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Edge degree Zagreb indices of certain class of trees and their application

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Abstract

The edge degree of a vertex of a graph G is defined as sum of degrees of all the edges incident to it. In this article, with respect to edge degree of a vertex, we introduce first and second Edge degree Zagreb indices of graph G and are defined as $EDZ_1 = \sum_{uv \in E(G)} \left[ed_{(u)} + ed_{(v)}\right]$ and $EDZ_2 = \sum_{uv \in E(G)} \left[ed_{(u)}\ ed_{(v)}\right]$ respectively. Later, we compute first and second edge degree Zagreb indices of well known trees such as Kragujevac trees, bistar trees and tristar trees. Further carried out linear regression analysis of first and second edge degree Zagreb indices of underlying molecular graphs of octane isomers which are trees.

Keywords: Edge degree of a vertex, Edge degree Zagreb indices, Kragujevac tree, Bistar tree, Tristar tree.

2020 MSC: 05C07, 05C92.

1. Introduction

In this article, we consider finite, connected and undirected graphs with many edges and no loops. Regarding all terms and notations that follow [14, 2].

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of edges incident to u and $\delta_G(u)$ is the sum of degrees of vertices v, where v is adjacent to u in G. Chemical graph theory is one of the branch of mathematical chemistry that greatly influences the development of the chemical sciences. A graph's topological index is a single number that characterises a feature of the graph of the underlying molecule. Numerous molecular descriptors, commonly known as topological indices[7, 8, 13], have been employed in theoretical chemistry, especially in QSPR/QSAR investigations [1, 6, 15]. The Zagreb indices $M_1(G)$ and $M_2(G)$ were introduced in 1972 by Gutman and Trinajstic [11] and are defined as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$$
$$M_2(G) = \sum_{uv \in E(G)} [d_G(u)\ d_G(v)].$$

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Current research on the Zagreb indices is provided in [3, 4, 5, 9, 10, 18, 19].

In the current work, we introduce here first Edge degree Zagreb index and second edge degree Zagreb index of graph G and defined as

$$EDZ_1(G) = \sum_{uv \in E(G)} \left[ed_{(u)} + ed_{(v)} \right]$$

$$EDZ_2(G) = \sum_{uv \in E(G)} \left[ed_{(u)} \, ed_{(v)} \right]$$

where,

$$ed_{(u)} = \sum_{e \sim u} [d_G(e)] = \sum_{uv \in E(G)} [d_G(u) + d_G(v) - 2]$$

We compute edge degree Zagreb indices of Kragujevac trees, bistar trees and tristar trees. We also derive linear regression model to check predictive potential of properties of octane isomers using first and second edge degree Zagreb indices of underlying molecular graphs of octane isomers.

A method for determining a relationship between chemical structure and physical or chemical properties is quantitative structure-property relationship (QSPR) analysis. Topological indices, molecular weight, and electro-negativity are examples of molecular descriptors, which are numerical values that describe the structure of molecules. Target properties include things like the entropy, acentric factor, and other physical or chemical characteristics.

2. Preliminaries

In the present work, we compute edge degree Zagreb indices of Kragujevac trees, bistar trees and tristar trees. We also demonstrate Edge degree Zagreb indices tress effectiveness in examining the properties of octane isomers.

Definition 2.1. A Kragujevac tree is a tree having a central vertex of degree atleast 2 to which branches of the form B_1 and (or) B_2 and (or) B_3 and (or)...and (or) B_k are attached as shown in 1. A Kragujevac tree is denoted by $Kg_{n,k}$ where $n \geqslant 2$ is the degree of the central vertex and $k \geqslant 1$ is branches attached vertex adjacent central vertex [16, 12, 2].

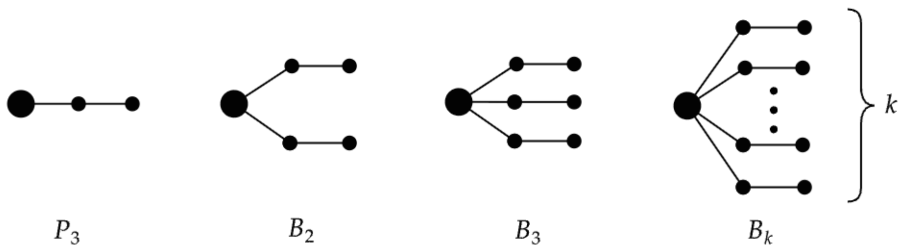

Figure 1: Branches of Kragujevac trees [2].

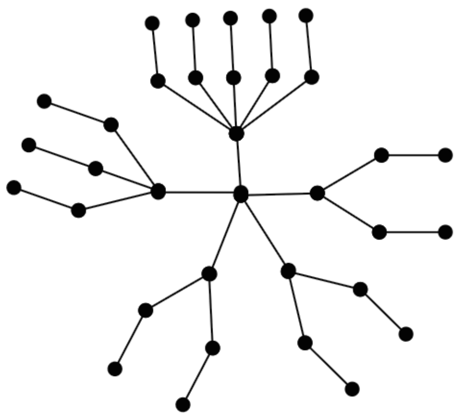

Figure 2: A Kragujevac tree ($Kg_{n,k}$) with $n = 5$ and $K = 14$ [2].

Definition 2.2. The bistar graph of two star graphs $K_{1,x}$ and $K_{1,y}$ is obtained by combining the centre nodes a and b of two star graphs $K_{1,x}$ and $K_{1,y}$ respectively by adding an edge ab as shown in figure 3.

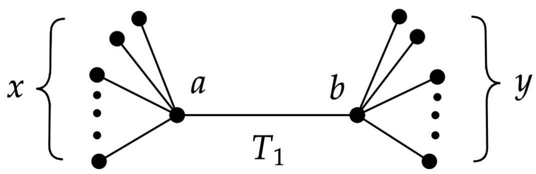

Figure 3: A bistar tree (T_1).

Definition 2.3. The tristar graph of three star graphs $K_{1,x}$, $K_{1,y}$ and $K_{1,z}$ is obtained by combining the centre nodes a,b and c of three star graphs $K_{1,x}$, $K_{1,y}$ and $K_{1,z}$ respectively by adding edges ab and bc as shown in figure 4.

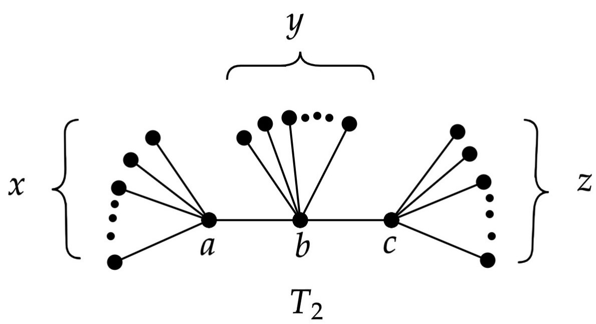

Figure 4: A tristar tree (T_2).

Lemma 2.4. for any simple connected graph G, edge degree of a vertex u is given by [17]

$$\begin{aligned} ed_{(u)} &= \sum_{uv\in E(G)} [d_G(u)+d_G(v)-2] \\ &= \sum_{u\in V(G)} [d_G(u)-2] + \sum_{v\sim u} d_G(v) \\ &= d_G(u)[d_G(u)-2]+\delta_G(u) \\ &= d_G^2(u)-2d_G(u)+\delta_G(u) \end{aligned}$$

where $\delta_G(u)$ is neighbors degree sum of a vertex u

3. Main Results

Theorem 3.1. Let Kg_{n,k_i} be a Kragujevac tree with $n \geqslant 2$ and $k_i \geqslant 1$ where $i = 1, 2, 3, ..., n$. then first edge Zagreb index and second edge Zagreb index of $Kg_{n,k}$ is given by

$$EDZ_1(Kg_{n,k}) = (6+2n)K+\sum_{i=1}^{n} k_i^3+5\sum_{i=1}^{n} k_i^2+n^3-n$$

and

$$EDZ_2(Kg_{n,k}) = \sum_{i=1}^{n} k_i^4+4\sum_{i=1}^{n} k_i^3+(n^2+K+4)\sum_{i=1}^{n} k_i^2+2K^2+(3n^2-n)K+n^4-2n^3+n^2$$

where $K=\sum_{i=1}^{n} k_i$.

Proof. The edge degree of vertex u in $Kg_{n,k}$ is, using lemma 2.4.

$$d_e(u) = \begin{cases} n^2-n+K, & \text{if } u \text{ is a central vertex of } Kg_{n,k} \\ k_i^2+2k_i+n-1, & \text{if } u \text{ is a non pendant and adjacent to central vertex} \\ k_i+2, & \text{if } u \text{ in as pendant neighbor and } u\in V(B_k) \\ 1, & \text{if } u \text{ in as pendant vertex and } u\in V(B_k) \end{cases}$$

Here, the edge set $E(Kg_{n,k})$ of a graph $Kg_{n,k}$ can be partitioned into three sets E_1, E_2, E_3, where
$E_1 = \{uv/ed_{(u)} = n^2-n+k \text{ and } ed_{(v)} = k_i^2+k_i+n-1\}$,
$E_2 = \{uv/ed_{(u)} = k_i^2+k_i+n-1 \text{ and } ed_{(v)} = k_i+2\}$ and $E_3 = \{uv/ed_{(u)} = k_i+2 \text{ and } ed_{(v)} = 1\}$.
It is easy to check that $|E_1|$=n, $|E_2|$=K, $|E_3|$=K.

Therefore,

$$\begin{aligned} EDZ_1(Kg_{n,k}) &= \sum_{uv\in E(Kg_{n,k})} [ed_{(u)}+ed_{(v)}] \\ &= \sum_{uv\in E_1(Kg_{n,k})} [ed_{(u)}+ed_{(v)}] + \sum_{uv\in E_2(Kg_{n,k})} [ed_{(u)}+ed_{(v)}] \\ &\quad + \sum_{uv\in E_3(Kg_{n,k})} [ed_{(u)}+ed_{(v)}] \\ &= \sum_{uv\in E_1(Kg_{n,k})} [n^2-n+K+k_i^2+2k_i+n-1] + \sum_{uv\in E_2(Kg_{n,k})} [k_i^2+2k_i+n-1+k_i+2] \\ &\quad + \sum_{uv\in E_3(Kg_{n,k})} [k_i+2+1] \end{aligned}$$

$$\begin{aligned}
EDZ_1(Kg_{n,k}) &= \sum_{i=1}^{n}(n^2+K+k_i^2+2k_i-1)+\sum_{i=1}^{n}(k_i^2+3k_i+n+1)k_i+\sum_{i=1}^{n}(k_i+3)k_i\\
&= \sum_{i=1}^{n}(K+k_i^3+5k_i^2+(6+n)k_i+n^2-1)\\
&= (6+2n)K+\sum_{i=1}^{n}k_i^3+5\sum_{i=1}^{n}k_i^2+n^3-n.
\end{aligned}$$

and

$$\begin{aligned}
EDZ_2(Kg_{n,k}) &= \sum_{uv\in E(Kg_{n,k})}[ed_{(u)}\ ed_{(v)}]\\
&= \sum_{uv\in E_1(Kg_{n,k})}[ed_{(u)}\ ed_{(v)}]+\sum_{uv\in E_2(Kg_{n,k})}[ed_{(u)}\ ed_{(v)}]\\
&\quad+\sum_{uv\in E_3(Kg_{n,k})}[d_e(u)\ d_e(v)]\\
&= \sum_{uv\in E_1(Kg_{n,k})}(n^2-n+K)\ (k_i^2+2k_i+n-1)\\
&\quad+\sum_{uv\in E_2(Kg_{n,k})}(k_i^2+2k_i+n-1)\ (k_i+2)\\
&\quad+\sum_{uv\in E_3(Kg_{n,k})}(k_i+2)\ (1)\\
&= \sum_{i=1}^{n}(n^2k_i^2+2n^2k_i+n^3-n^2-nk_i^2-2nk_i-n^2+n+Kk_i^2+2Kk_i+nK-K)\\
&\quad+\sum_{i=1}^{n}(k_i^3+2k_i^2+nk_i-k_i+2k_i^2+4k_i+2n-2)k_i+\sum_{i=1}^{n}(k_i+2)k_i\\
&= \sum_{i=1}^{n}(k_i^4+4k_i^3+(n^2+K+4)k_i^2+(2n^2+2K)k_i+n^3-2n^2+nK+n-K\\
&= \sum_{i=1}^{n}k_i^4+4\sum_{i=1}^{n}k_i^3+(n^2+K+4)\sum_{i=1}^{n}k_i^2+2K^2+(3n^2-n)K+n^4-2n^3+n^2.
\end{aligned}$$

□

Theorem 3.2. Let T_1 be bistar tree with n vertices as shown in figure 3. Then

$$\begin{aligned}
EDZ_1(T_1) &= x^2+y^2+2(x+y)+x(x^2+2x+y)+(n-x-2)(y^2+2y+x)\\
&\text{and}\\
EDZ_2(T_1) &= x^3+y^3+x^2y^2+x^2+y^2+xy(x+y+2)+x(x^3+x^2+xy)\\
&\quad+(n-x-2)(y^3+y^2+xy)
\end{aligned}$$

where n = x+y+2.

Proof. Take into consideration the vertices a, b as displayed in figure 3 without losing generality, edge degree of vertices a, b, x and y are $ed_{(a)}=x^2+x+y$, $ed_{(b)}=y^2+y+x$, $ed_{(x)}=x$ and $ed_{(y)}=y$ using lemma 2.4. Partition the edge set $E(T_1)$ into three subsets E_1 ,E_2 and E_3. such that,
$E_1=\{uv/ed_{(u)}=x^2+x+y \text{ and } ed_{(v)}=y^2+y+x\}$,
$E_2=\{uv/ed_{(u)}=x \text{ and } ed_{(v)}=x^2+x+y\}$, $E_3=\{uv/ed_{(u)}=y \text{ and } ed_{(v)}=y^2+y+x\}$.

It is easy to check that $|E_1|=1$, $|E_2|=x$, $|E_3|=n-x-2$.
Therefore,

$$\begin{aligned}
EDZ_1(T_1) &= \sum_{uv\in E(T_1)} [ed_{(u)} + ed_{(v)}] \\
&= \sum_{uv\in E_1(T_1)} [ed_{(u)} + ed_{(v)}] + \sum_{uv\in E_2(T_1)} [ed_{(u)} + ed_{(v)}] + \sum_{uv\in E_3(T_1)} [ed_{(u)} + ed_{(v)}] \\
&= \sum_{uv\in E_1(T_1)} [(x^2+x+y) + (y^2+y+x)] + \sum_{uv\in E_2(T_1)} [(x) + (x^2+x+y)] \\
&\quad + \sum_{uv\in E_3(T_1)} [(y) + (y^2+y+x)] \\
&= x^2+y^2+2(x+y)+x(x^2+2x+y)+(n-x-2)(y^2+2y+x).
\end{aligned}$$

and

$$\begin{aligned}
EDZ_2(T_1) &= \sum_{uv\in E(T_1)} [ed_{(u)}\ ed_{(v)}] \\
&= \sum_{uv\in E_1(T_1)} [ed_{(u)}\ ed_{(v)}] + \sum_{uv\in E_2(T_1)} [ed_{(u)}\ ed_{(v)}] + \sum_{uv\in E_3(T_1)} [ed_{(u)}\ ed_{(v)}] \\
&= \sum_{uv\in E_1(T_1)} [(x^2+x+y)\ (y^2+y+x)] + \sum_{uv\in E_2(T_1)} [(x)\ (x^2+x+y)] \\
&\quad + \sum_{uv\in E_3(T_1)} [(y)\ (y^2+y+x)] \\
&= x^3+y^3+x^2y^2+x^2+y^2+xy(x+y+2)+x(x^3+x^2+xy)+(n-x-2)(y^3+y^2+xy).
\end{aligned}$$

□

Theorem 3.3. Let T_2 be tristar tree with n vertices as shown in figure 4. Then,

$$\begin{aligned}
EDZ_1(T_2) &= x^2+2y^2+z^2+3x+8y+3z+6+x(x^2+2x+y+1) \\
&\quad +y(y^2+4y+x+z+3)+z(z^2+2z+y+1) \\
&\text{and} \\
EDZ_2(T_2) &= x^3+2y^3+z^3+x^2(y^2+3y+z+3)+y^2(z^2+z+x+8)+z^2(x+3y+3) \\
&\quad +5xy+5yz+2xz+4x+10y+4z+4+x(x^3+x^2+xy+x) \\
&\quad +y(y^3+4y^2+xy+yz+x+5y+z+2)+z(z^3+z^2+zy+z)
\end{aligned}$$

where n = x+y+z+3.

Proof. By observation the vertices a, b and c as displayed in figure 4 without losing generality, where edge degree of vertices a, b, c, x, y and z are $ed_{(a)} = x^2+x+y+1$, $ed_{(b)} = y^2+3y+x+z+2$, $ed_{(c)} = z^2+z+y+1$, $ed_{(x)} = x$, $ed_{(y)} = y+1$ and $ed_{(z)} = z$ using lemma 2.4.
Partition the edge set $E(T_2)$ into five subsets E_1 ,E_2, E_3, E_4 and E_5.
such that,
$E_1 = \{uv/ed_{(u)} = x^2+x+y+1 \text{ and } ed_{(v)} = y^2+3y+x+z+2\}$,
$E_2 = \{uv/ed_{(u)} = y^2+3y+x+z+2 \text{ and } ed_{(v)} = z^2+z+y+1\}$,
$E_3 = \{uv/ed_{(u)} = x \text{ and } ed_{(v)} = x^2+x+y+1\}$,
$E_4 = \{uv/ed_{(u)} = y+1 \text{ and } ed_{(v)} = y^2+3y+x+z+2\}$,
$E_5 = \{uv/ed_{(u)} = z \text{ and } ed_{(v)} = z^2+z+y+1\}$.

It is easy to check that $|E_1|=1$, $|E_2|=1$, $|E_3|=x$, $|E_4|=y$, $|E_5|=z$.
Therefore,

$$\begin{aligned}
EDZ_1(T_2) &= \sum_{uv\in E(T_2)} [ed_{(u)} + ed_{(v)}] \\
&= \sum_{uv\in E_1(T_2)} [ed_{(u)} + ed_{(v)}] + \sum_{uv\in E_2(T_2)} [ed_{(u)} + ed_{(v)}] \\
&\quad + \sum_{uv\in E_3(T_2)} [ed_{(u)} + ed_{(v)}] + \sum_{uv\in E_4(T_2)} [ed_{(u)} + ed_{(v)}] \\
&\quad + \sum_{uv\in E_5(T_2)} [ed_{(u)} + ed_{(v)}] \\
&= \sum_{uv\in E_1(T_2)} [(x^2+x+y+1)+(y^2+3y+x+z+2)] \\
&\quad + \sum_{uv\in E_2(T_2)} [(y^2+3y+x+z+2)+(z^2+z+y+1)] \\
&\quad + \sum_{uv\in E_3(T_2)} [(x)+(x^2+x+y+1)] + \sum_{uv\in E_4(T_2)} [(y+1)+(y^2+3y+x+z+2)] \\
&\quad + \sum_{uv\in E_5(T_2)} [(z)+(z^2+z+y+1)] \\
&= x^2+2y^2+z^2+3x+8y+3z+6+x(x^2+2x+y+1)+y(y^2+4y+x+z+3) \\
&\quad +z(z^2+2z+y+1).
\end{aligned}$$

and

$$\begin{aligned}
EDZ_2(T_2) &= \sum_{uv\in E(T_2)} [ed_{(u)}\ ed_{(v)}] \\
&= \sum_{uv\in E_1(T_2)} [ed_{(u)}\ ed_{(v)}] + \sum_{uv\in E_2(T_2)} [ed_{(u)}\ ed_{(v)}] + \sum_{uv\in E_3(T_2)} [ed_{(u)}\ ed_{(v)}] \\
&\quad + \sum_{uv\in E_4(T_2)} [ed_{(u)}\ ed_{(v)}] + \sum_{uv\in E_5(T_2)} [ed_{(u)}\ ed_{(v)}]
\end{aligned}$$

$$\begin{aligned}
EDZ_2(T_2) &= \sum_{uv\in E_1(T_2)} [(x^2+x+y+1)\ (y^2+3y+x+z+2)] \\
&\quad + \sum_{uv\in E_2(T_2)} [(y^2+3y+x+z+2)\ (z^2+z+y+1)] \\
&\quad + \sum_{uv\in E_3(T_2)} [(x)\ (x^2+x+y+1)] + \sum_{uv\in E_4(T_2)} [(y+1)\ (y^2+3y+x+z+2)] \\
&\quad + \sum_{uv\in E_5(T_2)} [(z)\ (z^2+z+y+1)] \\
&= x^3+2y^3+z^3+x^2(y^2+3y+z+3)+y^2(z^2+z+x+8)+z^2(x+3y+3) \\
&\quad +5xy+5yz+2xz+4x+10y+4z+4+x(x^3+x^2+xy+x) \\
&\quad +y(y^3+4y^2+xy+yz+x+5y+z+2)+z(z^3+z^2+zy+z).
\end{aligned}$$

□

4. Linear Regression Analysis

We investigate the predictive potential of a physicochemical properties of octane isomers with respect to first Edge degree Zagreb index ($EDZ_1(G)$) and second Edge degree Zagreb index ($EDZ_2(G)$) using a data set of 18 octane isomers. Numeric Values of First and second Edge degree Zagreb indices of octane isomers and the experimental data of physicochemical properties of octane isomers are shown in Table 1. We studied the following linear regression models

$$Y = mX + B \tag{4.1}$$

where Y, X, B, and m stands for physico-chemical property, topological index, intercept, and slope. The linear regression models for Acentric factor and Entropy of octane isomers using the data of Table 1 obtained by the least square fitting procedure as shown in Eqs.(4.2) to Eqs.(4.5).

$$AcentFac = 0.4600(\pm 0.005870) - 0.001525(\pm 6.953 \times 10^{-}5)EDZ_1 \tag{4.2}$$
$$AcentFac = 0.4092(\pm 0.004309) - 0.0003352(\pm 1.787 \times 10^{-}5)EDZ_2 \tag{4.3}$$
$$Entropy = 120.9(\pm 1.161) - 0.1898(\pm 0.01375)EDZ_1 \tag{4.4}$$
$$Entropy = 114.6(\pm 0.770) - 0.04174(\pm 0.003222)EDZ_2 \tag{4.5}$$

Regression analysis was carried out using data analysis techniques in Microsoft Excel. Scatter plots showing the correlations between $EDZ_1(G)$ and $EDZ_2(G)$ of the corresponding molecular graphs of 18 octane isomers and their Acentric factor and Entropy are shown in figure 5 to figure 8. From Table 2, we observe that all models from Eqs.(4.2) to Eqs.(4.5) gives a good correlation of Acentric factor and Entropy of octane isomers with $EDZ_1(G)$ and $EDZ_2(G)$.

Table 1: Acentric factor, Entropy, EDZ_1 and EDZ_2 of Octane isomers

SI No.	Octane isomers	AcentFac(ω)	Entropy($Cal/mol.K$)	EDZ_1	EDZ_2
1	n-octane	0.3979	111.67	46	78
2	2-mthylheptane	0.3779	109.84	58	114
3	3-methylheptane	0.371	111.26	60	127
4	4-methylheptane	0.3715	109.32	56	113
5	3-ethylhexane	0.3625	109.43	62	143
6	2,2-dimethylhexane	0.3394	103.42	88	234
7	2,3-dimethylhexane	0.3482	108.02	74	185
8	2,4-dimethylhexane	0.3442	106.98	72	170
9	2,5-dimethylhexane	0.3568	105.72	70	141
10	3,3-dimethylhexane	0.3226	104.72	92	264
11	3,4-dimethylhexane	0.3403	106.59	76	197
12	3-ethyl, 2-methylhexane	0.3324	106.06	76	200
13	3-ethyl, 3-methylhexane	0.3069	101.48	96	285
14	2,2,3-trimethylpentane	0.3008	101.31	106	330
15	2,2,4-trimethylpentane	0.3054	104.09	100	285
16	2,3,3-trimethylpentane	0.2932	102.06	108	341
17	2,3,4-trimethylpentane	0.3174	102.39	88	244
18	2,2,3,3-tetramethylbutane	0.2553	93.06	138	495

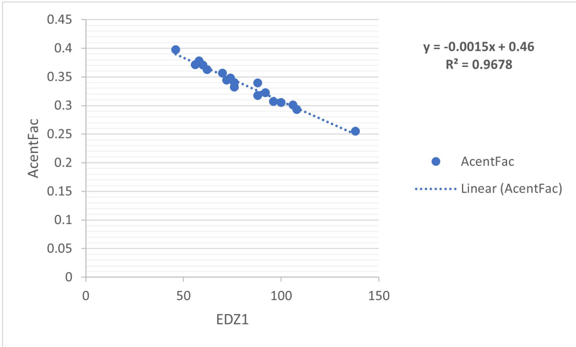

Figure 5: Scatter plot between the AcentFac and EDZ_1 of octane isomers.

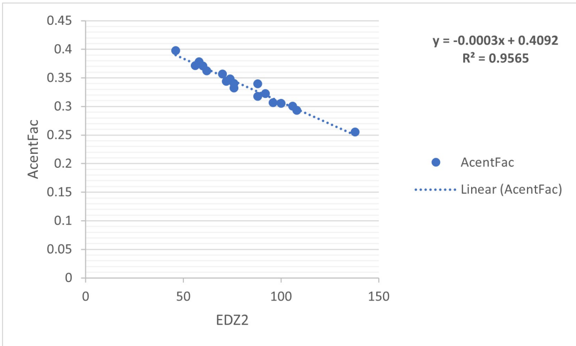

Figure 6: Scatter plot between the AcentFac and EDZ_2 of octane isomers.

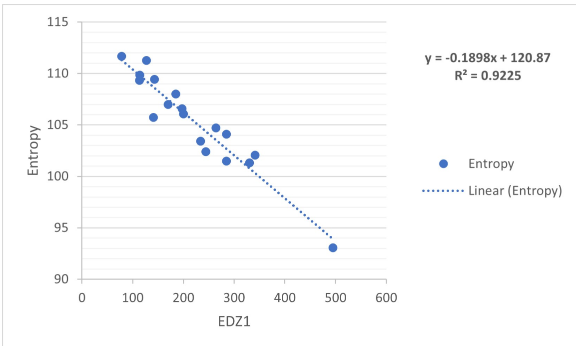

Figure 7: Scatter plot between the Entropy and EDZ_1 of octane isomers.

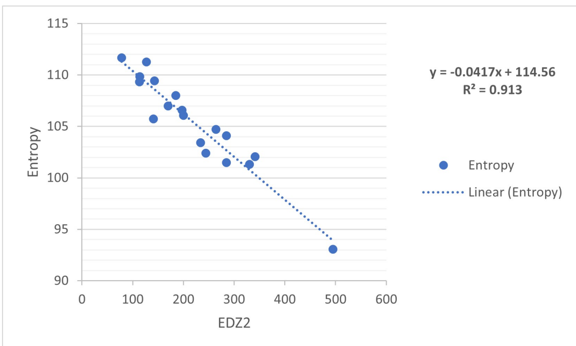

Figure 8: Scatter plot between the Entropy and EDZ_2 of octane isomers.

Table 2: Correlation coefficient (R) between EDZ_1 and EDZ_2 and physical properties of Octane isomers

Index	AcentFac	Entropy
EDZ_1	0.9837	0.9604
EDZ_2	0.9780	0.9555

5. Conclusion

We have introduced degree based topological index $EDZ_1(G)$ and $EDZ_2(G)$ and obtained explicit formula for Kragujevac tree, binary tree and tristar tree. Also carried out Linear regression analysis of edge degree Zagreb indices with Acentric factors and entropy of octane isomers. Edge degree Zagreb indices have good correlation to predicting physical properties of octane isomers as shown in table 2.

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