On New Variance of Zagreb Indices

Hanumantha Reddy D T and M V Chakradhara Rao

***Abstract*—In QSPR studies topological indices plays vital role. To enrich this field we put forward novel topological indices namely Mass Zagreb indices. In this paper first we study the mathematical properties of new variance of Zagreb indices then followed by its chemical applications in QSPR studies.**

***Index Terms*—first mass Zagreb index; second mass Zagreb index; QSPR-analysis.**

I. Introduction

A graph is said to be simple if it doesn't contain multiple edges or loops. Throughout this paper simple and undirected graphs are considered with vertex set V and edge set E. The order and size of G is denoted by $|V| = n$ and $|E| = m$ respectively. The degree of a vertex $v \in V$ is the number of edges incident to v and it is denoted by $d_G(v)$. The degree of an edge $e = uv$ is defined as $d_G(e) = d_G(u) + d_G(v) - 2$. For undefined terminology in this paper refer [5].

The topological index is just a number related to the molecular network. Many researchers have proposed a huge number of such values dating back to 1972 [2]. Prof. Gutman (Personal Communication) defines a relevant topological index as one that has a high predictive potential in QSPR investigations. As a result, topological indices can be divided into two categories: useful and not so useful TI's see [3], [4], [6], [7], [13], [15]. Zagreb indices are one of the most valuable topological indices, and they are defined as:

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_G(v)^2 \\ M_2(G) &= \sum_{uv \in E(G)} d_G(u) d_G(v) \end{aligned}$$

where M_1 and M_2 are the first and second Zagreb indices respectively.

In response to the Zagreb indices, we propose the Mass version of the first and second Zagreb indices. To begin, we must define the vertex and edge Mass of a graph G as follows:

Vertex Mass: Let $w_1, w_2, w_3 \cdots, w_n$ be the Mass of the vertices $v_1, v_2, v_3, \cdots, v_n$ such that $w_1 = d_G(v_1)$, $w_2 = d_G(v_2)$, $w_3 = d_G(v_3)$, $\cdots$, $w_n = d_G(v_n)$.

Edge Mass: Let $e_1, e_2, e_3, \cdots, e_m$ be the edges of a graph G. Then the edge Mass of $e = uv \in E(G)$ is defined as $w(e) = d_G(u) + d_G(v) - 2$.

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Mass Degree of a Vertex: The Mass degree of a vertex $v \in V(G)$ is defined as:

$$d_G^w(v) = \sum_{e=uv} w(e)$$

The maximum mass degree and minimum mass degree of a vertex $v \in V(G)$ is denoted by $\Delta_w(v)$ and $\delta_w(v)$ respectively.

II. Mass Zagreb Indices

The first Mass Zagreb index $Z_1^m(G)$ is defined as

$$Z_1^m(G) = \sum_{v \in V} d_G^w(v)^2 \quad (1)$$

The second Mass Zagreb index $Z_2^m(G)$ is defined as

$$Z_2^m(G) = \sum_{e=uv \in E} d_G^w(u) \cdot d_G^w(v) \quad (2)$$

Example 1: Consider the following graph G, with $V(G) = \{v_1, v_2, v_3, v_4, v_5\}$ and the edge set $E(G) = \{e_1, e_2, e_3, e_4, e_5\}$. Then clearly the Mass of vertices and edges are given by their corresponding degrees. Therefore, the Mass degree of each vertex is given by:

$$\begin{aligned} d_G^w(v_1) &= w(e_1) + w(e_2) = 2 + 3 = 5 \\ d_G^w(v_2) &= w(e_2) + w(e_4) = 2 + 2 = 4 \\ d_G^w(v_3) &= w(e_3) + w(e_4) = 3 + 2 = 5 \\ d_G^w(v_4) &= w(e_1) + w(e_3) + w(e_5) = 3 + 3 + 2 = 8 \\ d_G^w(v_5) &= w(e_5) = 2 = 2 \end{aligned}$$

Hence the first Mass Zagreb index $Z_1^m(G)$ of G is

$$\begin{aligned} Z_1^m(G) &= \sum_{v \in V} d_G^w(v)^2 \\ &= d_G^w(v_1)^2 + d_G^w(v_2)^2 + d_G^w(v_3)^2 \\ &+ d_G^w(v_4)^2 + d_G^w(v_5)^2 \\ &= 5^2 + 4^2 + 5^2 + 8^2 + 2^2 \\ &= 134. \end{aligned}$$

Observe that the first Zagreb index of G is

$$\begin{aligned} M_1(G) &= \sum_{v \in V} d_G(v)^2 \\ &= d_G(v_1)^2 + d_G(v_2)^2 + d_G(v_3)^2 \\ &+ d_G(v_4)^2 + d_G(v_5)^2 \\ &= 2^2 + 2^2 + 2^2 + 3^2 + 1^2 \\ &= 22. \end{aligned}$$

As a result, for any non-trivial graphs with at least three vertices, the values of the Mass first Zagreb index and the first Zagreb index differ dramatically. As a result, QSPR investigations of the Mass first Zagreb index will demonstrate the utility of this new parameter.

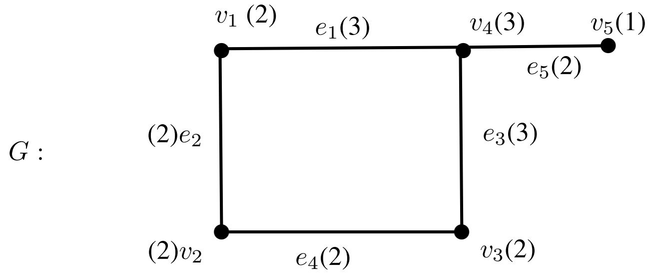


Figure 1. A graph on five vertices.

Proposition 1: $Z_1^w(K_n) = n[(n-1)(2n-4)]^2$ where ; $n \geq 2$.

Proof: Let $G = K_n; ngeq2$ represent the full graph with n vertices. Because $delta(G) = delta(G) = n-1$. As a result, the mass of an edge $einG$ is $2n-4$. As a result, using this information in (1) yields the desired result. ■

Proposition 2: $Z_1^w(C_n) = 16n$ where ; $n \geq 3$.

Proof: The proof stems from the fact that $G = C_n; n \geq 3$ is a two-regular graph with a mass of two edges. ■

Proposition 3: $Z_1^m(P_n) = 8n - 12$ where ; $n \geq 2$.

Proof: Let $G = P_n; n \geq 2$ represent a path of order n. Let v_1 and v_n represent the beginning and terminal vertices of G. Then $w(e_1) = w(e_n) = 1$ and $w(e_i); 2 \leq ileqm-1 = 2$ are obvious. Using this information in (1) yields the desired result. ■

Proposition 4: $Z_1^m(W_n) = n^2(n-1)^2 + 144(n-1)$ where ; $n \geq 4$.

Proof: Let $G = W_n; n \geq 4$ be an order n wheel. Let v_1 represent its central vertex. since $deg(v_1) = n-1$ and $deg(v_i); 2 \leq i = 3$. As a result, the mass of each edge may be divided into two groups, with $n-1$ edges having $w(e_i) = 3$ and the remaining $n-1$ edges having $w(e_i) = 4$. As a result, using (1) yields the desired outcome. ■

Proposition 5: For any $k-$regular graph $k \geq 1$ G,

$$Z_1^m(G) = 4nk^2(k-1)^2$$

Proof: Assume G is a $k-$regular graph with $k \geq 1$. The proof is then derived from the fact that the mass of each edge in G equals $2k-2$. ■

Observation 6: Let G be a with edge Mass $w_1, w_2, w_3, \cdots, w_m$. Then the following holds good:

$$\sum_{v \in V} d_G^w(v) = 2[M_1(G) - 2m]. \tag{3}$$

III. Bounds for $Z_1^m(G)$

We employed the mathematical inequalities from [1], [8]–[10], [12], [14] to get constraints for the first Mass Zagreb index.

Theorem 7: Let G be a simple connected graph with n vertices and m edges. Then

$$Z_1^m(G) \geq \frac{4M_1^2(G) - 16m(M_1(G)) + 16m^2}{n}$$

Proof: Let $v_1, v_2, v_3, \cdots, v_n$ be the vertices of a simple graph G with mass $w(v_1), w(v_2), w(v_3), \cdots, w(v_n)$. Let $deg_w(v_1), deg_w(v_2), deg_w(v_3), \cdots, deg_w(v_n)$ be the corresponding mass vertex degrees of G. Allow $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ to be non-negative integers. Then bythe Cauchy-Schrwz inequality. we have

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right) \cdot \left(\sum_{i=1}^{n} b_i^2\right) \tag{4}$$

by setting $a_i = deg_w(v_i)$ and $b_i = 1$ we have

$$\left(\sum_{i=1}^{n} deg_w(v_i) \cdot 1\right)^2 \leq \left(\sum_{i=1}^{n} deg_w(v_i)^2\right) \cdot \left(\sum_{i=1}^{n} 1^2\right)$$

By Observation 6, we have

$$\sum_{v \in V} d_G^w(v) = 2[M_1(G) - 2m].$$

Therefore,

$$\left(2[M_1(G) - 2m]\right)^2 \leq \left(Z_1^m(G)\right) \cdot \left(n\right)$$

Thus,

$$Z_1^m(G) \geq \frac{4M_1^2(G) - 16m(M_1(G)) + 16m^2}{n}$$

as asserted. ■

The equivalent bound is obtained by using the following inequalities:

Lemma 8: Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then

$$\sum_{i=1}^{n} a_i^r \geq n^{1-r}\left(\sum_{i=1}^{n} b_i\right)^r \tag{5}$$

Lemma 9: Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then

$$\sum_{i=1}^{n} \frac{a_i^{r+1}}{b_i^r} \geq \frac{\left(\sum\limits_{i=1}^{n} a_i\right)^{r+1}}{\left(\sum\limits_{i=1}^{n} b_i\right)^r} \tag{6}$$

Lemma 10: Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then

$$\left(\sum_{i=1}^{n} b_i\right)^{\alpha-1}\left(\sum_{i=1}^{n} b_i a_i^{\alpha}\right) \geq \left(\sum_{i=1}^{n} a_i b_i\right)^{\alpha} \tag{7}$$

where α is any positive integer.

Corollary 11: Let G be a simple connected graph with n vertices and m edges. Then by setting $a_i = deg_w(v_i)$ and $r = 2$ in (6) we get

$$Z_1^m(G) \geq \frac{4M_1^2(G) - 16m(M_1(G)) + 16m^2}{n}$$

Corollary 12: Let G be a simple connected graph with n vertices and m edges. Then by setting $a_i = deg_w(v_i)$, $b_i = 1$ and $r = 1$ in (7) we get

$$Z_1^m(G) \geq \frac{4M_1^2(G) - 16m(M_1(G)) + 16m^2}{n}$$

Corollary 13: Let G be a simple connected graph with n vertices and m edges. Then by setting $a_i = deg_w(v_i)$, $b_i = 1$ and $\alpha = 2$ in (7) we get

$$Z_1^m(G) \geq \frac{4M_1^2(G) - 16m(M_1(G)) + 16m^2}{n}$$

Theorem 14: Let G be a simple connected graph with n vertices and m edges with maximum(minimum) Mass degree $\Delta_w(\delta_w)$. Then

$$Z_1^m(G) \geq \frac{\alpha(n)(\Delta_w - \delta_w)^2 + (2M_1(G) - 4m)^2}{n}$$

where $\alpha(n) = n\lfloor \frac{n}{2} \rfloor (1 - \frac{1}{n}\lfloor \frac{n}{2} \rfloor)$. where $\lfloor x \rfloor$ smallest integer less than or equal to x.

Proof: Let $v_1, v_2, v_3, \cdots, v_n$ be the vertices of a simple graph G with Mass $w(v_1), w(v_2), w(v_3), \cdots, w(v_n)$. Let $deg_w(v_1), deg_w(v_2), deg_w(v_3), \cdots, deg_w(v_n)$ be the corresponding Mass vertex degrees of the vertices of G. Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \cdots, n, a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then the following inequality is valid

$$| \, n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \, | \leq \alpha(n)(A - a)(B - b) \quad (8)$$

We choose $a_i = deg_w(v_i) = b_i$, $A = \Delta_w = B$ and $a = \delta_w = b$, inequality (9), becomes

$$\begin{aligned} n\sum_{i=1}^{n} deg_w(v_i)^2 - \left(\sum_{i=1}^{n} deg_w(v_i)\right)^2 &\leq \alpha(n)(\Delta_w - \delta_w) \\ &\quad (\Delta_w - \delta_w) \\ nZ_1^w &\leq \alpha(n)(\Delta_w - \delta_w)^2 \\ &+ (2M_1(G) - 4m)^2 \end{aligned}$$

Thus,

$$Z_1^m(G) \geq \frac{\alpha(n)(\Delta_w - \delta_w)^2 + (2M_1(G) - 4m)^2}{n}$$

■

Theorem 15: Let G be a nontrivial graph of order n and size m. Then

$$Z_1^m(G) \leq (\delta_w + \Delta_w)(2M_1(G) - 4m) - \delta_w \Delta_w.$$

Proof: Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants r and R so that for each i, $i = 1, 2, \cdots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid.

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r + R)\sum_{i=1}^{n} a_i b_i. \quad (9)$$

We choose $b_i = deg_w(v_i)$, $a_i = 1$, $r = \delta_w$ and $R = \Delta_w$ in inequality (10), then

$$\begin{aligned} \sum_{i=1}^{n} deg_w(v_i)^2 + \delta_w \Delta_w \sum_{i=1}^{n} 1 &\leq (\delta_w + \Delta_w)\sum_{i=1}^{n} deg_w(v_i) \\ Z_1^m(G) + \delta_w \Delta_w n &\leq (\delta_w + \Delta_w) \\ &\quad (2M_1(G) - 4m) \\ Z_1^m(G) &\leq (\delta_w + \Delta_w) \\ &\quad (2M_1(G) - 4m) - \delta_w \Delta_w \end{aligned}$$

as desired. ■

IV. Applications of Mass first Zagreb Index in QSPR Studies

We chose a range of alkanes ranging from n-butanes to nonanes for chemical applications of the first mass Zagreb index. We used eight representative physical parameters for modeling: boiling points (BP), molar volumes (mv) at $20circ$C, molar refractions (mr) at 20○C, heats of vaporization (hv) at 25○C, surface tensions (st) at 20○C, and melting points (mp). The values for these properties were derived from Dejan Plavsi$acutec$ et. al [13].

V. Mass First Zagreb index $Z_1^m(G)$

1) Linear Model

$$\begin{aligned} bp &= 2.194 + [Z_1^m(G)]2.582 \\ mv &= 107.696 + [Z_1^m(G)]2.806 \\ mr &= 21.911 + [Z_1^m(G)]1.556 \\ hv &= 24.808 + [Z_1^m(G)]1.505 \\ ct &= 144.038 + [Z_1^m(G)]3.713 \\ cp &= 33.082 - [Z_1^m(G)]1.248 \\ st &= 16.125 + [Z_1^m(G)]1.198 \\ mp &= -146.169 + [Z_1^m(G)]2.462 \end{aligned}$$

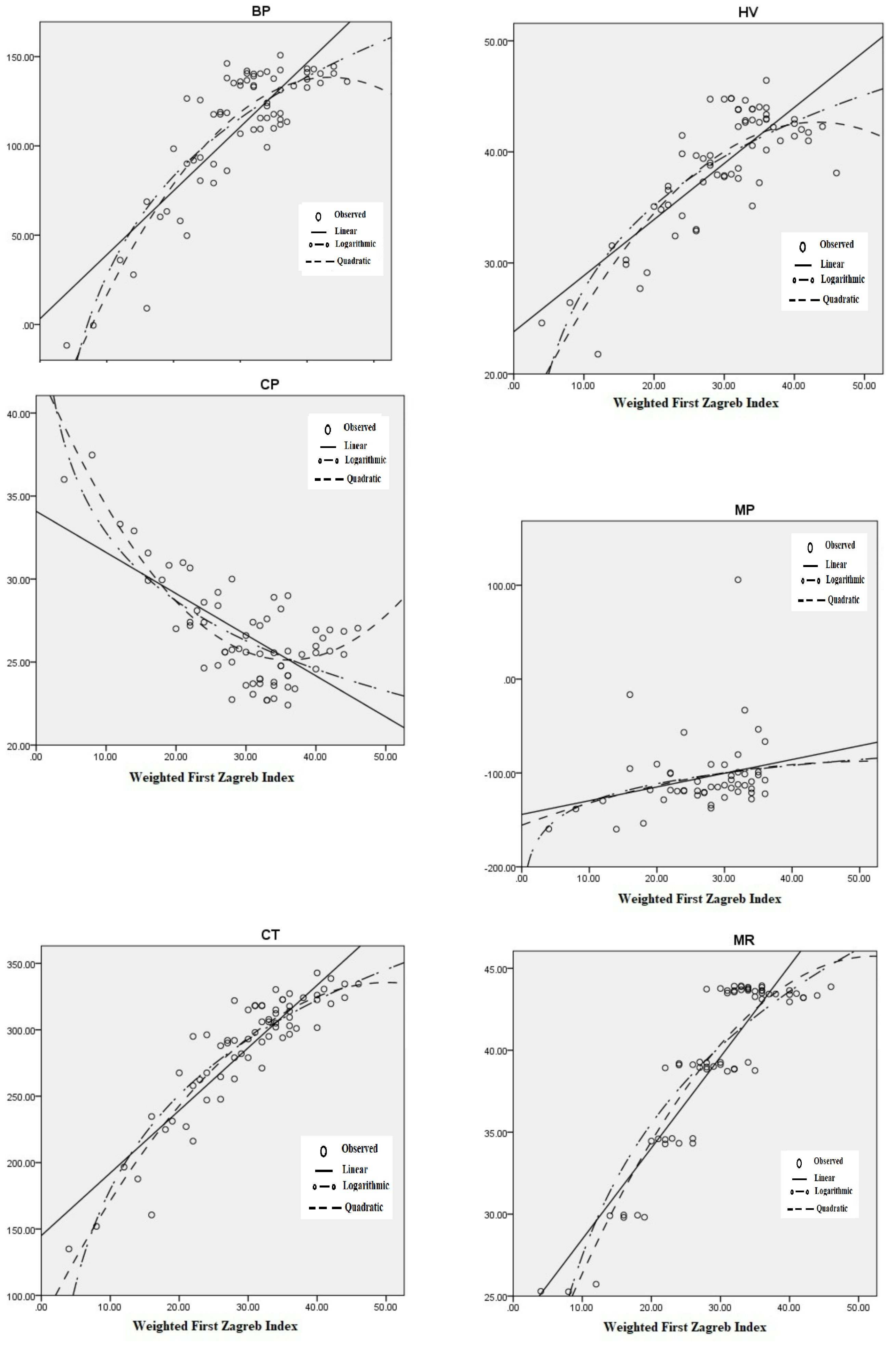
2) Quadratic Model

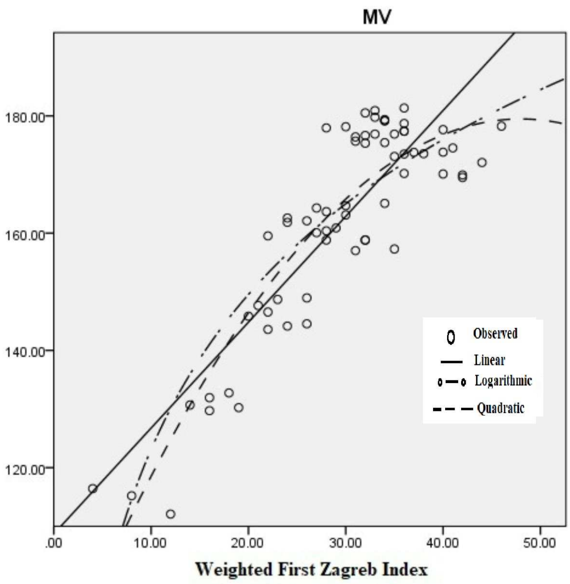
$$\begin{aligned} bp &= 8.5[Z_1^m(G)]^2 - 0.12[Z_1^m(G)] - 65.6 \\ mv &= 3.6[Z_1^m(G)]^2 - 0.42[Z_1^m(G)] + 81.2 \\ mr &= 2.1[Z_1^m(G)]^2 - 0.21[Z_1^m(G)] + 15.1 \\ hv &= 3.3[Z_1^m(G)]^2 - 0.15[Z_1^m(G)] + 13.2 \\ ct &= 9.1[Z_1^m(G)]^2 - 0.10[Z_1^m(G)] + 78.4 \\ cp &= -1.9[Z_1^m(G)]^2 + 0.14[Z_1^m(G)] + 41.9 \\ st &= 1.3[Z_1^m(G)]^2 - 0.3[Z_1^m(G)] + 12.4 \\ mp &= 3.6[Z_1^m(G)]^2 - 0.35[Z_1^m(G)] - 154.6 \end{aligned}$$

3) Logarithmic Model

$$\begin{aligned} bp &= -154.5 + \ln[Z_1^m(G)]81.3 \\ mv &= 34.3 + \ln[Z_1^m(G)]37.1 \\ mr &= 0.7 + \ln[Z_1^m(G)]12.6 \\ hv &= 22.8 + \ln[Z_1^m(G)]0.5 \\ ct &= -56.1 + \ln[Z_1^m(G)]101.8 \\ cp &= 44.4 - \ln[Z_1^m(G)]6.9 \\ st &= 8.2 + \ln[Z_1^m(G)]5.1 \\ mp &= -191.7 + \ln[Z_1^m(G)]27.1 \end{aligned}$$

The correlation of the first mass Zagreb index with the above-mentioned physical qualities of alkanes is depicted in the figures below:


BP
HV
CP
MP
CT
MR
Observed
Linear
Logarithmic
Quadratic
Weighted First Zagreb Index



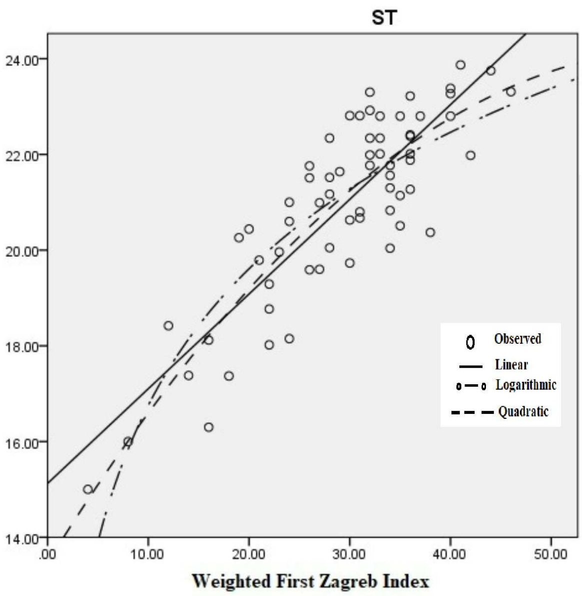


Figure2. The correlation of the first mass Zagreb index with the above-mentioned physical qualities of alkanes.

Table 2: Model summary for the boiling point of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.894	63.73	0.000
Logarithmic	0.753	93.65	0.000
Quadratic	0.771	51.72	0.000

According to the correlation coefficient value $r = 0.894$ for the linear model in Table 2, the prediction power of the mass first Zagreb index is good in predicting boiling points. In other words, our results indicate an accuracy of 89.4 percent in forecasting the boiling points of alkanes.

Table 3: Model summary for the critical pressure of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.819	41.96	0.000
Logarithmic	0.53	13.44	0.001
Quadratic	0.711	31.23	0.000

The correlation coefficient value $r = 0.819$ for the linear model in Table 3 reveals that the Mass first Zagreb index has strong predictive capacity in predicting the critical pressure of alkanes. In other words, our results indicate an 81.9% accuracy in forecasting the critical pressure of alkanes.

Table 4: Model summary for the critical temperature of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.059	0.83	0.456
Logarithmic	0.248	3.713	0.112
Quadratic	0.79	32.98	0.000

The correlation coefficient value $r = 0.79$ for the quadratic model in Table 4 demonstrated that the Mass first Zagreb index has strong predictive capacity in predicting the critical temperature of alkanes. In other words, our results indicate a 79% accuracy in forecasting the critical temperature of alkanes.

Table 5: Model summary for the heats of vaporization of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.814	60.77	0.000
Logarithmic	0.864	91.55	0.000
Quadratic	0.891	51.7	0.000

The correlation coefficient value $r = 0.891$ for the quadratic model in Table 5 reveals that the prediction power of the Mass first Zagreb index is good in predicting the temperatures of vaporization of alkanes. In other words, our results indicate an accuracy of 89.1% in forecasting the temperatures of vaporization of alkanes.

Table 6: Model summary for the melting point of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.571	15.843	0.001
Logarithmic	0.592	14.41	0.000
Quadratic	0.532	6.78	0.003

The correlation coefficient values for all models are less than 0.7, indicating that the prediction power of the Mass first Zagreb index is not very excellent in forecasting the melting point of alkanes.

Table 7: Model summary for the molar refraction of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.49	11.62	0.004
Logarithmic	0.486	13.355	0.001
Quadratic	0.583	7.662	0.003

The correlation coefficient value for all models is less than 0.7, indicating that the prediction capacity of the Mass first Zagreb index is not very excellent in forecasting the molar refraction of alkanes.

Table 8: Model summary for the molar volume of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.738	41.96	0.000
Logarithmic	0.534	13.43	0.001
Quadratic	0.819	31.35	0.000

According to the correlation coefficient value $r = 0.819$ for the quadratic model in Table 8, the prediction power of the Mass first Zagreb index is good in predicting molar volume of alkanes. In other words, our results demonstrate an 81.9% accuracy in forecasting the molar volume of alkanes.

Table 9: Model summary for the surface tension of alkanes and Mass first Zagreb index

Equation	R^2	F	Sig
Linear	0.068	0.90	0.65
Logarithmic	0.126	2.654	0.15
Quadratic	0.837	34.97	0.000

The correlation coefficient value $r = 0.837$ for the quadratic model in Table 9 reveals that the prediction capability of the Mass first Zagreb index is good in predicting the surface tension of alkanes. In other words, our results demonstrate an 83.7 percent accuracy in predicting the quadratic model of alkanes.

VI. Conclusion

We investigated the mathematical properties and chemical applications of the Mass first Zagreb index in this study. According to a QSPR investigation, the first Mass Zagreb index is a good option for predicting the physicochemical properties of alkanes. The interested reader might conduct additional research on the Second Mass Zagreb index.

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