

Article

# On $ve$ -Degree Irregularity Index of Graphs and Its Applications as Molecular Descriptor

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**Abstract:** Most of the molecular graphs in the area of mathematical chemistry are irregular. Therefore, irregularity measure is a crucial parameter in chemical graph theory. One such measure that has recently been proposed is the  $ve$ -degree irregularity index ( $irr_{ve}$ ). Quantitative structure property relationship (QSPR) analysis explores the capability of an index to model numerous properties of molecules. We investigate the usefulness of the  $irr_{ve}$  index in predicting different physico-chemical properties by carrying out QSPR analysis. It is established that the  $irr_{ve}$  index is efficient to explain the acentric factor and boiling point of molecules with powerful accuracy. An upper bound of  $irr_{ve}$  for the class of all trees is computed with identifying extremal graphs. We noticed that the result is not correct. In this report, we provide a counter example to justify our argument and determine the correct outcome.

**Keywords:** molecular graph; QSPR analysis;  $ve$ -degree; irregularity index; tree

**MSC:** 05C50; 11F72; 05C92



**Citation:** Das, K.C.; Mondal, S. On  $ve$ -Degree Irregularity Index of Graphs and Its Applications as Molecular Descriptor. *Symmetry* **2022**, *14*, 2406. <https://doi.org/10.3390/sym14112406>

Academic Editors: Juan Luis García Guirao

Received: 2 October 2022

Accepted: 8 November 2022

Published: 14 November 2022

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## 1. Introduction

Mathematical chemistry is an interdisciplinary area of research that explains chemical phenomena from a mathematical point of view. The topological index is one of the crucial tools in this field which describes the structural features of molecules. A topological index can be thought of mathematically as a function from the collection of all molecular graphs to the set of real numbers such that it remains unchanged under graph isomorphism. By “molecular graph”, we mean a simple connected graph whose nodes and edges correspond to atoms and chemical bonds between them, respectively. The journey of the topological index was started through the Weiner’s work [1] on the boiling point of alkanes in 1947. Due to their significant applications [2–9], topological indices have attracted considerable attention of researchers and many indices have been put forward based on different graph parameters [5,10–22]. Let  $G = (V, E)$  be a simple graph having  $n$  nodes and  $m$  edges. For a node  $v_i \in V(G)$ , the open neighborhood of  $v_i$  is the set  $N_G(v_i) = \{v_j \in V(G) : v_i v_j \in E(G)\}$ . The degree of a node  $v_i$ , denoted by  $deg(v_i)$ , is the cardinality of  $N_G(v_i)$ . A graph is known as regular if  $deg(v_i) = deg(v_j)$ , for all  $v_i, v_j \in V(G)$ . If a graph is not regular, it is obviously irregular. The substantial proportion of molecular graphs are irregular. Therefore, the following question naturally arises: how irregular is it? A topological index  $T$  is useful to measure such irregularity if  $T(G) \geq 0$  with  $T(G) = 0$  iff  $G$  is regular [23]. This kind of indices are known as irregularity indices. There are many indices to measure the irregularity in the literature [23–31]. The Albertson index [32] is one of them defined on the degree of end nodes of edges as follows:

$$Alb(G) = \sum_{v_i v_j \in E(G)} |deg(v_i) - deg(v_j)|.$$

In 2017, two new graph parameters were put forward parallel in degree: *ve*-degree and *ev*-degree [33]. The present report deals with the *ve*-degree of vertex ( $v_i \in V(G)$ ), which is a count of different edges that are incident to a vertex from the closed neighborhood of  $v_i$ . In [34], Ediz defined different *ve*-degree-based indices parallel to their corresponding classical degree versions. The regularity and irregularity concepts in view of *ve*-degree and *ev*-degree are studied by Horoldagva et al. [35]. In [36], Şahin and Şahin introduced the *ve*-degree version of the Albertson index as an irregularity measure, which is formulated as

$$irr_{ve}(G) = \sum_{v_i, v_j \in E(G)} |deg_{ve}(v_i) - deg_{ve}(v_j)|.$$

They named it as the *ve*-degree irregularity index of  $G$ . Quantitative structure property relationship (QSPR) analysis [2,37–41] is a promising approach to correlate structural features with properties of chemicals. It is a remarkable statistical approach for investigating drug activity or the binding mode for different receptors. The usefulness of topological indices as efficient molecular descriptors can be determined by QSPR study. Our goal is to explore the application potential of the *ve*-degree irregularity index in modelling structural properties of molecules employing QSPR analysis.

The upper bound of this index for the class of all trees is derived with characterizing extremal graphs in [36]. But we observe that this finding is not correct. The methodology used to prove the result is totally incorrect, but fortunately, the upper bound is right. Moreover, the extremal graphs are not completely determined. We intend to present a counter example to assure our claim, and then to establish the correct result.

Now we explain some notations that will be used throughout the article. The star of order  $n$  is denoted by  $K_{1,n-1}$ . A tree  $S_k^*$  [42] of order  $n (= 2k + 1)$  is obtained from a star  $K_{1,k}$  by adding a pendant edge to every pendant vertex of the star. A tree  $T_{n,k}$  of order  $n (= 2k + 2)$  is obtained from  $S_k^*$  such that a vertex of degree one has to be attached to the center of  $S_k^*$ . If  $K_n$  represents the complete graph of order  $n$ , then the graph generated from  $K_2$  by joining  $p$  and  $q$  pendant edges to two ends of  $K_2$  is termed as a double star  $DS_{p,q}$ .

Let  $T_{n,4}$  be a tree of order  $n$  with diameter 4 (see, [43,44]). We now define tree  $T_{n,4}$  as follows: Consider a node  $v$  of degree  $k (\geq 2)$  in  $T_{n,4}$  such that  $T_{n,4} \setminus \{v\} = K_{1,a_1} \cup K_{1,a_2} \cup \dots \cup K_{1,a_q} \cup p K_1$ , where  $a_i \geq 1$  for  $1 \leq i \leq q$  and  $k = p + q$  ( $p \geq 0, q > 1$ ). Let  $v_i \in N_{T_{n,4}}(v)$  ( $1 \leq i \leq q$ ) with  $deg(v_i) = a_i + 1 \geq 2$ , and  $v_i \in N_{T_{n,4}}(v)$  ( $q + 1 \leq i \leq q + p$ ) with  $deg(v_i) = 1$  in  $T_{n,4}$ . Therefore vertex  $v_i$  ( $1 \leq i \leq q$ ) is adjacent to vertex  $v$  &  $a_i$  pendant vertices, and  $v_i$  ( $q + 1 \leq i \leq q + p$ ) is adjacent to vertex  $v$  only. From Figure 1, one can easily see that  $n = \sum_{i=1}^q a_i + q + p + 1$ , that is,  $\sum_{i=1}^q a_i = n - k - 1$  as  $k = p + q$ . When  $p + q = \lfloor \frac{n}{2} \rfloor$  or  $\lceil \frac{n}{2} \rceil$ , we assume that  $T_{n,4} \cong T'_{n,p,q}$ . In particular, for  $T'_{n,2,r-1}$  with  $a_i = 1$  ( $1 \leq i \leq r - 1$ ), we have  $n = 2r + 1, p = 2, q = r - 1$ , and  $p + q = \lfloor \frac{n}{2} \rfloor$ . The structure of  $T_{n,4}$  is shown in Figure 1.

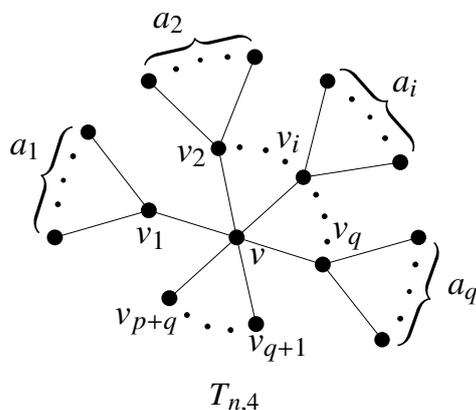


Figure 1. Structure of  $T_{n,4}$ .

## 2. Usefulness as Molecular Descriptor

The evaluation of possible implementations of topological indices is the foundation of chemical graph theory research, which is a motivating factor underneath the mathematical study of indices. The present section demonstrates the applicability of ve-degree irregularity index  $irr_{ve}$  in explaining structural features of molecules by employing the QSPR approach. To examine the chemical significance of a graph invariant, Randić and Trinajstić [45], pillars of mathematical chemistry, suggested to correlate theoretical indices with experimental properties of a benchmark dataset. In this report, we consider the octane isomers and benzenoid hydrocarbons as benchmark datasets. The hydrogen-deleted molecular graphs of octanes are created by the ChemDraw software (see Figure 2).

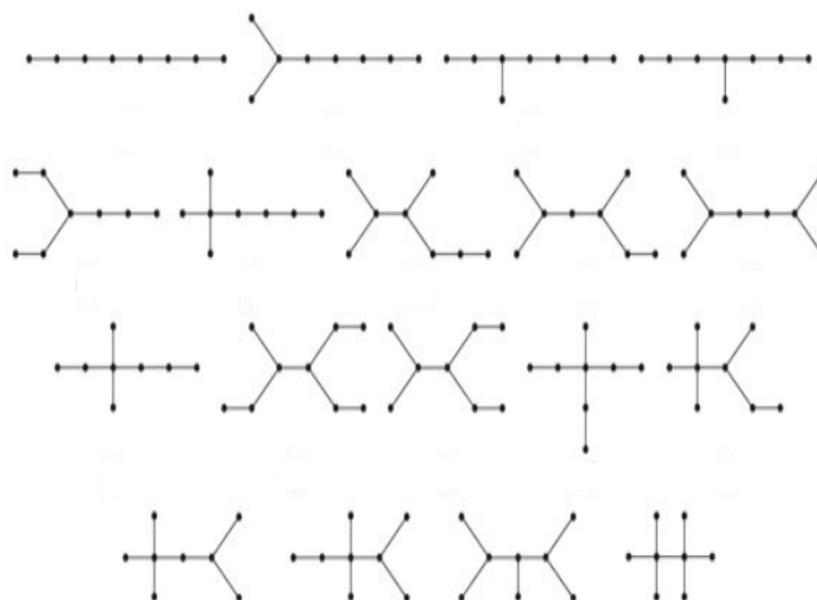


Figure 2. Hydrogen-deleted molecular graph of octane isomers.

The theoretical indices, computed by in-house Matlab script, are reported in Table 1. When we correlate  $irr_{ve}$  with experimental properties of octanes [46–48], no significant outcome is observed. In the case of the boiling point (BP), entropy (S), enthalpy of vaporization (HVAP) and the acentric factor (AF), the linear relations are depicted in Figure 3. The coefficient of determination ( $r^2$ ) for each case is considerably low.

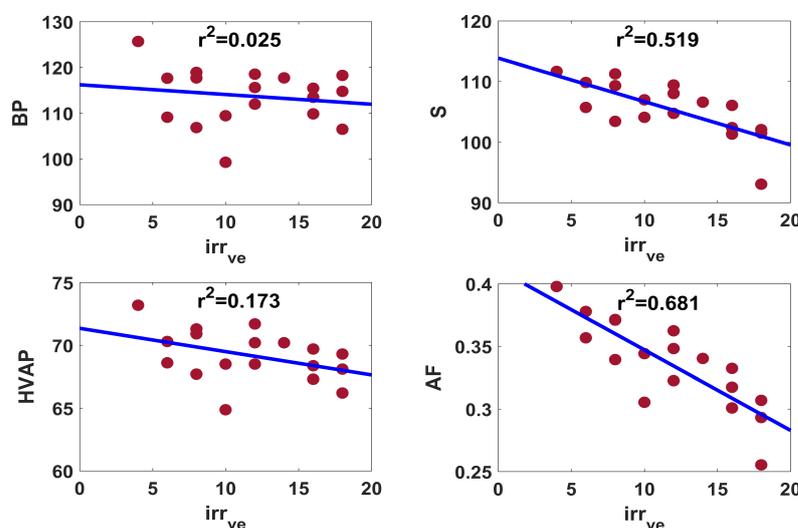


Figure 3. Linear relation of  $irr_{ve}$  with different properties of octanes.

**Table 1.** Experimental physico-chemical properties and theoretical indices for octane isomers. M: methyl, E: ethyl, Hept: Heptane, Hex: Hexane, Pent: Pentane, But: Butane.

Octanes	$irr_{ve}$	$Alb$	BP	S	HVAP	AF
n-Oct	4	2	125.665	111.67	73.19	0.397898
2-M-Hept	6	6	117.647	109.84	70.3	0.377916
3-M-Hept	8	6	118.925	111.26	71.3	0.371002
4-M-Hept	8	6	117.709	109.32	70.91	0.371504
3-E-Hex	12	6	118.534	109.43	71.7	0.362472
2,2-M-Hex	8	12	106.84	103.42	67.7	0.339426
2,3-M-Hex	12	8	115.607	108.02	70.2	0.348247
2,4-M-Hex	10	10	109.429	106.98	68.5	0.344223
2,5-M-Hex	6	10	109.103	105.72	68.6	0.35683
3,3-M-Hex	12	12	111.969	104.74	68.5	0.322596
3,4-M-Hex	14	8	117.725	106.59	70.2	0.340345
2-M-3-E-Pent	16	8	115.45	106.06	69.7	0.332433
3-M-3-E-Pent	18	12	118.259	101.48	69.3	0.306899
2,2,3-M-Pent	16	14	109.841	101.31	67.3	0.300816
2,2,4-M-Pent	10	16	99.238	104.09	64.87	0.30537
2,3,3-M-Pent	18	14	114.76	102.06	68.1	0.293177
2,3,4-M-Pent	16	10	113.467	102.39	68.37	0.317422
2,2,3,3-M-But	18	18	106.47	93.06	66.2	0.255294

But if we combine the  $irr_{ve}$  with  $Alb$  index, then the scenario alters dramatically and considerable correlation with the aforesaid properties is noticed. Consequently, our interest is to investigate the following regression model:

$$P = C_1(\pm e_1)irr_{ve} + C_2(\pm e_2)Alb + C_3(\pm e_3), \quad (1)$$

where  $P$  represents property,  $C_1$ ,  $C_2$  and  $C_3$  are fitting parameters, and  $e_1$ ,  $e_2$  and  $e_3$  indicate standard error of coefficients. Some additional statistical factors like coefficient of determination ( $r$ ), standard error of model ( $SE$ ), the F-test ( $F$ ) and the significance F ( $SF$ ) are also discussed with the model (1). Now in view of relation (1), we obtain the following regression equations for octane isomers.

$$BP = 0.68(\pm 0.177)irr_{ve} - 1.672(\pm 0.197)Alb + 122.229(\pm 1.925), \\ r^2 = 0.832, \quad SE = 2.666, \quad F = 37.239, \quad SF = 1.52 \times 10^{-6}. \quad (2)$$

$$S = -0.288(\pm 0.119)irr_{ve} - 0.802(\pm 0.133)Alb + 116.73(\pm 1.304), \\ r^2 = 0.859, \quad SE = 1.806, \quad F = 45.69, \quad SF = 4.16 \times 10^{-7}. \quad (3)$$

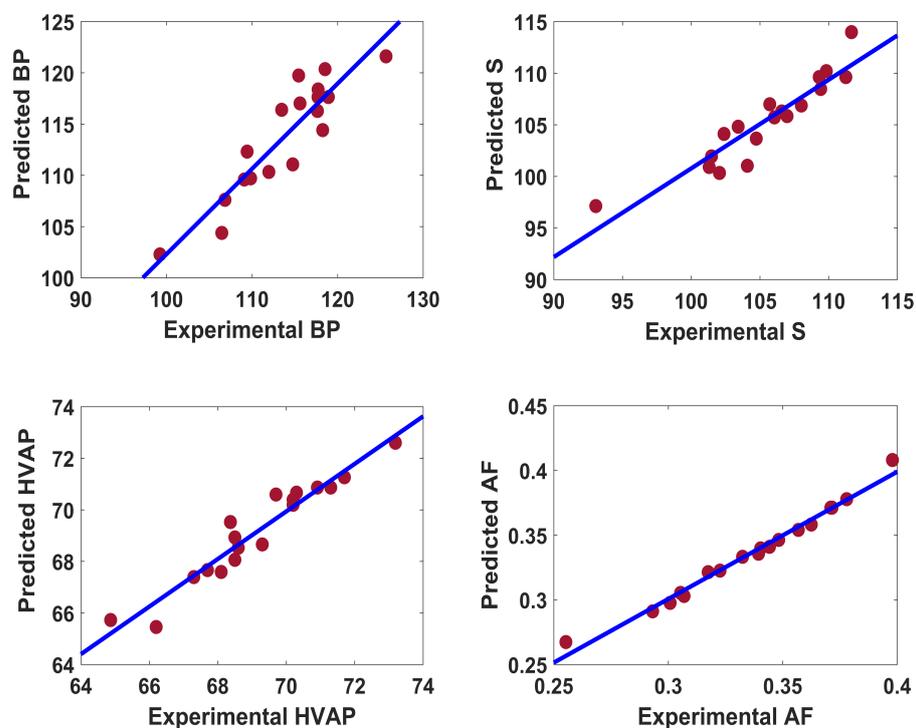
$$HVAP = 0.099(\pm 0.039)irr_{ve} - 0.534(\pm 0.044)Alb + 73.269(\pm 0.433), \\ r^2 = 0.923, \quad SE = 0.599, \quad F = 89.665, \quad SF = 4.54 \times 10^{-9}. \quad (4)$$

$$AF = -0.003(\pm 0.0003) - 0.006(\pm 0.0003)Alb + 0.433(\pm 0.003), \\ r^2 = 0.984, \quad SE = 0.005, \quad F = 450.084, \quad SF = 4.07 \times 10^{-14}. \quad (5)$$

From Equations (2)–(5), many interesting remarks can be drawn. The data variances for  $BP$ ,  $S$ ,  $HVAP$ , and  $AF$  are almost 83%, 86%, 92% and 98%, respectively, which are better than the  $irr_{ve}$  and  $Alb$ , when they are considered individually. Standard errors are very low, in fact, for the model (5), since it is significantly small. The consistency of model improves as well as the  $F$ -value increases. It is remarkably large in the case of  $AF$ .

The predicted properties by the model (1) are plotted against the experimental properties in Figure 4. From this figure, one can conclude that experimental and predicted data

align well with each other. In view of all parameters, we can claim that  $irr_{ve}$  and  $Alb$  exert superior ability to predict  $AF$  compared to other properties.



**Figure 4.** Relation between experimental and predicted properties for octane isomers.

Now we correlate the experimental boiling points [49] with theoretical values of  $irr_{ve}$  and  $Alb$  for benzenoid hydrocarbons (see Table 2). Chemical graphs of benzenoid hydrocarbons under consideration are shown in Figure 5.

**Table 2.** Experimental boiling points and theoretical indices for benzenoid hydrocarbons.

Compounds	$irr_{ve}$	$Alb$	BP	Compounds	$irr_{ve}$	$Alb$	BP
BHC1	12	4	218	BHC12	36	10	542
BHC2	20	6	338	BHC13	28	10	535
BHC3	16	8	340	BHC14	32	12	536
BHC4	26	8	431	BHC15	32	12	531
BHC5	24	10	425	BHC16	32	10	519
BHC6	24	6	429	BHC17	36	12	590
BHC7	20	12	440	BHC18	36	10	592
BHC8	32	10	496	BHC19	28	16	596
BHC9	32	8	493	BHC20	36	12	594
BHC10	36	8	497	BHC21	36	10	595
BHC11	36	12	547				

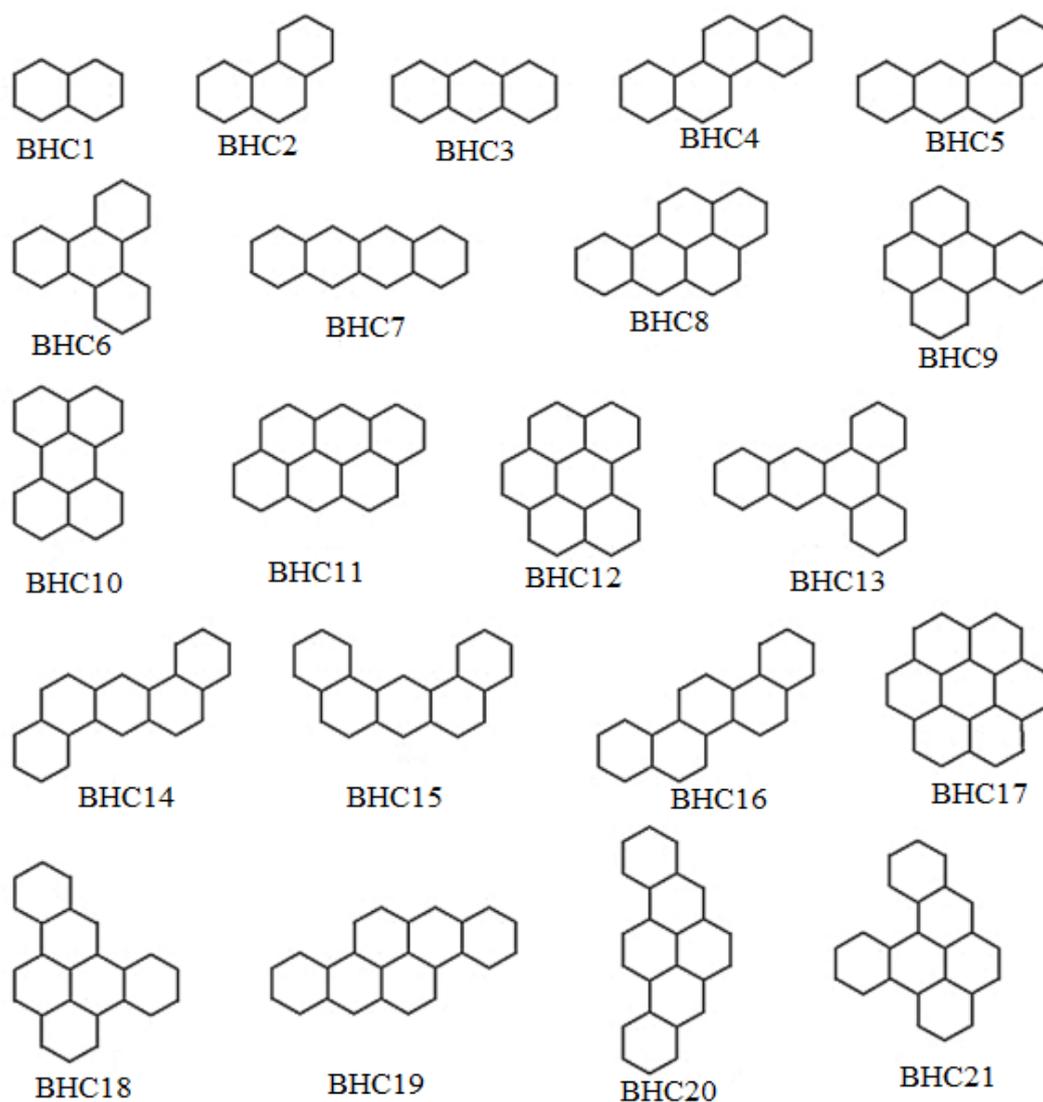


Figure 5. Chemical graphs of 21 benzenoid hydrocarbons.

Linear fitting of both the invariants with  $BP$  for benzenoid hydrocarbons is shown in Figure 6. Performance of  $irr_{ve}$  ( $r^2 = 0.805$ ) is better than  $Alb$  ( $r^2 = 0.591$ ). However, the combined effect of the indices is found to be better than the individuals. Equation (1) generates the following model.

$$BP = 9.332(\pm 0.953)irr_{ve} + 15.672(\pm 2.602)Alb + 64.924(\pm 26.995), \quad (6)$$

$$r^2 = 0.935, \quad SE = 26.762, \quad F = 130.422, \quad SF = 1.95 \times 10^{-11}.$$

In this case, the  $SE$  value is little bit high. The rest of the parameters are significant to state that  $irr_{ve}$  and  $Alb$  can predict the  $BP$  of benzenoid hydrocarbons. The relation between the experimental and predicted  $BP$  is depicted in Figure 7.

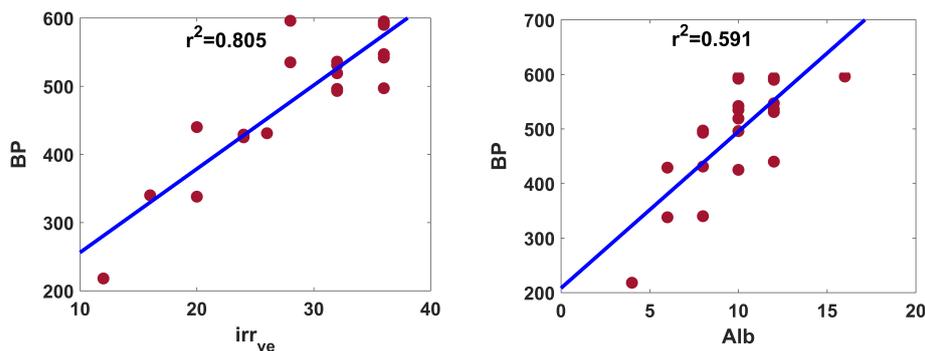


Figure 6. Linear fitting of  $irr_{ve}$  and  $Alb$  with  $BP$  for benzenoid hydrocarbons.

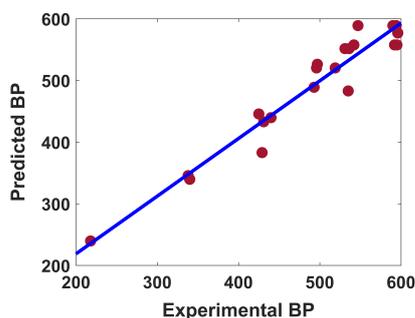


Figure 7. Relation between experimental and predicted  $BP$  for benzenoid hydrocarbons.

To check the independence of the  $ve$ -degree irregularity index  $irr_{ve}$ , it is correlated with some well known indices including the first Zagreb ( $M_1$ ), second Zagreb ( $M_2$ ), forgotten, Randić ( $R$ ), symmetric division deg ( $SDD$ ), and Albertson ( $Alb$ ) index, which is reported in Table 3. From Table 3 it is clear that  $irr_{ve}$  is not well correlated with existing indices, which makes its appearing in chemical graph theory purposeful.

Table 3. Correlation coefficient ( $r$ ) of  $irr_{ve}$  with some well known indices.

	$M_1$	$M_2$	$F$	$SCI$	$R$	$SDD$	$Alb$
$irr_{ve}$	0.688	0.874	0.667	−0.588	−0.539	0.517	0.594

### 3. On $ve$ -Degree Irregularity Index of Trees

First, we recall the Theorem of [36] concerning the upper bound of  $irr_{ve}$  for the class of all trees and provide two counter examples to it.

**Theorem 1** ([36]). *Let  $T$  be a tree of order  $n$ . Then*

$$irr_{ve}(T) \leq \begin{cases} \frac{n^2 - 4n + 3}{2} & \text{if } n \text{ is odd,} \\ \frac{n^2 - 4n + 4}{2} & \text{if } n \text{ is even.} \end{cases}$$

Moreover, the equality holds if and only if  $T \cong S_k^*$  ( $n = 2k + 1$ ) and  $T \cong T_{n,k}$  ( $n = 2k + 2$ ).

This result is not correct, as is shown in the following two counter examples.

**Example 1.** Let  $T \cong DS_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}$ . Also let  $v_1$  and  $v_2$  ( $deg(v_1) \geq deg(v_2)$ ) be two non-pendant vertices in  $T$ . We have  $deg(v_1) = \lceil \frac{n}{2} \rceil$ ,  $deg(v_2) = \lfloor \frac{n}{2} \rfloor$ ,  $deg_{ve}(v_1) = n - 1$ ,  $deg_{ve}(v_2) =$

$n - 1$ ,  $deg_{ve}(v_i) = \lceil \frac{n}{2} \rceil$  for  $v_i \in N_T(v_1)$  with  $deg(v_i) = 1$ , and  $deg_{ve}(v_j) = \lfloor \frac{n}{2} \rfloor$  for  $v_j \in N_T(v_2)$  with  $deg(v_j) = 1$ . Now,

$$\begin{aligned}
 irr_{ve}(T) &= \left( n - 1 - \left\lfloor \frac{n}{2} \right\rfloor \right) \left\lfloor \frac{n-2}{2} \right\rfloor + \left( n - 1 - \left\lceil \frac{n}{2} \right\rceil \right) \left\lceil \frac{n-2}{2} \right\rceil \\
 &= 2 \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil = \begin{cases} \frac{n^2 - 4n + 3}{2} & \text{if } n \text{ is odd,} \\ \frac{n^2 - 4n + 4}{2} & \text{if } n \text{ is even.} \end{cases}
 \end{aligned}$$

**Example 2.** Let  $T \cong T'_{n,p,q}$ . Then  $p + q = \lceil \frac{n}{2} \rceil$  or  $\lfloor \frac{n}{2} \rfloor$ . Moreover,  $deg_{ve}(v) = n - 1$ ,  $deg_{ve}(v_i) = p + q + a_i$  for  $v_i \in N_T(v)$  with  $deg(v_i) > 1$ ,  $deg_{ve}(v_i) = p + q$  for  $v_i \in N_T(v)$  with  $deg(v_i) = 1$ , and  $deg_{ve}(v_i) = a_j + 1$  for  $v_i \in N_T(v_j)$ ,  $1 \leq j \leq q$  with  $deg(v_i) = 1$ . Since  $\sum_{i=1}^q a_i = n - p - q - 1$  and  $p + q = \lceil \frac{n}{2} \rceil$  or  $\lfloor \frac{n}{2} \rfloor$ , we obtain

$$\begin{aligned}
 irr_{ve}(T) &= \sum_{i=1}^q (n - 1 - p - q - a_i) + \sum_{i=q+1}^{p+q} (n - 1 - p - q) + \sum_{i=1}^q (p + q - 1) a_i \\
 &= \sum_{i=1}^q \left( n - 1 - p - q + (p + q - 2) a_i \right) + (n - 1 - p - q) p \\
 &= (n - p - q - 1) (p + q) + (p + q - 2) (n - p - q - 1) \\
 &= 2 (n - p - q - 1) (p + q - 1) = 2 \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil.
 \end{aligned}$$

Now we present the corrected statement of Theorem 1 of [36] as follows, along with a detailed proof.

**Theorem 2.** Let  $T$  be a tree of order  $n$ . Then

$$irr_{ve}(T) \leq 2 \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil \tag{7}$$

with equality if and only if  $T \cong T'_{n,p,q}$  ( $p + q = \lceil \frac{n}{2} \rceil$  or  $\lfloor \frac{n}{2} \rfloor$ ) or  $T \cong DS_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}$ .

**Proof.** Let  $d$  be the diameter of tree  $T$ . If  $d = 2$ , then  $T \cong K_{1,n-1}$ . In this case  $deg_{ve}(v_i) = n - 1$  for all  $v_i \in V(T)$ . Thus, we have

$$irr_{ve}(T) = \sum_{v_i, v_j \in E(T)} |deg_{ve}(v_i) - deg_{ve}(v_j)| = 0 < 2 \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil.$$

Otherwise,  $d \geq 3$ . We consider the following cases:

**Case 1:**  $d = 3$ . In this case  $T \cong DS_{p,q}$  ( $p + q = n - 2$ ,  $p \geq q$ ). Let  $v_1$  and  $v_2$  ( $deg(v_1) \geq deg(v_2)$ ) be two non-pendant vertices in  $T$ . We have

$$deg(v_i) = \begin{cases} p + 1 & \text{if } i = 1, \\ q + 1 & \text{if } i = 2, \\ 1 & \text{otherwise.} \end{cases}$$

Moreover,  $deg_{ve}(v_1) = n - 1, deg_{ve}(v_2) = n - 1, deg_{ve}(v_i) = p + 1$  for  $v_i \in N_T(v_1)$  with  $deg(v_i) = 1$ , and  $deg_{ve}(v_j) = q + 1$  for  $v_j \in N_T(v_2)$  with  $deg(v_j) = 1$ . Since  $p + q = n - 2$ , using these results, we obtain

$$\begin{aligned}
 irr_{ve}(T) &= \sum_{v_i v_j \in E(T)} |deg_{ve}(v_i) - deg_{ve}(v_j)| \\
 &= p(n - p - 2) + q(n - q - 2) \\
 &= 2pq \leq 2 \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor
 \end{aligned}$$

with equality if and only if  $T \cong DS_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor}$ .

**Case 2:**  $d = 4$ . Since  $T$  has  $n$  vertices with diameter 4, we have  $T \cong T_{n,4}$ . Then there exists a vertex  $v$  in  $T$  such that  $T - v = pK_1 \cup_{i=1}^q K_{1, a_i}$ , where  $n = \sum_{i=1}^q a_i + q + p + 1$ . We have

$$deg(v_i) = \begin{cases} p + q & v_i = v, \\ a_i + 1 & 1 \leq i \leq q, \\ 1 & \text{otherwise.} \end{cases}$$

Moreover,  $deg_{ve}(v) = n - 1, deg_{ve}(v_i) = p + q + a_i$  for  $v_i \in N_T(v)$  with  $deg(v_i) > 1$ ,  $deg_{ve}(v_i) = p + q$  for  $v_i \in N_T(v)$  with  $deg(v_i) = 1$ , and  $deg_{ve}(v_i) = a_j + 1$  for  $v_i \in N_T(v_j), 1 \leq j \leq q$  with  $deg(v_i) = 1$ . We obtain

$$\begin{aligned}
 irr_{ve}(T) &= \sum_{v_i v_j \in E(T)} |deg_{ve}(v_i) - deg_{ve}(v_j)| \\
 &= \sum_{j=1}^q |deg_{ve}(v) - deg_{ve}(v_j)| + \sum_{j=1}^p |deg_{ve}(v) - deg_{ve}(v_{q+j})| \\
 &\quad + \sum_{j=1}^q \sum_{\substack{v_i \in N_T(v_j), \\ deg(v_i)=1}}^{a_j} |deg_{ve}(v_i) - deg_{ve}(v_j)| \\
 &= \sum_{j=1}^q \left[ \sum_{i=1}^q a_i - a_j \right] + p \sum_{j=1}^q a_j + (p + q - 1) \sum_{j=1}^q a_j \\
 &= \sum_{j=1}^q \sum_{i=1}^q a_i + p \sum_{j=1}^q a_j + (p + q - 2) \sum_{j=1}^q a_j \\
 &= (p + q)(n - p - q - 1) + (p + q - 2)(n - p - q - 1) \\
 &= 2(p + q - 1)(n - p - q - 1). \tag{8}
 \end{aligned}$$

Let us consider a function

$$f(x) = (x - 1)(n - x - 1).$$

Then  $f'(x) = n - 2x$ . Therefore  $f(x)$  is an increasing function on  $x \leq n/2$  and a decreasing function on  $x \geq n/2$ . Hence,

$$f(x) \leq \max \left\{ f \left( \left\lceil \frac{n}{2} \right\rceil \right), f \left( \left\lfloor \frac{n}{2} \right\rfloor \right) \right\} = \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor,$$

with equality holding if and only if  $x = \lfloor \frac{n}{2} \rfloor$  or  $\lceil \frac{n}{2} \rceil$ . Using the above result in (8), we obtain

$$irr_{ve}(T) \leq 2 \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor,$$

with equality holding if and only if  $T \cong T_{n,4}$  with  $p + q = \lceil \frac{n}{2} \rceil$  or  $\lfloor \frac{n}{2} \rfloor$ , that is, if and only if  $T \cong T'_{n,p,q}$  ( $p + q = \lceil \frac{n}{2} \rceil$  or  $\lfloor \frac{n}{2} \rfloor$ ).

**Case 3:**  $d \geq 5$ . Let  $P_{d+1} : v_1 v_2 \dots v_d v_{d+1}$  be a diametral path in  $T$ . Without loss of generality, we can assume that  $deg(v_3) \leq deg(v_{d-1})$ . Then  $deg(v_3) \leq \frac{n-2}{2}$ . Let  $T' = T - v_1$ . Also, let  $V(T') = \{v'_2, v'_3, \dots, v'_n\} = V(T) - v_1$ , where  $v'_i = v_i$  for  $i = 2, 3, \dots, n$ . For any  $v_i v_j \in E(T')$ ,

$$|deg_{ve}(v'_i) - deg_{ve}(v'_j)| = \begin{cases} |deg_{ve}(v_i) - deg_{ve}(v_j)| & \text{if } i = 2, \\ |deg_{ve}(v_i) - deg_{ve}(v_j) - 1| & \text{if } i = 3, j \neq 2, \\ |deg_{ve}(v_i) - deg_{ve}(v_j)| & \text{if } i, j \notin \{2, 3\}. \end{cases}$$

For any edge  $v_3 v_j \in E(T - v_1)$  ( $j \neq 2$ ), one can easily check that

$$|deg_{ve}(v_3) - deg_{ve}(v_j)| \leq |deg_{ve}(v_3) - deg_{ve}(v_j) - 1| + 1$$

and, hence,

$$\sum_{\substack{v_j: v_3 v_j \in E(T-v_1) \\ j \neq 2}} \left[ |deg_{ve}(v_3) - deg_{ve}(v_j)| - |deg_{ve}(v_3) - deg_{ve}(v_j) - 1| \right] \leq deg(v_3) - 1.$$

Using the above results, we obtain

$$\begin{aligned} & irr_{ve}(T) - irr_{ve}(T - v_1) \\ &= \sum_{v_i v_j \in E(T)} |deg_{ve}(v_i) - deg_{ve}(v_j)| - \sum_{v'_i v'_j \in E(T-v_1)} |deg_{ve}(v'_i) - deg_{ve}(v'_j)| \\ &= deg_{ve}(v_2) - deg_{ve}(v_1) + \sum_{v_i v_j \in E(T-v_1)} \left[ |deg_{ve}(v_i) - deg_{ve}(v_j)| - |deg_{ve}(v'_i) - deg_{ve}(v'_j)| \right] \\ &= deg(v_3) - 1 + \sum_{v_j: v_2 v_j \in E(T-v_1)} \left[ |deg_{ve}(v_2) - deg_{ve}(v_j)| - |deg_{ve}(v'_2) - deg_{ve}(v'_j)| \right] \\ &\quad + \sum_{\substack{v_j: v_3 v_j \in E(T-v_1), \\ j \neq 2}} \left[ |deg_{ve}(v_3) - deg_{ve}(v_j)| - |deg_{ve}(v'_3) - deg_{ve}(v'_j)| \right] \\ &\quad + \sum_{\substack{v_i v_j \in E(T-v_1), \\ i, j \notin \{2, 3\}}} \left[ |deg_{ve}(v_i) - deg_{ve}(v_j)| - |deg_{ve}(v'_i) - deg_{ve}(v'_j)| \right] \\ &= deg(v_3) - 1 + \sum_{\substack{v_j: v_3 v_j \in E(T-v_1) \\ j \neq 2}} \left[ |deg_{ve}(v_3) - deg_{ve}(v_j)| - |deg_{ve}(v_3) - deg_{ve}(v_j) - 1| \right] \\ &\leq 2 \left( deg(v_3) - 1 \right) \leq n - 4. \end{aligned}$$

Therefore, by the mathematical induction hypothesis with the above result, we obtain

$$\begin{aligned} irr_{ve}(T) &\leq irr_{ve}(T - v_1) + n - 4 \leq 2 \left\lceil \frac{n-3}{2} \right\rceil \left\lfloor \frac{n-3}{2} \right\rfloor + n - 4 \\ &< 2 \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor \end{aligned}$$

and (7) holds strictly by induction. This completes the proof of the theorem.  $\square$

#### 4. Concluding Remarks

In this report, we have unveiled the application potential of  $irr_{ve}$  in structure-property modelling. It has been found that  $irr_{ve}$  can model the acentric factor of octanes and the boiling point of benzenoid hydrocarbons in combination with  $Alb$  index with powerful accuracy. We have established that  $irr_{ve}$  is weakly correlated with existing indices, which indicates its appearance as a meaningful molecular descriptor. Furthermore, it has been observed that the upper bound and corresponding extremal graphs of  $ve$ -degree irregularity index for the class of all trees are determined incorrectly in [36]. Later, the updated result was demonstrated. We have found some extra classes of graphs as extremal structure, when compared with the previous version. Future research on this index might focus on tight bounds estimation for the unicyclic, bicyclic, and tricyclic classes of graphs with identifying extremal structures.

**Author Contributions:** Conceptualization, K.C.D.; investigation, K.C.D., S.M.; writing—original draft preparation, K.C.D., S.M.; writing—review and editing, K.C.D., S.M. All authors have read and agreed to the submitted version of the manuscript.

**Funding:** The first author is supported by National Research Foundation funded by the Korean government (Grant No. 2021R1F1A1050646). The second author is grateful to the Department of Science and Technology (DST), Government of India for the INSPIRE Fellowship [IF170148].

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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