

## Original Research Article

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# A theoretical study on correlation analysis between eccentricity of VL-index and the physical properties of alkanes

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## Abstract

Topological indices are mathematical techniques used to mathematically correlate the relationship between the chemical structure and various physical attributes, chemical reactivity, or biological activity. In this research studies, the interaction of various chemical compounds(alkanes), their structures, and the eccentricity of the VL-Index., using the First and Second Zagreb, and reformulated First Zagreb indices, we investigate the  $\xi$ VL index may be considered as an useful tool in predicting the physical properties of lower alkanes.

*Keywords:* VL-Index, Status, Reciprocal status index and Temperature index and Graph operations.

AMS Subject Classification: 05C35; 05C90; 05C12.

## 1 Introduction

The definition of a topological index is a real function that converts a chemical graph into a real value. The quantitative structure activity relationship (QSAR) and the quantitative structure property relationship (QSPA) are well correlated with topological indices. Vertex degree-based topological indices have been utilized for more than 40 years. The Topological Index is a mathematical indicator of chemical nature that seeks to correlate chemical structure with various physical properties, chemical reactivity, or biological activity. If  $Gr$  denotes the class of all finite graphs. Clearly, the number of vertices and the number of edges are the two fundamental parameters in topological indices. Numerous topological indices have been developed and used in recent years for a variety of purposes, including chemical documentation, isomer discrimination, molecular complexity research, chirality, similarity/dissimilarity, QSAR/QSPR, drug design, database selection, lead optimization, etc. The first and second Zagreb indices[8] are two of the most helpful topological graph indices. In several mathematical and chemical applications, particularly in the study of molecular graphs in chemistry[7], both Zagreb indices are employed to offer information about the structural characteristics of the graph. They belong to a group of graph indices that have been successful in evaluating and contrasting various kinds of networks because they capture numerous facets of a graph's topology.

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## 2 Materials and Methods

Many scholars have found bounds for many topological indices. Only a few of those indices are listed below.

The Gutman and Trinajestic[8,9] are define the Zagreb indices as

$$M_1(G) = \sum_{uv \in E(G)} [d_u + d_v]$$

$$M_2(G) = \sum_{uv \in E(G)} [d_u \cdot d_v]$$

The Kulli et al.[5,6] defined the first Gourava index as follows

$$GO_1(G) = \sum_{uv \in E(G)} [d_u + d_v + d_u d_v]$$

The Furtula et al.[3,11]defined the Forgotten topological index as

$$F(G) = \sum_{uv \in E(G)} [d_u + d_v]^2$$

The V.S. Shegehalli et al.[12] defined the SK indices as follows

$$SK_1(G) = \sum_{uv \in E(G)} \left[ \frac{d_u + d_v}{2} \right]$$

The Milicevic et al.[10] defined the first reformulated Zagreb index as follows[12][13]

$$EM_1(G) = \sum_{uv \in E(G)} [d_u + d_v - 2]^2$$

The second Zagreb index  $M_2(G)$  is equivalent to the sum of the products of the degrees of pairs of adjacent vertices, while the first Zagreb index  $M_1(G)$  is equivalent to the sum of squares of the degrees of the vertices of the underlying molecular graph  $G$ . Many academics are working on the Zagreb indices. Due to their applicability in the realm of chemical sciences, their extended versions ended up being the most fascinating aspect of the research[14][15]. The V L index was created in 2020 and was inspired by the works of the Zagreb indices. Invoking Veerabhadraiah Lokesha index introduced by Deepika T. The VL index is defined as[16]

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} [d_e + d_f + 4]$$

where  $d_e = d_u + d_v - 2$  and  $d_f = d_u \cdot d_v - 2$ , such that  $d_u$  and  $d_v$  are the degree vertices of  $u$  and  $v$  in  $G$ , respectively.

The above VL-Index can also be written as

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} [d_u + d_v + d_u \cdot d_v]$$

**VL status index and Co-index:** The VL status index of a graph  $G$  is defined as,

$$VLS(G) = \frac{1}{2} \sum_{uv \in E(G)} [\sigma(u) + \sigma(v) + \sigma(u) \cdot \sigma(v)]$$

and, VL status Co-index of a graph G is defined as,

$$\overline{VLS(G)} = \frac{1}{2} \sum_{uv \notin E(G)} [\sigma(u) + \sigma(v) + \sigma(u) \cdot \sigma(v)]$$

**VL reciprocal status index and Co-index:**The VL reciprocal status index of a graph G is defined as,

$$VLR(S(G)) = \frac{1}{2} \sum_{uv \in E(G)} [rs(u) + rs(v) + rs(u) \cdot rs(v)]$$

and, VL reciprocal status co-index of a graph G is defined as,

$$\overline{VLR(S(G))} = \frac{1}{2} \sum_{uv \notin E(G)} [rs(u) + rs(v) + rs(u) \cdot rs(v)]$$

Be aware that Siemion Fajlowictas introduced the concept of the temperature of a vertex of a graph G. This temperature of a vertex u of a connected graph G is defined as

$$T_u(G) = \left[ \frac{d_u}{n - d_u} \right]$$

Where,  $d_u$  is the degree of a vertex u of a connected graph G and n is the total number of vertices of a graph G

**VL-Temperature index:**The VL-Temperature index of a graph G is defined as,

$$VLTI(G) = \frac{1}{2} \sum_{uv \in E(G)} [T_u + T_v + T_u \cdot T_v]$$

where  $T_u$  and  $T_v$  are the temperature of the vertex u and v, respectively.

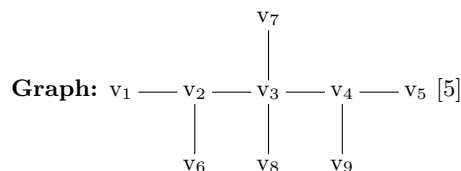
### Eccentricity of VL-Index

**Definition 2.1:** The Eccentricity of VL-Index of a graph G is defined as[16],

$$\xi[VL(G)] = \frac{1}{2} \sum_{uv \in E(G)} [\xi_u + \xi_v + \xi_u \cdot \xi_v]$$

Where,  $\xi_u$  and  $\xi_v$  are the Eccentricity of the vertex u and v in G, respectively.

For example, **2,3,3,4-Tetramethyl Pentane**,



Here,  $\xi_{v_1} = 4$ ,  $\xi_{v_4} = 3$ ,  $\xi_{v_3} = 2$ ,  $\xi_{v_2} = 3$ ,  $\xi_{v_5} = 4$ ,  $\xi_{v_6} = 4$ ,  $\xi_{v_7} = 3$ ,  $\xi_{v_8} = 3$ ,  $\xi_{v_9} = 4$

from the above figure

$$\xi[VL(G)] = \frac{1}{2} [19 + 19 + 11 + 11 + 11 + 11 + 19 + 19] = 60$$

### 3 Preliminary results:

Table 1: The interaction of various chemical compounds, their structures, and the eccentricity of the VL-Index

Sl. No.	Name of the Chemical Compound	Graph( Structure)	Total $\xi_{VL}$ -Index
01	Ethane	$v_1 - v_2$	1.5
02	Propane	$v_1 - v_2 - v_3$	5
03	Butane	$v_1 - v_2 - v_3 - v_4$	15
04	2-Methyl Propane	$v_1 - v_4 - v_2$   $v_3$	7.5
05	Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$	30
06	2- Methyl Butane	$v_1 - v_2 - v_3 - v_4$   $v_5$	20.5
07	2, 2- Dimethyl Profane	$v_1 - v_2 - v_3$   $v_4$   $v_5$	10
08	Hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$	55.5
09	2- Methyl Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$   $v_6$	39.5
10	3- Methyl Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$   $v_6$	35.5
11	2, 2- Dimethyl Butane	$v_1 - v_2 - v_3 - v_4$   $v_5$   $v_6$	26
12	2,3- Dimethyl Butane	$v_1 - v_2 - v_3 - v_4$   $v_5$   $v_6$	26
13	Heptane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7$	89
14	2- Methyl hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$   $v_7$	70
15	3- Methyl hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$   $v_7$	65

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16	3-ethyl hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$ $ $ $v_7 - v_8$	79.5
17	2,2 - Dimethyl Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$ $ $ $v_6$ $ $ $v_7$	49
18	2,3 - Dimethyl Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$ $ $ $v_6$ $ $ $v_7$	45
19	2,4 - Dimethyl Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$ $ $ $v_6$ $ $ $v_7$	49
20	3,3 - Dimethyl Pentane	$v_1 - v_2 - v_3 - v_4 - v_5$ $ $ $v_6$ $ $ $v_7$	41
21	2,3,3 - Trimethyl Butane	$v_1 - v_2 - v_3 - v_4$ $ $ $v_5$ $ $ $v_6$ $ $ $v_7$	31.5
22	Octane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7 - v_8$	55.5
23	2- Methyl heptane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7$ $ $ $v_8$	109.5
24	3- Methyl heptane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7$ $ $ $v_8$	103.5
25	4- Methyl heptane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7$ $ $ $v_8$	98.5
26	2,2 - Dimethyl hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$ $ $ $v_7$ $ $ $v_8$	84.5
27	2,3 - Dimethyl hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$ $ $ $v_7$ $ $ $v_8$	89
28	2,4 - Dimethyl hexane	$v_1 - v_2 - v_3 - v_4 - v_5 - v_6$ $ $ $v_7$ $ $ $v_8$	79.5

*Continued on next page*









71	2,2,4,4-Tetramethyl, Pantane	$  \begin{array}{ccccccc}  & & v_6 & & v_8 & & \\  & &   & &   & & \\  v_1 & - & v_2 & - & v_3 & - & v_4 & - & v_5 \\  & &   & & & &   & & \\  & & v_7 & & & & v_9 & &   \end{array}  $	68
72	2,3,3,4-Tetramethyl, Pantane	$  \begin{array}{ccccccc}  & & & & v_7 & & \\  & & & &   & & \\  v_1 & - & v_2 & - & v_3 & - & v_4 & - & v_5 \\  & &   & &   & &   & & \\  & & v_6 & & v_8 & & v_9 & &   \end{array}  $	60
73	4-Ethyl Pantane	$  \begin{array}{ccccccccccc}  v_1 & - & v_2 & - & v_3 & - & v_4 & - & v_5 & - & v_6 & - & v_7 \\  & & & & & &   & & & & & & \\  & & & & & & v_8 & & & & & & v_9 \\  & & & & & &   & & & & & & \\  & & & & & & v_8 & - & v_9 & & & &   \end{array}  $	113

## 4 Correlation between $\xi$ VL-Index and the physical properties

[11] We carry a correlation analysis to find relations between the physical properties - Boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of lower alkanes with  $\xi$ VL-index indices of their molecular graphs. Table 1 gives the  $\xi$ VL-index of molecular graphs of the considered lower alkanes. For the analysis the experimental values of the physical properties - Boiling points ( $bp$ )  $^{\circ}C$ , molar volumes ( $mv$ )  $cm^3$ , molar refractions ( $mr$ )  $cm^3$ , heats of vaporization ( $hv$ )  $kJ$ , critical temperatures ( $ct$ )  $^{\circ}C$ , critical pressures ( $cp$ )  $atm$ , and surface tensions( $st$ )  $dyne\ cm^{-1}$  of considered alkanes are taken from Seybold et al. [2] and Needham et al. [1] (the same values can be found in the research articles [3, 4]). The correlation coefficient  $r$  is computed and tabulated in Table 2:  $r$  for the physical properties and  $\xi$ VL-index.

Table 2:  $r$  for the physical properties and  $\xi$ VL-index

Physical Properties	$r$
$bp$	0.720224306
$mv$	0.736004494
$mr$	0.693701013
$hv$	0.790991841
$ct$	0.605809051
$cp$	-0.849864306
$st$	0.54576317

## 5 Conclusions

As per statistical theories, if we wish to label the strength of the association, for absolute values of  $r$ , 0-0.19 is regarded as very weak, 0.2-0.39 as weak, 0.40-0.59 as moderate, 0.6-0.79 as strong and 0.8-1 as very strong correlation.

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Table 2:  $r$ , reveals that the  $\xi$ VL index shows strong correlation with boiling points, molar volumes, molar refractions, heats of vaporization and critical temperatures, where as it shows very strong correlation with critical pressures. But it shows moderate correlation with surface tensions.

Hence, we can conclude that the  $\xi$ VL index may be considered as an useful tool in predicting the physical properties of lower alkanes.

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