 10$.

• For $\Delta = 3$. By Lemma 3.1, we have only two molecular trees:

(1) one edge of degree four, denotes it T_1,
(2) two edges of degree four, denotes it by T_2.

Further, $EM_1(T_1) = 4n$ and $EM_1(T_2) = 4n - 2$, clearly $EM_1(T_1) > EM_1(T_2)$.

• For $\Delta = 4$. By Lemmas 3.2 and 3.3, we have the following molecular trees:

(1) two edges of degree nine, denotes it T_3,
(2) three edges of degree nine, denotes it by T_4.

Further, $EM_1(T_3) = 4n + 24$ and $EM_1(T_4) = 4n + 20$, and clearly $EM_1(T_3) > EM_1(T_4)$, which completes the proof. □

4. Application to octane isomers

In this section, we will present a possible application of our work. The acentric factor is a measure of the non-centricity of molecules. As the acentric factor increases, the vapor pressure goes down, resulting in higher boiling points [30, 31]. Entropy is a measure of the unavailability of a system's energy to do work. It is a measure of disorder. The greater the disorder in a molecule, the greater the entropy [32, 33]. Here, 18 octane isomers [34, 35] with their acentric factors and entropy measure are considered, as well as the first reformulated Zagreb indices of these octane isomers. This information is provided in Table 1. Several papers have been written on the correlation between properties and topological indices of molecular graphs, and we refer [12, 15] and references therein. A linear regression through Microsoft Excel is performed on the data in Table 1. We obtain the following linear equations that can predict the acentric factor and entropy of octane isomers. Further, from Table 1 we can notice that the 2,2,3,3,-tetramethyl butane (18th isomer) has the maximum reformulated Zagreb index with the minimum acentric factor and entropy. In Theorem 2.1, we can notice that the same molecular tree attained the maximum value. This implies that the chemical trees with the maximum reformulated Zagreb index have the minimum acentric factor and entropy measure.

$$Acentric \; factor = -0.0021 \times RM_1 + 0.4351,$$
$$Entropy = -0.258 \times RM_1 + 117.77,$$

with the correlation coefficients (R) 0.9841 and 0.9608, respectively. These results are comparable with the models already discussed in the literature. Figures 1 and 2 show the close relation between the acentric factor and entropy and the reformulated Zagreb index. These results imply that the reformulated Zagreb index can be a good predictor of the acentric factor and entropy for octane isomers.

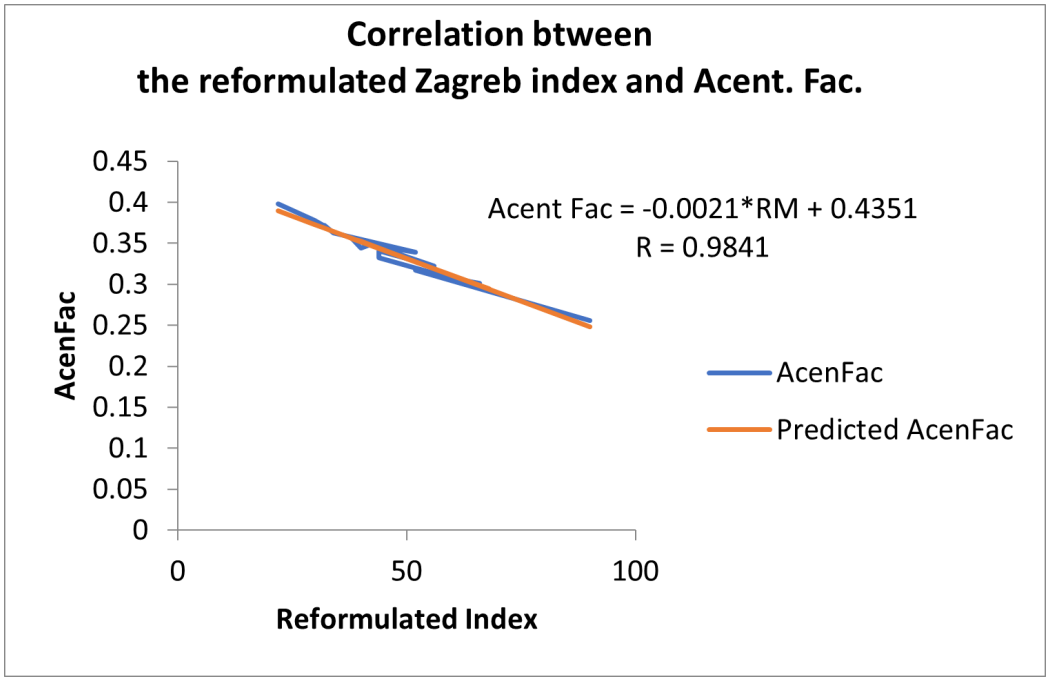


Figure 1. The relationship between acentric factor and the reformulated Zagreb index for 18 isomers.

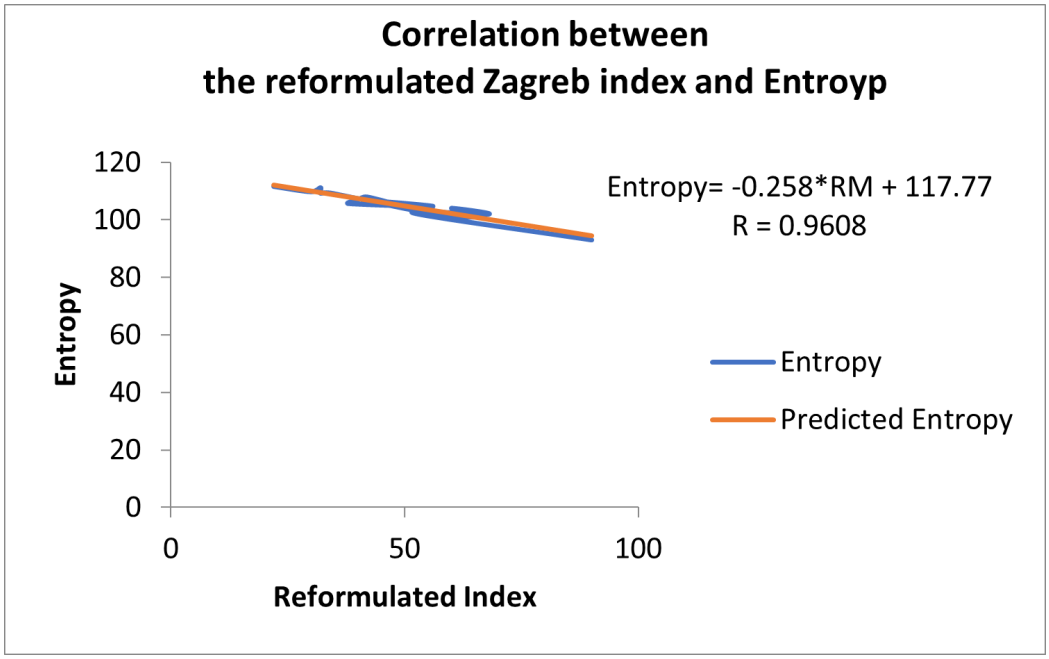
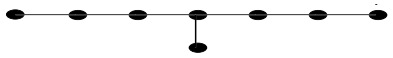
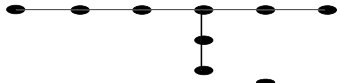
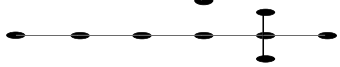
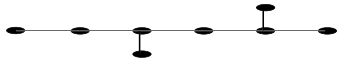
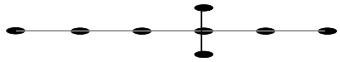
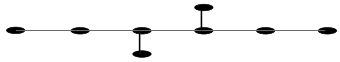
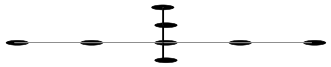
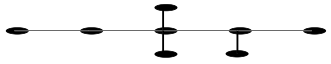
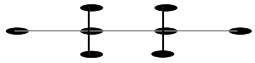


Figure 2. The relationship between entropy and the reformulated Zagreb index for 18 octane isomers.

Table 1. Acentric factor, entropy and the reformulated Zagreb index values of 18 octane isomers.

No.	Isomer	Acent. Fac.	Entropy	EM_1
1		0.397898	111.67	22
2		0.377916	109.84	30
3		0.371002	111.26	32
4		0.371504	109.32	32
5		0.362472	109.43	34
6		0.339426	103.42	52
7		0.348247	108.02	42
8		0.344223	106.98	40
9		0.356830	105.72	38
10		0.322596	104.74	56
11		0.340345	106.59	44
12		0.332433	106.06	44
13		0.306899	101.48	60
14		0.300816	101.31	66
15		0.305370	104.09	60
16		0.293177	102.06	68
17		0.317422	102.39	52
18		0.255294	93.06	90

5. Conclusions

In the field of chemical graph theory, topological indices play an important role. Topological indices are numerical values that are used to correlate the chemical structure of molecules by a graph with

chemical properties. Many distance-based and degree-based topological indices have been introduced. Among all existing topological indices, degree-based indices are very helpful in hydrocarbons, in the field of pharmacy and the preparation of drugs used against diseases like cancer. In this article, we discussed the behavior of the first reformulated Zagreb index for molecular trees, which is the generalized form of of the first Zagreb index. Here, we calculated the first reformulated Zagreb index for molecular trees of order n and then calculated the results for extremal (maximal, minimal) values. The results obtained can be useful in extracting data for molecular trees and in discussing many properties of these molecular tree graphs, like melting point, boiling point, latent heat of fusion, entropy, enthalpy etc. In the end, we presented an application of the proposed work to calculate the acentric factor and entropy of octane isomers, then compared the values of the first reformulated Zagreb index, acentric factor and entropy graphically.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

Authors declare there is no conflict of interest in publishing the article.

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