Extremal Values of the First Reformulated Zagreb Index for Molecular Trees With Application to Octane Isomers

Shabana Anwar¹, Muhammad Kamran Jamil¹,*, Amal S. Alali²,*, Mehwish Zegham¹, Aisha Javed ³

¹Department of Mathematics, Riphah International University, Lahore, Pakistan
² Department of Mathematical Sciences, College of Science, Princess Nourah bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia
³Abdus Salam School of Mathematical Sciences, Government College University, Lahore, Pakistan

*Corresponding author: asalali@pnu.edu.sa, m.kamran.sms@gmail.com

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.

Key words: Molecular tree; first reformulated Zagreb index; extremal trees; entropy; isomers.

1 Introduction

A graph is defined as \( J = (V_\alpha, E_\alpha) \), where \( V_\alpha \) is the graph’s vertex set and \( E_\alpha \) 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 \( u_\alpha \) and \( v_\alpha \) is denoted by \( u_\alpha v_\alpha \). The vertex degree denoted by \( \rho_\alpha(u_\alpha) \) of a vertex \( u_\alpha \) is measured by the total count of links connected with \( u_\alpha \). The maximum degree in a graph is denoted as \( \Delta(J) \), or simply \( \Delta \). A single-component graph having no cycle with \( \Delta = 4 \) 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 [3,4].

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 [5] reformulated 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 are 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 [7]. A relation between graph and its line graph is used to determine a relationship among original and reformulated Zagreb indices in [8]. In article [9], the authors discussed the maximum and minimum values of trees for $EM_1(\mathcal{J})$ and $EM_2(\mathcal{J})$. Some important results for dendrimers, related to above two indices are presented in [10].

Ji et al [6] investigated the extremal trees, unicyclic and bicyclic graphs with given order for the first reformulated Zagreb indices. In [11] authors found the extremal tricyclic graphs for the index. Bounds on $EM_1(\mathcal{J})$ were observed by Milovanović et al in [14] in terms of some graph parameters. Su et al. [17] studied with given connectivity and determined the extremal graphs for the same index. The exact expressions for the same index the first reformulated Zagreb index are presented in [18] for some familiar graph operations. In [1, 2] authors, investigated the first, second, and third maximum Randić indices of molecular trees. Husin et al [23] extended the results and determined the fourth maximum Randić index for the same class. 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], they also gave the extremal values of the harmonic descriptor of trees with $\triangle = 4$.

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 $\zeta_{ij}$.

For a molecular tree, $T$, we have the following information:

$$\begin{align*}
n_1 + n_2 + n_3 + n_4 &= n, \\
\zeta_{12} + \zeta_{13} + \zeta_{14} &= n_1, \\
\zeta_{21} + 2\zeta_{22} + \zeta_{23} + \zeta_{24} &= 2n_2, \\
\zeta_{31} + \zeta_{32} + 2\zeta_{33} + \zeta_{34} &= 3n_3, \\
\zeta_{41} + \zeta_{42} + \zeta_{43} + 2\zeta_{44} &= 4n_4, \\
n_1 + 2n_2 + 3n_3 + 4n_4 &= 2(n - 1).
\end{align*}$$

Applying the definition of $EM_1(T)$,

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

From Eqs. (1) and (6), we have

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

Using Eqs. (2), (3) and (4) in (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. (1) and (6), gives

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

Using Eqs. (3), (4) and (5) in (9), we get

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

Substituting the values of $\zeta_{14}$ and $\zeta_{44}$ in Eq. 7, we have

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

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

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

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 $T$ having 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 3, and $u_\alpha$ and $v_\alpha$ are three degree vertices i.e. $\rho(u_\alpha) = \rho(v_\alpha) = 3$. Based on adjacency of $u_\alpha$ and $v_\alpha$, we have the following two cases.

Case I. when $u_\alpha v_\alpha \notin E(T)$.

Suppose $u_{a1}, u_{a2}, u_{a3}$ are the neighbours of $u_\alpha$ in $T$ and $e_i = u_\alpha u_{ai}$ for $1 \leq i \leq 3$, and $v_{a1}, v_{a2}, v_{a3}$ are the neighbours of $v_\alpha$ in $T$ and $f_i = v_\alpha v_{ai}$ for $1 \leq i \leq 3$. Further, suppose that $\rho(u_{a1}) + \rho(u_{a2}) + \rho(u_{a3}) \leq \rho(v_{a1}) + \rho(v_{a2}) + \rho(v_{a3})$.

Now, we construct a new graph $T' = T - u_\alpha u_{a2} + v_\alpha u_{a2}$, 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,

$$EM_1(T) - EM_1(T') = \{1 + \rho(u_{a1})\}^2 + \{1 + \rho(u_{a2})\}^2 + \{1 + \rho(u_{a3})\}^2 - \{1 + \rho(v_{a1})\}^2 - \{1 + \rho(v_{a2})\}^2 - \{1 + \rho(v_{a3})\}^2 - \{2 + \rho(u_{a1})\}^2 - \{2 + \rho(u_{a2})\}^2 - \{2 + \rho(u_{a3})\}^2 - \{2 + \rho(v_{a1})\}^2 - \{2 + \rho(v_{a2})\}^2 - \{2 + \rho(v_{a3})\}^2 - \{\rho(v_{a2}) + 2\}^2 - \{\rho(v_{a3}) + 2\}^2 < 0$$

Case II. when $u_\alpha v_\alpha \in E(T)$.

Here we suppose that, $u_{a1} = u_\alpha$ and $v_{a1} = v_\alpha$ and $e_1 = u_\alpha v_\alpha = f_1$. Without loss of generality take $\rho(u_{a2}) + \rho(u_{a3}) \leq \rho(v_{a2}) + \rho(v_{a3})$. We construct a new tree $T' = T - u_\alpha u_{a3} + v_\alpha u_{a3}$. Let $A = \{e_2, e_3, f_2, f_3\}$, then,

$$EM_1(T) - EM_1(T') = \{1 + \rho(u_{a2})\}^2 + \{1 + \rho(u_{a3})\}^2 + \{1 + \rho(v_{a2})\}^2 + \{1 + \rho(v_{a3})\}^2 - \{\rho(u_{a2})\}^2 - \{1 + \rho(v_{a2})\}^2 - \{2 + \rho(v_{a3})\}^2 - \{2 + \rho(u_{a3})\}^2 < 0$$.
which is a contradiction. □

**Lemma 2.3.** If a molecular tree having 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 $u_{\alpha}$ and $v_{\alpha}$ have degree 2. There are two possibilities either $u_{\alpha}v_{\alpha} \notin \mathcal{E}(T)$ or $u_{\alpha}v_{\alpha} \in \mathcal{E}(T)$, 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

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

**Case II.** when $u_{\alpha}v_{\alpha} \in \mathcal{E}(T)$.
Since the degree of $u_{\alpha}$ and $v_{\alpha}$ is two, suppose $u_{\alpha 2}$ and $v_{\alpha 2}$ are their other neighbours. 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 $u_{\alpha}$ is one and the degree of $v_{\alpha}$ 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 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 2 and at least one vertex of degree 3, then $T$ cannot attain the maximum first reformulated Zagreb index.

**Proof.** Let $T$ be a molecular tree with a vertex $u_{\alpha}$ of degree 2 and a vertex $v_{\alpha}$ of degree 3.

**Case I.** vertices $u_{\alpha}$ and $v_{\alpha}$ are not adjacent.
Since the degree of $u_{\alpha}$ and $v_{\alpha}$ are 2 and 3, 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 $T'$.

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

**Case II.** Vertices $u_{\alpha}$ and $v_{\alpha}$ are adjacent.
Let the vertex $u_{\alpha 2}$ different from $v_{\alpha}$ is adjacent to $u_{\alpha}$ and vertices $v_{\alpha 1}$ and $v_{\alpha 2}$ different from $u_{\alpha}$ are adjacent the vertex $v_{\alpha}$.
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 $u_{\alpha}$ and $v_{\alpha}$ are
neighbours of each other. Then \( u_{\alpha 1} \) and \( v_{\alpha 1} \) are actually vertices \( u_{\alpha} \) and \( v_{\alpha} \). 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 above three Lemmas we draw following conclusion.

**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 degree either 1 or 4,
- exactly one vertex of the graph is of degree 2 and remaining vertices are of degree 1 or 4,
- exactly one vertex of the graph is of degree 3 and remaining vertices are of degree 1 or 4.

**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. 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 \( n = 3h \) and \( h \geq 2 \). From Eq. 9 we get

\[
n_2 + 2n_3 + 3n_4 = 3h - 2 \tag{11}
\]

Since \( T \) has the maximal first reformulated Zagreb index then by Lemmas 2.2, 2.3 and 2.4, solution of the Eq. 11 exists if and only if \( n_4 = h - 1, \ n_3 = 0 \) and \( n_2 = 1 \). Putting these values in Eq. 10, we have,

\[
EM_1(T) = 18n - 54 + \zeta_{12} - 11\zeta_{24}.
\]
Moreover,

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

But

\[
EM_1 (T) \leq 18n - 64,
\]

gives the maximum value and the equality holds if and only if \( T \) has exactly one edge of degree 1 and one vertex edge of degree 16.

**Case II.** When \( n \equiv 1 \mod (3) \).

Let \( n = 3h + 1, \) and \( h \geq 2 \). Then Eq. 9 becomes

\[
n_2 + 2n_3 + 3n_4 = 3h - 1. \tag{12}
\]

From Lemmas 2.2, 2.3 and 2.4, the solution of the Eq. 12 exists if and only if \( n_4 = h - 1, n_2 = 0 \) and \( n_3 = 1 \). In this case all \( \zeta_{ij} = 0 \), if any of \( i = 2 \) or \( j = 2 \) and \( \zeta_{33} = 0 \). So Eq. 10 reduces to,

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

Moreover,

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

Hence,

\[
EM_1 (T) \leq 18n - 66,
\]

and the equality holds if and only if degree of two edges of molecular tree are 4 and degree of one edge is 25.

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

Let \( n = 3h + 2 \), for \( h \geq 2 \), and from Eq. 9 we have \( n_2 + 2n_3 + 3n_4 = 3h \). As in previous cases the solution of the equation exists if and only if \( n_4 = h, n_3 = 0 \) 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 degree of all the edges are either 9 or 36. which completes the proof.

\[\square\]

### 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 $\Delta = 3$ and having 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 $\Delta = 3$ 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 $w_\alpha$ such that $\rho(w_\alpha) = 1$. Let $u_{\alpha 1}, u_{\alpha 2}, u_{\alpha 3}$ are neighbours of $u_\alpha$ and $w_{\alpha 1}$ is the neighbour of $w_\alpha$ in $T$. Let’s construct a new graph $T'$ as, $T' = T - u_\alpha u_{\alpha 1} + w_\alpha w_{\alpha 1}$, 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 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 are 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 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 $\Delta = 3$, and $\rho(u_\alpha) = 3$ and $\rho(w_\alpha) = 4$. Suppose that $u_\alpha$ has neighbours $u_{\alpha 1}, u_{\alpha 2}$ and $u_{\alpha 3}$ and $w_\alpha$ has neighbour $w_{\alpha 1}$. Now construct $T'$ such that $T' = T - u_\alpha u_{\alpha 1} + w_\alpha w_{\alpha 1}$, 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

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

Proof. If $\Delta = 2$, then obviously 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;
  
  i. one edge of degree four, denotes it $T_1$,
  ii. 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
i. two edges of degree nine, denotes it $T_3$,
ii. three edges of degree nine, denotes it by $T_4$.
Further, $EM_1(T_3) = 4n + 24$ and $EM_1(T_2) = 4n + 20$, 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 [24,25]. Entropy is a measure of the unavailability of a systems energy to do work. It is a measure of disorder. The greater the disorder in a molecule, the greater the entropy [26,27]. Here, 18 octane isomers [28,29], with their acentric factors and entropy measure [12,13,16] are considered, and the 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, 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.

\[
\begin{align*}
\text{Acentric factor} &= -0.0021 \times RM_1 + 0.4351 \\
\text{Entropy} &= -0.258 \times RM_1 + 117.77
\end{align*}
\]

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 shows the close relation between the acentric factor and entropy, and the reformulated Zagreb index. These results implies that the reformulated Zagreb index can be a good predictor of 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.

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5 Conclusion

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 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, like melting point, boiling point, latent heat of fusion, entropy, enthalpy, etc. of these molecular tree graphs. In the end, we presented an application of the proposed work, to calculate the acentric factor and entropy of octane isomers. Then compare the values of the first reformulated Zagreb index, acentric factor, and entropy graphically.

References


