70(8A): 1-479; 2022. DOI: 10.18311/jmmf/2022/32009

Print ISSN : 0022-2755
Journal of Mines, Metals and Fuels
Contents available at: www.informaticsjournals.com/index.php/jmmf

QSPR Analysis of Polycyclic Aromatic Hydrocarbons

Ishita Sarkar[1], Manjunath N[2], K. Ramesha[3]

[1]*Department of Mathematics, CHRIST (Deemed to be University) Bengaluru, Karnataka. e-mail: ishita.sarkar@res.christuniversity.in*
[2]*Department of Sciences and Humanities, School of Engineering and Technology, CHRIST (Deemed to be University) Bengaluru, Karnataka. e-mail: manjunath.nanjappa@christuniversity.in*
[3]*Dept. of Mech. and Automobile Engg. CHRIST (Deemed to be University) Bengaluru, Karnataka. e-mail: ramesha.kra@gmail.com*

Abstract

Topological indices serve as a crucial component in chemical graph theory linked with some molecular structure. The First and Second Zagreb Indices are one among the earliest and extensively explored molecular descriptors. The study on equitable zagreb indices have been initiated earlier by Akram Alqesmah, Anwar Alwardi and R. Rangarajan based on the equitable degree of the vertices. In this paper, we introduce the first and second equitable and non-equitable zagreb polynomials and compute the exact values of the respective equitable and non-equitable zagreb indices for polycyclic aromatic hydrocarbons. We have also utilised certain formulations for the determination of the corresponding relative equitable and non-equitable zagreb indices of the chemical graph. Further, QSPR analysis is carried out for the topological indices with regard to the physico-chemical properties of the polycyclic hydrocarbon molecules.

Keywords: *Equitable zagreb index, polynomial, polycyclic aromatic hydrocarbon.*

Subject Classification: *05C07, 05C90.*

1.0 Introduction

We take into account the undirected, simple connected molecular graphs here in chemical graph theory. Its vertices correspond to the atoms and the edges to the bonds of a molecule. In this paper, vertex set and edge set of a molecular graph, ξ are represented by $V(\xi)$, $E(\xi)$ respectively. The open neighbourhood for node w is indicated by $N(w) = \{v \in V(\xi) | vw \in E(\xi)\}$ and the closed neighbourhood for node w is represented as $N(w) = N(w) \cup \{w\}$. d(w) denotes the degree of vertex w in ξ and $e=vw$ is the edge joining v with w. The minimum and maximum degree of the graph, ξ is denoted by δ_ξ and Δ_ξ respectively.

In ξ, the vertex v is equitable adjacent with w if they are neighboring vertices and $|d(v)-d(w)| < 1$. $N_e(w) = v \in V(\xi) : v$ is equitable to $w\}$ represents open equitable neighborhood for $v \in V(\xi)$ and the equitable degree of w is denoted by $d_e(w) = |N_e(w)|$. An edge $e = vw$ is said to be an equitable edge if $|d(v)-d(w)| < 1$ (Al-Kenani et al., 2013) (Anitha et al., 2009). The minimum and maximum equitable degree of the graph, ξ is denoted by $\delta_e(\xi)$ and $\Delta_e(\xi)$ respectively where $\delta_e(\xi) = min\{d_e(w) | w \in V(\xi)\}$ and $\Delta_e(\xi) = max\{d_e(w) | w \in V(\xi)\}$. Non-equitable neighborhood for w as $N_{ne}(w) = \{v \in n(w) : |d(w) - d(v)| > 2$, $d_{ne}(w) = |N_{ne}(w)|$. Clearly, $d(w) = d_e(w) + d_{ne}(w)$. In ξ, summation of equitable degrees equals twice the number of equitable links, qe i.e. for $w \in V(\xi)$, $d_e(w) = 2q_e$.

[2]*Corresponding Author*

Wiener index is one of the earliest and extensively explored molecular descriptors (Wiener, 1947). The First and Second Zagreb Indices are the widely known graph invariants defined by Gutman to specify π-electron energy of the molecules (Gutman et al., 2020) (Gutman & Trinajstiæ, 1972).

$$M_1(\xi) = \sum_{w \in V(\xi)} d(w)^2$$

$$M_2(\xi) = \sum_{vw \in E(\xi)} d(v)d(w)$$

Further many properties related to the zagreb index have been studied in (Zhou, 2004)(Zhou & Gutman, 2005).

Preliminaries

Study on first equitable zagreb index ($M_1^e(\xi)$) and second equitable zagreb index ($M_2^e(\xi)$) of a graph ξ was initiated in (Alqesmah, 2016) as:

$$M_1^e(\xi) = \sum_{w \in V(\xi)} [d_e(w)]^2$$

and

$$M_2^e(\xi) = \sum_{vw \in E(\xi)} [d_e(v)d_e(w)]$$

We define the First Equitable Zagreb Polynomial ($M_1^e(\xi, x)$) and Second Equitable Zagreb Polynomial ($M_2^e(\xi, x)$) as:

$$M_1^e(\xi, x) = \sum_{w \in V(\xi)} x^{(d_e(w))^2}$$

and

$$M_2^e(\xi, x) = \sum_{vw \in E(\xi)} x^{d_e(v)d_e(w)}$$

We define the First Non-Equitable Zagreb ($M_1^{ne}(\xi, x)$) Polynomial and Second Non- Equitable Zagreb Polynomial ($M_2^{ne}(\xi, x)$) as:

$$M_1^{ne}(\xi, x) = \sum_{w \in V(\xi)} x^{(d_{ne}(w))^2}$$

and

$$M_2^{ne}(\xi, x) = \sum_{vw \in E(\xi)} x^{d_{ne}(v)d_{ne}(w)}$$

We can obtain the respective indices from their polynomials by finding out the derivative at the point x=1. According to the equitable and non-equitable degree of the vertices, we have certain divisions of vertex $V(\xi)$ and edge $E(\xi)$ set of graph ξ:

$$\forall r, \delta_{e/ne}^2 \le r \le \Delta_{e/ne}^2, E_r^* = \{vw \in E(\xi) | d_{e/ne}(v)d_{e/ne}(w) = r\} \quad \text{... (1)}$$

$$\forall s, \delta_{e/ne} \le s \le \Delta_{e/ne}, V_s = \{w \in E(\xi) | d_{e/ne}(w) = s\} \quad \text{... (2)}$$

Such that $V(\xi) = \bigcup_{i=\delta}^{\Delta} V_i$

Equitable zagreb polynomials and equitable zagreb indices of polycyclic aromatic hydrocarbons

In this section, we discuss the computation of Equitable Zagreb Polynomials and Equitable Zagreb Indices of Polycyclic Aromatic Hydrocarbons (PAH_n).

Polycyclic Aromatic Hydrocarbons, PAH_n is afamily of hydrocarbon molecules, so that its framework is composed of six cycles (benzene).

According to the equitable degree of the vertices, the vertex set have three divisions:

$$V_3 = \{w \in V(\xi) | d_e(w) = 3\}$$
$$V_2 = \{w \in V(\xi) | d_e(w) = 2\}$$
$$V_0 = \{w \in V(\xi) | d_e(w) = 0\}$$

The number of vertices in vertex sets are: $|V_3| = 6n^2$–
–6n, $|V_2| = 6n$, and $|V_0| = 6n$. The edge set of molecular graph, ξ can be partitioned into four divisions e.g. E_0^*, E_4^*, E_6^* and E_9^* as follows:

- For every e=vw $\in E_0^*$;
  $d_e(v) = 2, d_e(w) = 0,$
  $E_0^* = \{e \in E(PAH_n) | d_e(v)d_e(w) = 0\}$
- For every e=vw $\in E_4^*$;
  $d_e(v) = 2, d_e(w) = 2,$
  $E_4^* = \{e \in E(PAH_n) | d_e(v)d_e(w) = 4\}$
- For every e=vw $\in E_6^*$;
  $d_e(v) = 3, d_e(w) = 2,$
  $E_6^* = \{e \in E(PAH_n) | d_e(v)d_e(w) = 6\}$
- For every e=vw $\in E_9^*$;
  $d_e(v) = 3, d_e(w) = 3,$
  $E_9^* = \{e \in E(PAH_n) | d_e(v)d_e(w) = 9\}$

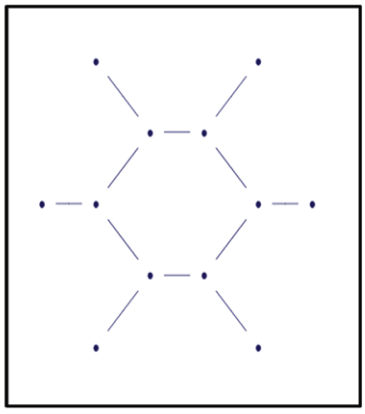

Figure 1: PAH_1

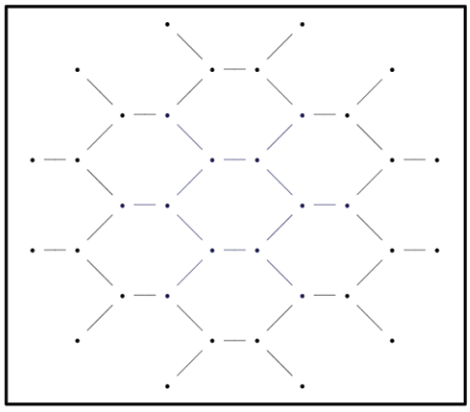

Figure 1: PAH_2

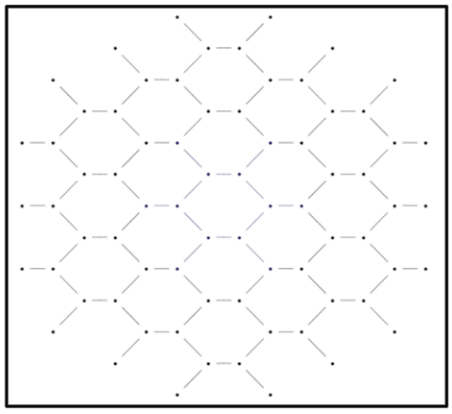

Figure 1: PAH_2

Now by using the above definitions and notations, we have the main result of the paper in the following theorem:

Theorem 1: For the Polycyclic Aromatic Hydrocarbon molecule (PAH_n),

- The First Equitable Zagreb Polynomial equals

$M_1^e(PAH_n, x) = 6n(n-1)x^9 + (6n)x^4 + 6n$

The First Equitable Zagreb Index is:

$54n^2 - 30n$

- The Second Equitable Zagreb Polynomial equals

$$M_2^e(PAH_n, x) = 3(3n^2 - 5n + 2)x^9 + 12(n-1)x^6 + 6x^4 + 6n$$

The Second Equitable Zagreb Index is:

$81n^2 - 58n + 6$

Proof. Assume PAH_n indicate the basic illustration of polycyclic hydrocarbons. It has $6n^2 + 6n$ nodes. The cardinality of equitable links in molecular graph:

$$|E_e(PAH_n)| = \frac{(3 \times 6n^2) - (1 \times 6n)}{2} = 9n^2 - 3n$$

The respective cardinalities of the edge sets of Polycyclic Aromatic Hydrocarbon, PAH_n are $|E_0^*| = 6n$, $|E_4^*| = 6$, $|E_6^*| = 12(n-1)$, and $|E_9^*| = 9n^2 - 15n + 6$. According to the definition of First Equitable Zagreb Polynomial and Second Equitable Zagreb Polynomial,

$$M_1^e(PAH_n, x) = \sum_{w \in V(PAH_n)} x^{(d_e(w))^2} = \sum_{w \in V_3} x^{3^2} + \sum_{w \in V_2} x^{2^2} + \sum_{w \in V_0} x^{0^2} = \sum_{w \in V_3} x^9 + \sum_{w \in V_2} x^4 + \sum_{w \in V_0} 1 = 6n(n-1)x^9 + (6n)x^4 + 6n$$

and

$$M_2^e(PAH_n, x) = \sum_{vw \in E(PAH_n)} x^{(d_e(v)d_e(w))} = \sum_{vw \in E_9^*} x^{3*3} + \sum_{vw \in E_6^*} x^{3*2} + \sum_{vw \in E_4^*} x^{2*2} + \sum_{vw \in E_0^*} x^{0*2} = \sum_{vw \in E_9^*} x^9 + \sum_{vw \in E_6^*} x^6 + \sum_{vw \in E_4^*} x^4 + \sum_{vw \in E_0^*} x^0 = 3(3n^2 - 5n + 2)x^9 + 12(n-1)x^6 + 6x^4 + 6n$$

Hence, the first equitable zagreb index and second equitable zagreb index of Polycyclic Aromatic Hydrocarbons (PAH_n) are:

$$M_1^e(PAH_n) = \frac{\partial M_1^e(PAH_n, x)}{\partial x}|_{x=1} = 9(6n^2 - 6n) + 4(6n) + 0 = 54n^2 - 30n$$

and

$$M_2^e(PAH_n) = \frac{\partial M_2^e(PAH_n, x)}{\partial x}|_{x=1} = 9(9n^2 - 15n + 6) + 72(n-1) + 24 = 81n^2 - 58n + 6$$

This proves the result.

Non-equitable zagreb polynomials and non-equitable zagreb indices of polycyclic aromatic hydrocarbons

In this section, we discuss the computation of Non-Equitable Zagreb Polynomials and Non-Equitable

Zagreb Indices of Polycyclic Aromatic Hydrocarbons (PAH_n). According to the non-equitable degree of the vertices, the vertex set have two divisions:

$V_{ne}^0 = \{w \in V(\xi) | d_{ne}(w) = 0\}$
$V_{ne}^1 = \{w \in V(\xi) | d_{ne}(w) = 1\}$

The respective cardinalities of the vertex $|V_{ne}^0| = 6n^2 - 6n$, $|V_{ne}^1| = 12n$ edge set of molecular graph, ξ is partitioned in two divisions i.e. E_{ne}^{0*} and E_{ne}^{1*}:

- For every e=vw $\in E_{ne}^0$;
  $d_{ne}(v) = 0, d_{ne}(w) = 0$ or
  $d_{ne}(v) = 0, d_{ne}(w) = 1,$
  $E_{ne}^{0*} = \{e \in E(PAH_n) | d_{ne}(v) d_{ne}(w) = 0\}$

- For every e=vw $\in E(PAH_n)$;
  $d_{ne}(v) = 1, d_{ne}(w) = 1,$
  $E_{ne}^{1*} = \{e \in E(PAH_n) | d_{ne}(v) d_{ne}(w) = 1\}$

Theorem 2: For the Polycyclic Aromatic Hydrocarbon molecule (PAH_n), then

- The first Non-Equitable Zagreb Polynominal equals

$M_1^{ne}(PAH_n, x) = 6n(2x + n - 1)$

The first Non-Equitable Zagreb Index is: $12n$

- The second Non-Equitable Zagreb Polynominal equals

$M_2^{ne}(PAH_n, x) = 3[2(n+1)x + (3n^2 - n - 2)]$

The second Non-Equitable Zagreb Index is: $6(n+1)$.

Proof. Assume PAH_n indicate the basic illustration of polycyclic hydrocarbons. The molecular graph of PAH_n has $6n^2+6n$ nodes. Since $d(w) = d_e(w) + d_{ne}(w)$ (Alqesmah, 2016), the cardinality of non-equitable links in the molecular graph are:

$|E_{ne}(PAH_n)| = |E(PAH_n)| - |E_e(PAH_n)| = 6n$

We have $|E_{ne}^{0*}| = 9n^2 - 3n - 6$ and $|E_{ne}^{1*}| = 6(n+1)$ for PAH_n by the definition first and second non-equitable Zagreb Polynominal, we have

$$M_1^{ne}(PAH_n, x) = \sum_{w \in V(PAH_n)} x^{(d_{ne}(w))^2}$$
$$= \sum_{w \in V_{ne}^0} x^{0^2} + \sum_{w \in V_{ne}^1} x^{1^2}$$
$$= \sum_{w \in V_{ne}^0} 1 + \sum_{w \in V_{ne}^1} x$$
$$= 6n(2x + n - 1)$$

and

$$M_2^{ne}(PAH_n, x) = \sum_{vw \in E(PAH_n)} x^{(d_{ne}(v) d_{ne}(w))}$$
$$= \sum_{vw \in E_{ne}^{0*}} x^{0*0} + \sum_{vw \in E_{ne}^{0*}} x^{0*1} + \sum_{vw \in E_{ne}^{1*}} x^{1*1}$$
$$= (9n^2 - 3n - 6) + (6(n+1))x$$
$$= 3[2(n+1)x + (3n^2 - n - 2)]$$

Now, the first Non Equitable Zagreb index and Second Non Equitable Zagreb index for PAH_n are :

$$M_1^{ne}(PAH_n) = \frac{\partial M_1^{ne}(PAH_n, x)}{\partial x}|_{x=1} = 12n$$

and

$$M_2^{ne}(PAH_n) = \frac{\partial M_2^{ne}(PAH_n, x)}{\partial x}|_{x=1} = 6(n+1)x$$

This proves the result.

Relative equitable and non-equitable zagreb indices of polycyclic aromatic hydrocarbons

In this section, we discuss the computation of Relative Equitable and Non-Equitable Zagreb Indices of PAH_n by the formulations involving equitable and non-equitable zagreb indices.

Theorem 3 For the Polycyclic Aromatic Hydrocarbon molecule (PAH_n), then

- The First Relative Equitable Zagreb Index PAH_n is: $RM_1^e(\xi) = 18n(3n - 1)$
- The Second Relative Equitable Zagreb PAH_n is: $RM_2^e(\xi) = 162n^2 - 67n$
- The First Relative Non-Equitable Zagreb Index of PAH_n is: $RM_1^{ne}(\xi) = 24n$
- The Second Relative Non-Equitable Zagreb Index of PAH_n is: $RM_2^{ne}(\xi) = 61n$

Proof. From (Alqesmah et al., 2016), (Farahani, 2013), we have certain formulations involving the zagreb indices, equitable, non-equitable and relative equitable and non-equitable zagreb indices. We utilise those computations for finding our required results:

For finding the First Relative Equitable Zagreb Index,

$$M_1^{ne}(\xi) = M_1(\xi) + M_1^e(\xi) - 2RM_1^e(\xi)$$
$$2RM_1^e(\xi) = M_1(\xi) + M_1^e(\xi) - M_1^{ne}(\xi)$$
$$= (54n^2 + 6n) + (54n^2 - 30n) - 12n$$
$$= 108n^2 - 36n$$
$$RM_1^e(\xi) = 18n(3n-1)$$

For finding the Second Relative Equitable Zagreb Index,

$$M_2^{ne}(\xi) = M_2(\xi) + M_2^e(\xi) - RM_2^e(\xi)$$
$$RM_2^e(\xi) = M_2(\xi) + M_2^e(\xi) - M_2^{ne}(\xi)$$
$$= (81n^2 - 3n) + \big(81n^2 - 58n + 6 - 6(n+1)\big)$$
$$RM_2^e(\xi) = 162n^2 - 67n$$

For finding the First Relative Non-Equitable Zagreb Index,

$$M_1(\xi) = RM_1^e(\xi) + RM_1^{ne}(\xi)$$
$$RM_1^{ne}(\xi) = M_1(\xi) - RM_1^e(\xi)$$
$$= (54n^2 + 6n) - 18n(3n-1)$$
$$RM_1^{ne}(\xi) = 24n$$

For finding the Second Relative Non-Equitable Zagreb Index,

$$2M_2(\xi) = RM_2^e(\xi) + RM_2^{ne}(\xi)$$
$$RM_2^{ne}(\xi) = 2M_2(\xi) - RM_2^e(\xi)$$
$$= 2(81n^2 - 3n) - (162n^2 - 67n)$$
$$RM_2^{ne}(\xi) = 61n$$

This proves the result.

QSPR Analysis of the hydrocarbon families

This section demonstrates the quantitative structure property relationship (QSPR) connecting several specified graph invariants with some physico-chemical molecular attributes. The potency of the descriptors is investigated by such analysis. Some topological indices are represented with few physico-chemical properties such as density, molar refractivity, polarizability, surface tension and molar volume of the hydrocarbon molecules. The values for the respective physico-chemical properties, were acquired from ChemSpider as shown in Table (2). Table (1) enlists the calculated equitable and non-equitable degree-based topological indices of related molecular graphs. The correlation coefficient (r) values for the characteristics are expressed with specified equitable and non-equitable topological index in the Table (3).

From Table (3), it is to be noted:

- First Relative Equitable Zagreb Index shows a very strong correlation with Molar Refractivity (R^2=0.999998), Polarizability (R^2=0.999999) and Surface Tension (R^2=0.997709).
- First, Second Non-Equitable and the respective Relative Non-Equitable Zagreb Indices having equal correlation values shows good correlation with Density (R^2=0.986842) and Molar volume (R^2=0.996613).

Table 1: PAH_n with related equitable and non-equitable zagreb indices

PAH_n	M_1^e	M_2^e	M_1^{ne}	M_2^{ne}	RM_1^e	RM_2^e	RM_1^{ne}	RM_2^{ne}
PAH_1	24	29	12	12	36	95	24	61
PAH_2	156	214	24	18	180	514	48	122
PAH_3	396	561	36	24	432	1257	72	183

Table 2: PAH_n • with their physico-chemical attributes

PAH_n	Molar refractivity	Density	Polarizability	Surface Tension	Molar Volume
PAH_1	26.3	0.9	10.4	28.9	89.4
PAH_2	111.4	1.5	44.1	85.8	204.7
PAH_3	259.6	1.9	102.9	169.1	345.9

Table 3: the correlation values between the equitable and non-equitable topological indices					
Topological Index	Molar Refractivity	Density	Polarizability	Surface Tension	Molar Volume
M_1^e	0.999937609	0.960768923	0.999943051	0.998331037	0.994190669
M_2^e	0.999817069	0.958531603	0.999826475	0.994142241	0.993302746
M_1^{ne}	0.988026449	0.993399268	0.987949451	0.994142241	0.998305006
M_2^{ne}	0.988026449	0.993399268	0.987949451	0.994142241	0.998305006
RM_1^e	0.999999189	0.963466788	0.999999699	0.998853698	0.995207218
RM_2^e	0.99998891	0.962540827	0.999991132	0.998683326	0.994865336
RM_1^{ne}	0.988026449	0.993399268	0.987949451	0.994142241	0.998305006
RM_2^{ne}	0.988026449	0.993399268	0.987949451	0.994142241	0.998305006

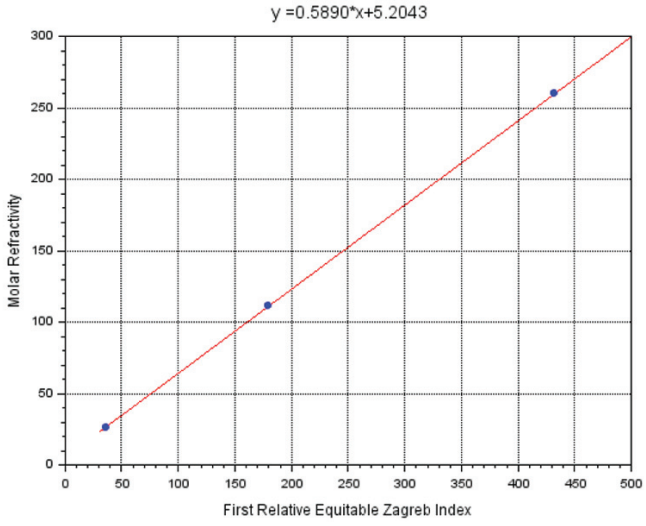

Figure 4: Correlation of RM_1^e with Molar Refractivity

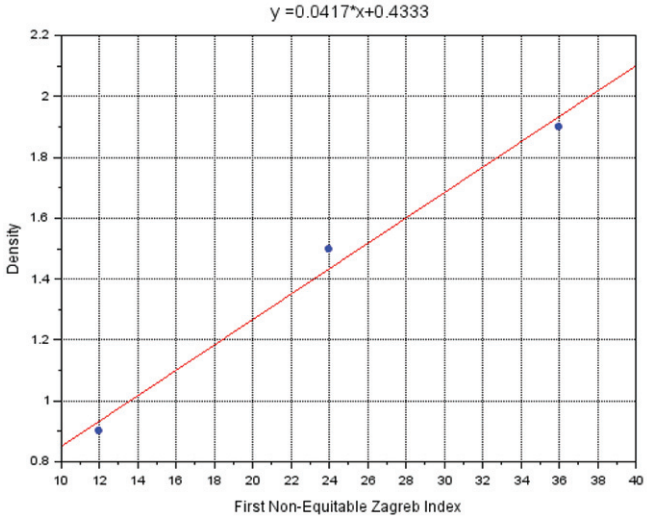

Figure 5: Correlation of M_1^{ne} with Density

Further, the correlation of First Relative Equitable Zagreb Index with Molar Refractivity and of First Non-Equitable Zagreb Index with Density is depicted in figure (4) and (5) respectively. The noted observations on the correlation reveal the utility of molecular descriptors for the physico-chemical properties of the specified family of hydrocarbon molecules during QSPR model.

Conclusion

In this paper, the computation of the equitable, non-equitable zagreb polynomials and their respective indices is carried out. We have implied the formulations related to the topological indices for the determination of the relative equitable and non-equitable zagreb indices of the molecular graph.

Furthermore, some very strong correlations are also obtained between the descriptors and the physico-chemical properties for specified hydrocarbon families. The outcomes procured have favourable angles towards further research for the analysis of equitable degree and distance dependent descriptors and their applications.

References

1. (Al-Kenani et al., 2013) Al-Kenani, A. N., Soner, N. D., & Alwardi, A. (2013). Graphs and Degree Equitability. *Applied Mathematics*, 04(08),1199–1203.
2. (Alqesmah, 2016) Alqesmah, A. Alwardi, and R. Rangarajan. (2016). Equitable and Non-Equitable Zagreb Indices of Graphs. *International*

Journal of Mathematics And its Applications, 4(2), 57–65.

3. (Anitha et al., 2009) Anitha, A., Arumugam, S., & Sampathkumar, E. (2009). Degree Equitable Sets in a Graph. In *International J.Math. Combin* (Vol. 3), 32-47.
4. (Farahani, 2013) Farahani, M. R. (2013). Zagreb Indices and Zagreb Polynomials of Polycyclic Aromatic Hydrocarbons PAHs. *In Journal of Chemica Acta* (Vol. 2).
5. (Gutman et al., 2020) Gutman, I., Milovanoviæ, E., & Milovanoviæ, I. (2020). Beyond the Zagreb indices. *AKCE International Journal of Graphs and Combinatorics*, 17(1), 74–85.
6. (Gutman & Trinajstiæ, 1972) Gutman, I., & Trinajstiæ, N. (1972). Graph theory and molecular orbitals. Total ð-electron energy of alternant hydrocarbons. *Chemical Physics Letters*, 17(4), 535–538.
7. (Wiener, 1947) Wiener, H. (1947). Structural Determination of Paraffin Boiling Points. Journal of the American Chemical Society, 69(1), 17–20.
8. (Zhou, 2004) Zhou, B. (2004). Zagreb indices. MATCH Commun. *Math. Comput. Chem*., 52(1), 113-118.
9. (Zhou & Gutman, 2005) Zhou, B., & Gutman, I. (2005). Further properties of zagreb indices. MATCH Commun. *Math. Comput. Chem*., 54(1), 233–239.