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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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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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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 ξVL 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 Classication: 05C35, 5C90, 05C12.

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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 [1] are two of the most helpful topological graph indices.In several mathematical and chemical applications, particularly in the study of molecular graphs in chemistry[2], 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.

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[1,3] 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.[4,5] 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.[6,7]defined the Forgotten topological index as

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

The V.S. Shegehalli et al.[8] 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.[9] defined the first reformulated Zagreb index as follows[8][10]

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

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[11][12]. 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[12]:

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

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,

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

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

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

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.

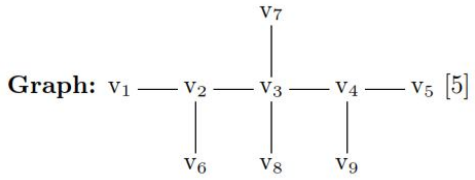
Eccentricity of VL-Index

Definition 2.1: The Eccentricity of VL-Index of a graph G is defined as[15],

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

Where , ξ_u and ξ_v are the Eccentricity of the vertex u and v in G, respectively.

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



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 ξVL-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_4 | v_1 — v_2 — v_3 | 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_5 | v_1 — v_2 — v_3 — v_4 | 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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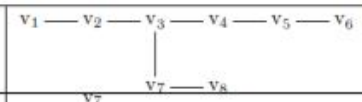
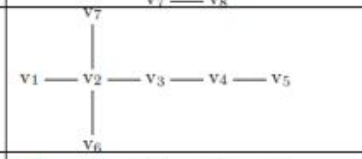
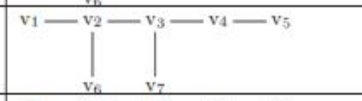
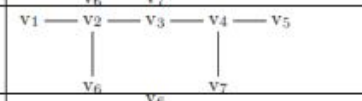
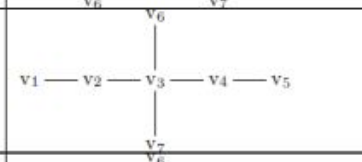
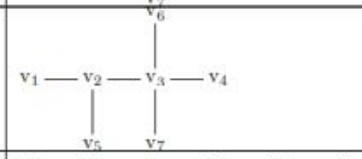
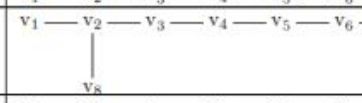
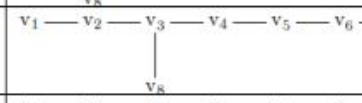
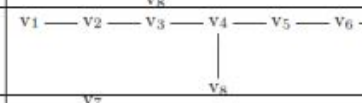
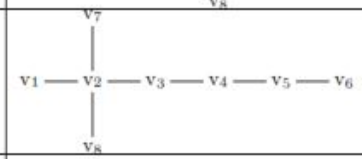
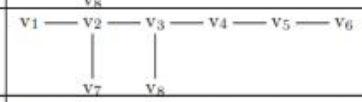
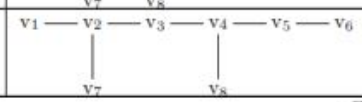
16	3-ethyl hexane		79.5
17	2,2 - Dimethyl Pentane		49
18	2,3 - Dimethyl Pentane		45
19	2,4 - Dimethyl Pentane		49
20	3,3 - Dimethyl Pentane		41
21	2,3,3 - Trimethyl Butane		31.5
22	Octane		55.5
23	2- Methyl heptane		109.5
24	3- Methyl heptane		103.5
25	4- Methyl heptane		98.5
26	2,2 - Dimethyl hexane		84.5
27	2,3 - Dimethyl hexane		89
28	2,4 - Dimethyl hexane		79.5

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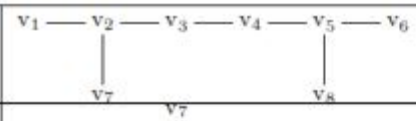
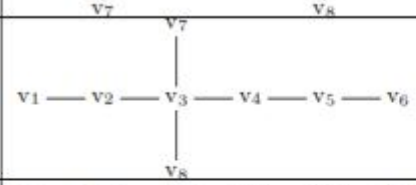
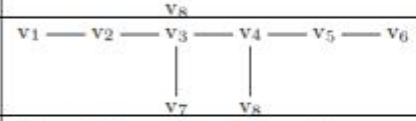
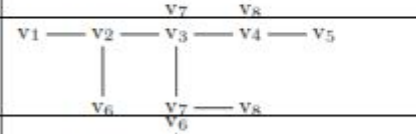
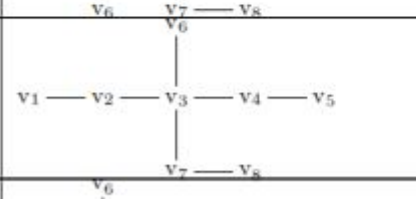
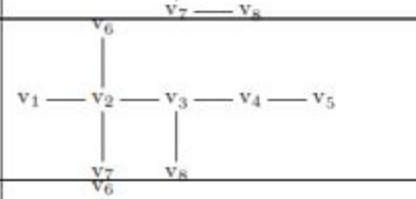
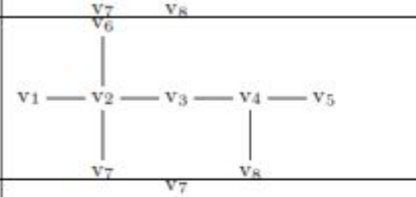
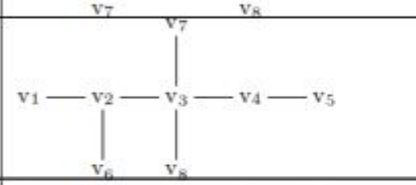
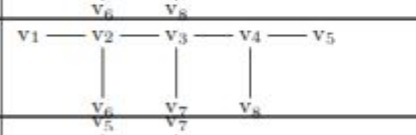
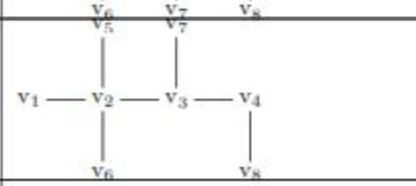
29	2,5 - Dimethyl hexane		84.5
30	3,3 - Dimethyl hexane		74.5
31	3,4 - Dimethyl hexane		74.5
32	3-ethyl, 2-Methyl pentane		54.5
33	3-ethyl, 3-Methyl pentane		50.5
34	2,2,3 - Dimethyl Pentane		54.5
35	2,2,4 - Dimethyl Pentane		58.5
36	2,3,3 - Trimethyl Pentane		50.5
37	2,3,4 - Trimethyl Pentane		54.5
38	2,2,3,3 - Tetra Methyl Butane		37
39	Nonane		196

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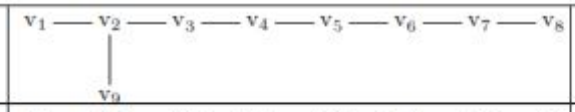
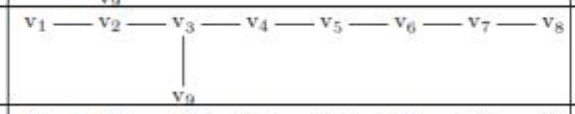
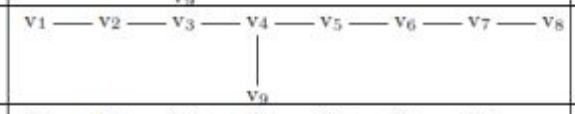
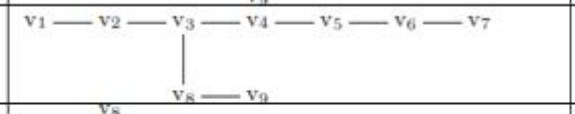
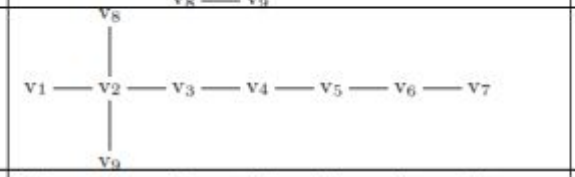
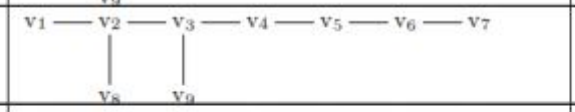
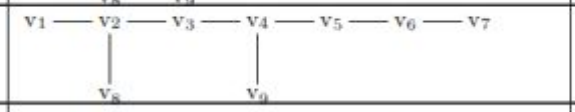
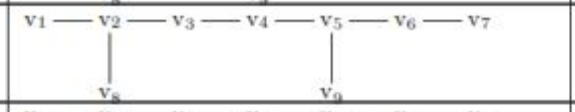
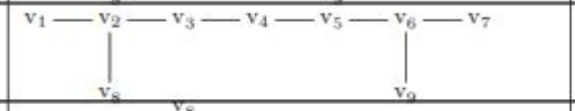
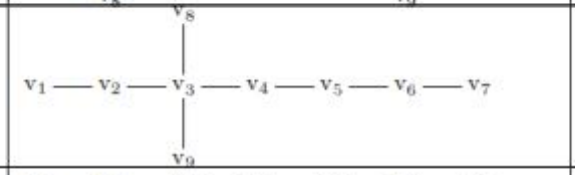
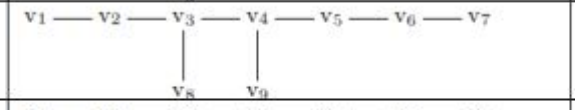
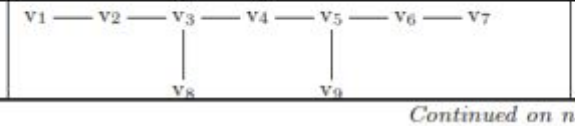
40	2-Methyl Octane		164.5
41	3-Methyl Octane		157.5
42	4-Methyl Octane		151.5
43	3-Ethyl Heptane		124
44	2,2 -Dimethyl heptane		130
45	2,3 -Dimethyl heptane		124
46	2,4 -Dimethyl heptane		119
47	2,5 -Dimethyl heptane		124
48	2,6 -Dimethyl heptane		130
49	3,3 -Dimethyl heptane		118
50	3,4-Dimethyl heptane		113
51	3,5-Dimethyl heptane		118

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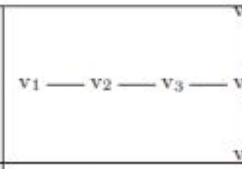
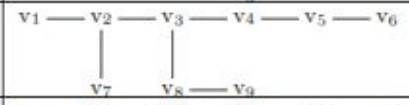
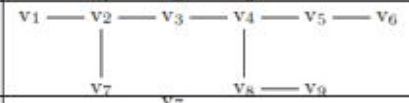
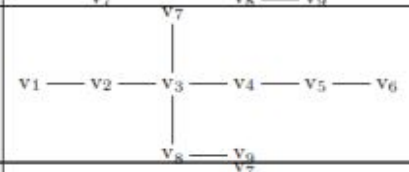
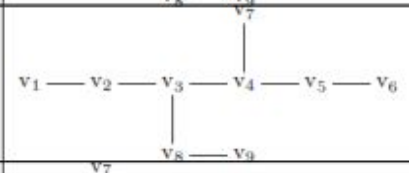
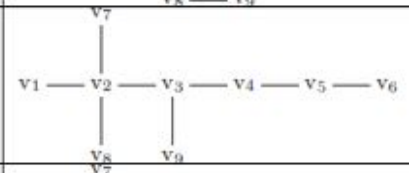
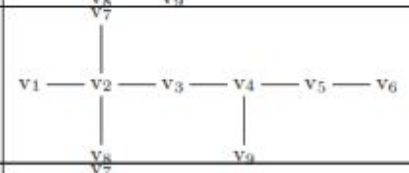
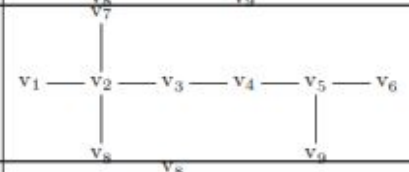
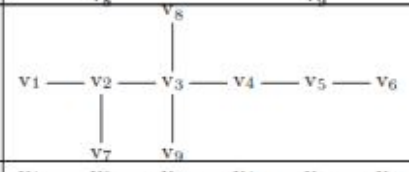
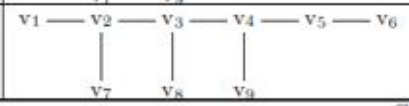
52	4,4 -Dimethyl heptane		108
53	3-Ethyl,2-Methyl Hexane		94
54	4-Ethyl,2-Methyl Hexane		94
55	3-Ethyl,3-Methyl Hexane		89
56	3-Ethyl,4-Methyl Hexane		87
57	2,2,3 -Trimethyl hexane		94
58	2,2,4 -Trimethyl hexane		94
59	2,2,5 -Trimethyl hexane		99
60	2,3,3 -Trimethyl hexane		89
61	2,3,4 -Trimethyl hexane		89

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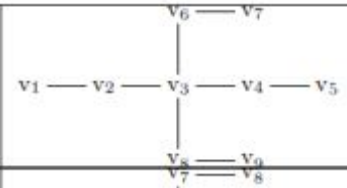
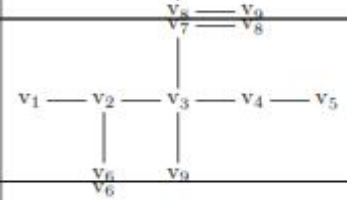
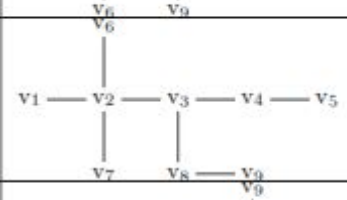
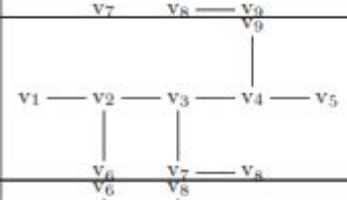
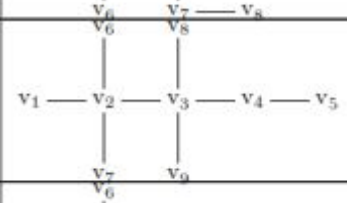
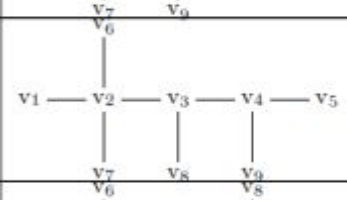
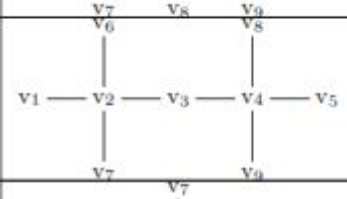
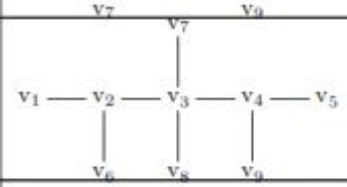
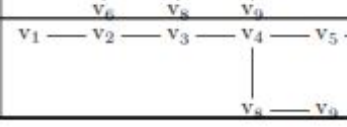
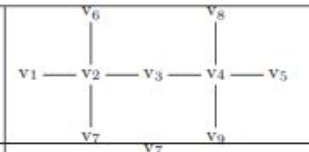
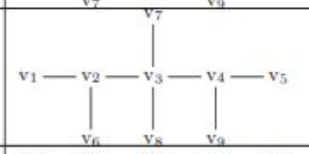
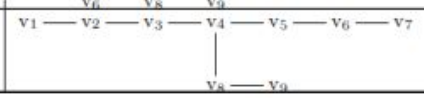
65	3,3-Diethyl Pantane		60
66	2,3-Diethyl,3-Ethyl Pantane		60
67	2,2-Diethyl,3-Ethyl Pantane		64
68	2,2-Diethyl,3-Ethyl Pantane		64
69	2,2,3,3-Tetramethyl, Pantane		60
70	2,2,3,4-Tetramethyl, Pantane		64
71	2,2,4,4-Tetramethyl, Pantane		68
72	2,3,3,4-Tetramethyl, Pantane		60
73	4-Ethyl Pantane		113

71	2,2,4,4-Tetramethyl, Pantane		68
72	2,3,3,4-Tetramethyl, Pantane		60
73	4-Ethyl Pantane		113

4 Correlation between ξVL-Index and the Physical Properties

[7] 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 ξVL-index indices of their molecular graphs. Table 1 gives the ξVL-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. [13] and Needham et al. [14] (the same values can be found in the research articles [6, 15]). The correlation coefficient r is computed and tabulated in Table 2: r for the physical properties and ξVL-index.

Table 2. r for the physical properties and ξVL-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.

Table 2: **r**, reveals that the ξVL 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 ξVL index may be considered as an useful tool in predicting the physical properties of lower alkanes.

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Competing Interests

Authors have declared that no competing interests exist.

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