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On The Correlation Analysis Between Vector Index Of Alkanes

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Abstract: The primary aim of this article is to introduce the Zagreba Vector Index for the chemical graphs. Here in this research article, the topological indices were partially replaced by the new approach, Vector index for graphs. The vector index is named as Zagreb vector index, and used to study the physical properties of various chemical compounds (alkanes), their structures, the correlativity with the Vector-Index. In determining the Vector index, I have used total degree of the vertex (du), as the first component of the vector along with two more components to create a vector index. In the vector index of an atom, there will be three components, the first component of the vector is it's total degree du, second component is number of similar atoms adjacent to it d1u and the third component is number of heterogeneous atoms adjacent to it d2u. After a thorough investigate, the Vector index found to be a useful tool in predicting the physical properties of lower alkanes..

Keywords: Vector-Index; Topological index, Chemical graphs, Graph operations AMS Subject Classication: 05C35, 5C90, 05C12.

1 **Introduction**: From it's inception, the topological index of a graph, is used as a mathematical tool that converts a chemical graph into a real value based set of indexes. The Topological Index gives various impetus over the years, as a mathematical indicator of chemical nature that seeks to correlate chemical structure with various physical properties, chemical reactivity, or biological activity. Clearly, the number of vertices and the number of edges were 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. Even though the topological indices formed a strong valuable tool in predicting properties of certain family of Chemical compounds, still it needs major changes to correlate more precisely with physical properties of substances. The major challenge is to distinguish between isomers of the chemical compounds. This draw back may be rectified in this article by considering the positon of atoms. A new approach of indexing the graph is introduced in this article, to overcome the draw backs of overlooking of the position of the vertices in the graph. In space, the position of a point is described with respect to three rectilinear components, which is as an ordered triple(x, y, z), thus vectors were introduced. Here the in this article, the atom in the straight chain n-Alkane is indexed by a Vector, with three components. Vector is an ordered n-tuple of numbers[13] used to represent various physical quantities and properties, geometrical shapes. Vectors plays important rules in Physics, Chemistry and all branches of life sciences. The quantitative structure activity relationship (QSAR) and the quantitative structure property relationship (QSPA) are also well correlated with new

vector indices. Now in this article, as mentioned in the abstract, I am modified the topological indices as vector indices. Such type of study not only concentrates on the chain form of compounds but also includes the isomers in the study. Vector indices are similar to the Topological indices, but have more than one component and provide very closely estimated values to the practical values. In Vector index of an atom, vertex degree-based numbers are used as in topological indices. The first and second Zagreb indices [1] are two of the most helpful topological graph indices, which are modified here in this article, to include vector indices. In several mathematical and chemical applications, particularly in the study of molecular graphs in chemistry, these type of indices may be employed to offer information about the structural characteristics of the graph. Further the study of applications of Vector indices, connected to various type of graphs like completely connected graphs, degree regular graphs etc will be presented in the forth coming publications. Here, we mention the new vector index, naming it as Zagreb[] Vector Index, and study the variation of indexes in case of straight chain n-Alkanes.

2 **Materials and Methods**: Most of the materials were brought from the earlier literature on the topological indices. As many scholars defined various topological indices and obtained bounds for those topological indices, my effort is only to use similar topological indices along with the number of similar atoms in adjacent vertices, to create vector indices. While creating vector indices, counting or numbering of edges in the alkanes are started from left side C-H bound and numbered the edges in anti-cyclic way. The study shows these vector indices gives more precise correlation between the vector indices and physical properties of the chemical compounds. Following list provides few type of topological indices that are used in the earlier literatures. But in this article these indices are modified to include corresponding vector indices of Chemical graphs.

The Gutman and Trinajestic[] were defined the Zagreb indices as

$M1(G)= \sum_{uv\in E(G)}[du + dv]$

$M2(G)= \sum_{uv\in E(G)}[du \,.\, dv]$

The Kulli et al.[4,5] defined the first Gourava index as follows

$GO1(G)= \sum_{uv\in E(G)}[du + dv] + du.dv$

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 recent research articles like, Narendra and Mahalakshmi; Asian Res. J. Math., vol. 19, no. 10, pp. 103-113, 2023; Article no.ARJOM.104981 research[ ][ ]. 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[ ]: $V L(G) = \sum_{uv\in E(G)}[de + df + 4]$ where de=du+dv −2 and df=du ·dv −2, such that du and dv are the degree vertices of u and v in G, respectively. In this article also, all the above type of activities are considered on the same lines, but the topological indices were replaced by vector indices of the vertices. A vector index of a vertex u in the graph is defined as lu=(du, d1u, d2u), where du is the degree (total number of atoms adjacent to u) of the vertex u, d1u is the number of similar atoms adjacent to the vertex u, d2u is the number of different atoms adjacent to u. Further similar to the Zagreb index, I define First and Second Zagreb vector index as follows

$MV1(G)= \| \sum_{uv\in E(G)}(lu + lv) \|$

$MV2(G)= \|\sum_{uv\in E(G)}(l(u) + l(y))\|$

Where || (a, b, c) || is the two norm of the vector (a, b, c), that is (a, b, c)|=$\sqrt{a^2 + b^2 + c^2}$

Lemma 1: The Zagreb vector index of the Methane is ||(20, 0, 20)|| =.$\sqrt{800}$

Prrof: The Methane molecule has the following chemical structure, with the chemical formula CH_4,

$$H-\begin{array}{c}H\\|\\C\\|\\H\end{array}-H$$ Each edge is a bound between an H atom and a C atom, the vector index of C atom is (4, 0, 4) and vector index of each H atom is (1, 0, 1). So the Zagreb vector index of entire Methane molecule is

$\sum_{H-C\in E(G)} (l(C) + l(H))$ =4{(4, 0, 4) + (1, 0, 1)}=(20, 0, 20)

Lemma 2: The Zagreb vector index of the Ethane is ||(38, 8, 30)||= $\sqrt{2408}$.

Prrof: The Ethane molecule has the following chemical structure, with the chemical formula C_2H_6,

$$H-\begin{array}{c}H\\|\\C\\|\\H\end{array}\begin{array}{c}H\\|\\-C\\|\\H\end{array}-H$$ Each edge is a bound between an H atom and a C atom, except the middle edge E3, here the vector index of C atom is (4, 1, 3) and vector index of each H atom in the edges E1,E2, E4, E5, E6, E7 is (1, 0, 1). So the Zagreb vector index of entire Ethane molecule is

$\sum_{H-C\in E(G)} (l(C) + l(H)) + (l(C) + l(C))$ =6{(4, 1, 3) + (1, 0, 1)}+{2(4, 1, 3)}=(30, 6, 24) + (8, 2, 6) = (38, 8, 30)

Lemma 3: The Zagreb vector index of the Alkane $C_nH_{(2n+2)}$, (when n is greater than or equal to 3) is $||(n-3)(8,4,4) + 2(8,3,5) + (n-2)(5,2,3) + 6(5,1,4)||$

Proof: Alkanes $C_nH_{(2n+2)}$ in it's chain form has (2n+3) edges(where n ≥ 3). There are four cases t o consider

1. Total C – C edges except E3 and E2n-1 edges are (n-3). Hence for these edges $\sum_{(u,v)gE_c(G)}(l(C) + l(C))$ =(n – 3)(8, 4, 4)
2. The two edges E3 and E2n-1 where each C-atom is connected to only one C atom =$\sum_{(u,v)gE_c(G)}(l(C) + l(C))$ =2(8, 3, 5) = (16, 6, 10)
3. Out of all those C-H edges except on the 1st and nth C-atom $\sum_{(u,v)gE_c(G)}(l(C) + l(H))$ = (n-2)(5, 2, 3)
4. Six edges with C-H bonding on the 1st and nth C-atom = 6(5, 1, 4)

Hence for the total (2n + 3) edges

$\sum_{(u,v)gE(G)}(l(u) + l(v))$ = (n – 3)(8, 4, 4) + 2(8, 3, 5) + (n – 2)(5, 2, 3) + 6(5, 1, 4).

Hence the result. We use maxima software to calculate the above values, for n=3 to n=10, as follows. The function f(n):=(n-3)*[8,4,4]+2*[8,3,5]+(n-2)*[5,2,3]+6*[5,1,4]; is used, with the arguments as n. Then we find the norm each resulting vector. The results obtained gives the ZAGREB vector indexes for each straight chain alkanes, which are listed in the table 1 as MV1 index.

Correlation between MV1-Index and the Physical Properties of lower alkanes are analysed to find relations between the physical properties - Boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions considering their molecular graphs. Following Table 1 gives the MV1-index of molecular graphs of the considered lower straight chain alkanes along with

the boiling points, melting points, and similar properties. For the analysis the experimental values of the physical properties - Boiling points (bp) ◦C, molar mass, molar refractions (mr) cm3 , heats of vaporization (hv) kJ, critical temperatures (ct) ◦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]).

Table 1:

Alkane	MV!-index	Bp/C	Molar Mass	Melting point	St/dyne cm^{-1}
Methane(CH_4)	28.3	-164	16	-188	Gas
Ethane(C_2H_6)	49.07	-89	30	-186	0.48
Propane(C_3H_8)	64.54	-42	44	-183	7.0
Butane(C_4H_{10})	80.20	-1	58	-138	13
Pentane	95.94	36.1	72	-130	16
Hexane	111.75	68.7	86	-95	18.42
Heptane	127.59	98.4	100	-91	20.26
Octane	143.44	125.7	114	-57	21.76
Nonane	159.32	150.8	128	-54	22.92
Decane	175.20	174	142	-30	24.75

The co-relation coefficient between MV1 – index and Boiling point is 0.988396. Similarly the co-relation coefficient of MV1 – index with Molar Mass, Melting Point, and surface tension are 0.999658, 0.960999 , 0.951689 respectively. Hence all the physical properties are positively co-related with MV1 – index, with the co-relation coefficient nearly equal to 1. This shows the close proximity of MV1 – index with basic properties straight chain Alkanes.

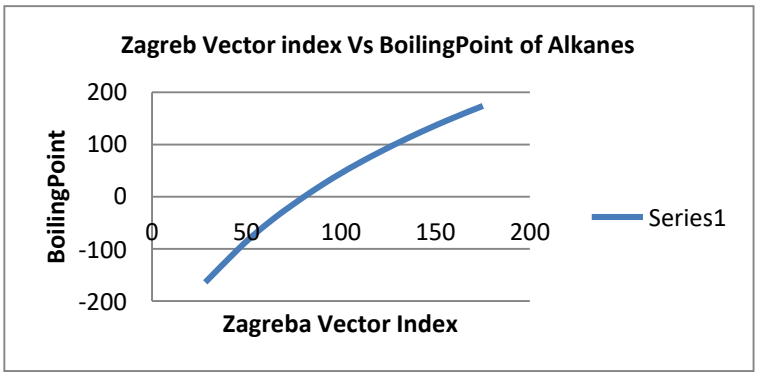
The following table gives the predicted values of n – Alkanes (Straight chain Alkanes), Zagreb Vector index MV1. A slight deviation in the Zagreb vector index for Alkanes shows that the chemical is not a Straight chain n-Alkane. Hence the Zagreb vector index for Alkanes can be used to distinguish the isomers from it's straight chain n-Alkanes. The formula connecting MV1 – index and the various parameters like Boiling point, Melting point, Surface tension etc are obtained using mathematical modelling techniques. Then the values are approximated upto n=111, are with a close proximaty to practical values.

Sl no	Formula	Alkane	MV1 – index
2	C_2H_6	Ethane	49.07
3	C_3H_8	Propane	64.54
4	C_4H_{10}	*n*-Butane	80.1997506 2
5	C_5H_{12}	*n*-Pentane	95.9479025 3
6	C_6H_{14}	*n*-Hexane	111.749720 4
7	C_7H_{16}	*n*-Heptane	127.585265 6
8	C_8H_{18}	*n*-Octane	143.443368 6
9	C_9H_{20}	*n*-Nonane	159.317293 5
10	$C_{10}H_{22}$	*n*-Decane	175.202739 7
11	$C_{11}H_{24}$	*n*-Undecane	191.096834 1
12	$C_{12}H_{26}$	*n*-Dodecane	206.997584 5
13	$C_{13}H_{28}$	*n*-Tridecane	222.903566 6
14	$C_{14}H_{30}$	*n*-Tetradecane	238.813734 9
15	$C_{15}H_{32}$	*n*-Pentadecane	254.727305 2
16	$C_{16}H_{34}$	*n*-Hexadecane	270.643677 2
17	$C_{17}H_{36}$	*n*-Heptadecane	286.562384 1
18	$C_{18}H_{38}$	*n*-Octadecane	302.483057 4
19	$C_{19}H_{40}$	*n*-Nonadecane	318.405402
20	$C_{20}H_{42}$	*n*-Eicosane	334.329179 1
21	$C_{21}H_{44}$	*n*-Heneicosane	350.254193 4
22	$C_{22}H_{46}$	*n*-Docosane	366.180283 5
23	$C_{23}H_{48}$	*n*-Tricosane	382.107314 8
24	$C_{24}H_{50}$	*n*-Tetracosane	398.035174 3
25	$C_{25}H_{52}$	*n*-Pentacosane	413.963766 5
26	$C_{26}H_{54}$	*n*-Hexacosane	429.893009 9
27	$C_{27}H_{56}$	*n*-Heptacosane	445.822834 8
28	$C_{28}H_{58}$	*n*-Octacosane	461.753180 8
29	$C_{29}H_{60}$	*n*-Nonacosane	477.683996
30	$C_{30}H_{62}$	*n*-Triacontane	493.615234 8
31	$C_{31}H_{64}$	*n*-Hentriacontane	509.546857 5
32	$C_{32}H_{66}$	*n*-Dotriacontane	525.478829 3
33	$C_{33}H_{68}$	*n*-Tritriacontane	541.411119 2
34	$C_{34}H_{70}$	*n*-Tetratriacontane	557.343700 1
35	$C_{35}H_{72}$	*n*-Pentatriacontane	573.276547 6
36	$C_{36}H_{74}$	*n*-Hexatriacontane	589.209640 1
37	$C_{37}H_{76}$	*n*-Heptatriacontane	605.142958 3
38	$C_{38}H_{78}$	*n*-Octatriacontane	621.076484 8
39	$C_{39}H_{80}$	*n*-Nonatriacontane	637.010204
40	$C_{40}H_{82}$	*n*-Tetracontane	652.944101 7
41	$C_{41}H_{84}$	*n*-Hentetracontane	668.878165 3
42	$C_{42}H_{86}$	*n*-Dotetracontane	684.812383 1
43	$C_{43}H_{88}$	*n*-Tritetracontane	700.746744 6
44	$C_{44}H_{90}$	*n*-Tetratetracontane	716.681240 2
45	$C_{45}H_{92}$	*n*-Pentatetracontane	732.615861 1

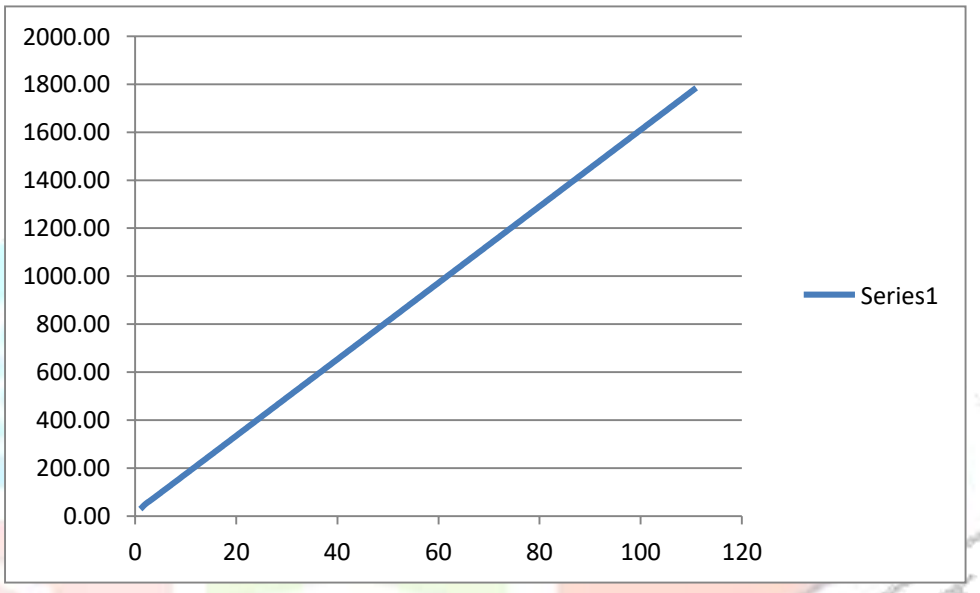
46	$C_{46}H_{94}$	*n*-Hexatetracontane	748.5505995
47	$C_{47}H_{96}$	*n*-Heptatetracontane	764.4854479
48	$C_{48}H_{98}$	*n*-Octatetracontane	780.4203995
49	$C_{49}H_{100}$	*n*-Nonatetracontane	796.3554483
50	$C_{50}H_{102}$	*n*-Pentacontane	812.2905884
51	$C_{51}H_{104}$	*n*-Henpentacontane	828.2258146
52	$C_{52}H_{106}$	*n*-Dopentacontane	844.1611221
53	$C_{53}H_{108}$	*n*-Tripentacontane	860.0965062
54	$C_{54}H_{110}$	*n*-Tetrapentacontane	876.0319629
55	$C_{55}H_{112}$	*n*-Pentapentacontane	891.9674882
56	$C_{56}H_{114}$	*n*-Hexapentacontane	907.9030785
57	$C_{57}H_{116}$	*n*-Heptapentacontane	923.8387305
58	$C_{58}H_{118}$	*n*-Octapentacontane	939.774441
59	$C_{59}H_{120}$	*n*-Nonapentacontane	955.7102071
60	$C_{60}H_{122}$	*n*-Hexacontane	971.6460261
61	$C_{61}H_{124}$	*n*-Henhexacontane	987.5818953
62	$C_{62}H_{126}$	*n*-Dohexacontane	1003.517812
63	$C_{63}H_{128}$	*n*-Trihexacontane	1019.453775
64	$C_{64}H_{130}$	*n*-Tetrahexacontane	1035.389782
65	$C_{65}H_{132}$	*n*-Pentahexacontane	1051.32583
66	$C_{66}H_{134}$	*n*-Hexahexacontane	1067.261917
67	$C_{67}H_{136}$	*n*-Heptahexacontane	1083.198043
68	$C_{68}H_{138}$	*n*-Octahexacontane	1099.134205
69	$C_{69}H_{140}$	*n*-Nonahexacontane	1115.070401
70	$C_{70}H_{142}$	*n*-Heptacontane	1131.006631
71	$C_{71}H_{144}$	*n*-Henheptacontane	1146.942893
72	$C_{72}H_{146}$	*n*-Doheptacontane	1162.879185
73	$C_{73}H_{148}$	*n*-Triheptacontane	1178.815507
74	$C_{74}H_{150}$	*n*-Tetraheptacontane	1194.751857
75	$C_{75}H_{152}$	*n*-Pentaheptacontane	1210.688234
76	$C_{76}H_{154}$	*n*-Hexaheptacontane	1226.624637
77	$C_{77}H_{156}$	*n*-Heptaheptacontane	1242.561065
78	$C_{78}H_{158}$	*n*-Octaheptacontane	1258.497517
79	$C_{79}H_{160}$	*n*-Nonaheptacontane	1274.433992
80	$C_{80}H_{162}$	*n*-Octacontane	1290.370489

81	$C_{81}H_{164}$	*n*-Henoctacontane	1306.307008
82	$C_{82}H_{166}$	*n*-Dooctacontane	1322.243548
83	$C_{83}H_{168}$	*n*-Trioctacontane	1338.180107
84	$C_{84}H_{170}$	*n*-Tetraoctacontane	1354.116686
85	$C_{85}H_{172}$	*n*-Pentaoctacontane	1370.053284
86	$C_{86}H_{174}$	*n*-Hexaoctacontane	1385.989899
87	$C_{87}H_{176}$	*n*-Heptaoctacontane	1401.926532
88	$C_{88}H_{178}$	*n*-Octaoctacontane	1417.863181
89	$C_{89}H_{180}$	*n*-Nonaoctacontane	1433.799847
90	$C_{90}H_{182}$	*n*-Nonacontane	1449.736528
91	$C_{91}H_{184}$	*n*-Hennonacontane	1465.673224
92	$C_{92}H_{186}$	*n*-Dononacontane	1481.609935
93	$C_{93}H_{188}$	*n*-Trinonacontane	1497.54666
94	$C_{94}H_{190}$	*n*-Tetranonacontane	1513.483399
95	$C_{95}H_{192}$	*n*-Pentanonacontane	1529.420152
96	$C_{96}H_{194}$	*n*-Hexanonacontane	1545.356917
97	$C_{97}H_{196}$	*n*-Heptanonacontane	1561.293694
98	$C_{98}H_{198}$	*n*-Octanonacontane	1577.230484
99	$C_{99}H_{200}$	*n*-Nonanonacontane	1593.167286
100	$C_{100}H_{202}$	*n*-Hectane	1609.104099
101	$C_{101}H_{204}$	*n*-Henihectane	1625.040923
102	$C_{102}H_{206}$	*n*-Dohectane	1640.977757
103	$C_{103}H_{208}$	*n*-Trihectane	1656.914603
104	$C_{104}H_{210}$	*n*-Tetrahectane	1672.851458
105	$C_{105}H_{212}$	*n*-Pentahectane	1688.788323
106	$C_{106}H_{214}$	*n*-Hexahectane	1704.725198
107	$C_{107}H_{216}$	*n*-Heptahectane	1720.662082
108	$C_{108}H_{218}$	*n*-Octahectane	1736.598975
109	$C_{109}H_{220}$	*n*-Nonahectane	1752.535877
110	$C_{110}H_{222}$	*n*-Decahectane	1768.472787
111	$C_{111}H_{224}$	*n*-Undecahectane	1784.41

The following graph shows the relation between Zagreb vector index and boiling point, which is in the form of parabolic curve.



The following graph shows the variation of the Zagreb vector index with n= the number of Carbon atoms, which is linear for the straight chain n-Alkanes.



4. **Conclusions and Advantages:** The vector indices consider more than one fact at a time. Hence useful in distinguishing the entities more precisely than the topological indices. Hence the primary intension was to introduce the Vector indices based vertex degree of chemical graphs. The co-relation co-efficient between the vector indices and Physical properties of Alkanes add strength to such studies. 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. Our calculation yields, the Vector index shows very strong correlation with boiling points, molar volumes, melting points and Surface tension. Hence, we can conclude that the Vector index may be considered as a more useful tool in predicting the physical properties of lower alkanes comparative to the topological indices. One more advantage is, the Vector index distinguishes isomers and straight chain alkanes, rather than as in Topological indices. The vector index remains the same on similar compounds like methane and CCl_4. The vector index becomes large number for calculation and needs computing aids as the number of Carbon atoms increases. Thus it has few disadvantages also.

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