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VL TEMPERATURE INDEX OF CERTAIN ARCHIMEDEAN LATTICE

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Abstract: In $QSPR$ study, a prediction about the bioactivity of chemical compounds is made on the basis of physico-chemical properties and topological indices such as Zagreb index, Harmonic index and VL index etc. Inspired by many degree based topological indices, we propose here a new topological index, called the VL temperature index $VLTI(G)$ of a molecular graph G. Our study showcases some important results on the correlation between Surface Tension, Complexity, Heavy Atomic Count, Density and Index of refraction of Butane derivatives with VL temperature index ($VLTI$). In this paper we compute the VL temperature index of line graphs of subdivision graphs of Archimedean Lattices.

Keywords and Phrases: Temperature of a vertex, VL temperature index, Archi -medean Lattice.

2020 Mathematics Subject Classification: 05C07, 05C10, 05C76.

1. Introduction

The branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena is known as chemical graph theory. Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Topological indices have a prominent place in Molecular descriptors. There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in $QSPR$ [14] [15] research.

Topological indices are numerical parameters of a graph which are invariant under graph isomorphism. Let $V(G)$ and $E(G)$ be its vertex and edge sets of a connected graph $G = (V, E)$, respectively. As usual order $n = |V(G)|$ and size $m = |E(G)|$ denote the number of vertices and edges at a graph G, respectively. The edge joining the vertices u and v is denoted by uv. The degree of a vertex u in a graph G is the number of edges incidence to u and is denoted by $d(u)$. For graph theoretic terminology, the reader may refer the books [1] [2].

The temperature of a vertex u of a connected graph G is defined by Siemion Fajtlowiczas [12].

$$T(u) = \frac{d_u}{n - d_u}$$

where d_u is the degree of a vertex u of a connected graph G.

T. Deepika [5], introduced the VL index of a graph G is defined as,

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

where $d_e = d(u) + d(v) - 2$ and $d_f = (d(u).d(v)) - 2$. The VL index shows a good correlation with the physical properties of octane isomers and polychlorinated biphenyl (PCB).

The VL index which can also be written as,

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} [d(u) + d(v) + d(u).d(v)].$$

Recently, Kishori P. N., Afework Teka Kahsay [6] has introduced Harmonic temperature index of a graph and is defined as $HTI(G) = \sum_{uv \in E(G)} \frac{2}{T_u + T_v}$ and we extend this study for VL temperature index. Inspired by the work on degree based topological indices and VL index, we now define the VL temperature index $(VLTI(G))$ of a molecular graph G as follows.

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

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

Also, we inspired by the work on Sharp bounds for SZ, PI and GA_2 indices in terms of the number of triangles [3], Operations on Dutch Windmill Graph of

Topological indices [7], New results on the F-index of graphs based on corona-type products of graphs [8], Computation of Adriatic indices of certain operators of regular and complete bipartite graphs [9] and M-Polynomial of subdivision and complementary graphs of Banana tree graph [10].

The Archimedean lattices [4] [11] [13] are the infinite transitive planar graphs that can be drawn in the plane such that all faces are regular polygons. A regular polygon with m edges is a polygon, where all edges have the same length, and the inner angle between any two adjacent edges $[(m-2)\pi/m]$ radians. It follows that all vertices are equivalent and have the same coordination number. In this paper, our aim to study different types of Archimedean lattices are $L_{4,8^2}$, L_{4^4} and L_{6^3}.

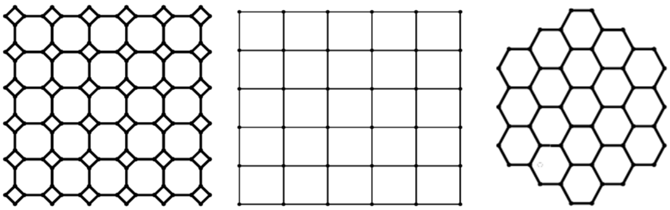


Figure 1: (a) $L_{4,8^2}$ Archimedean Lattice. (b) L_{4^4} Archimedean Lattice. (c) L_{6^3} Archimedean Lattice.

2. Result for Archimedean Lattice $L_{4,8^2}$

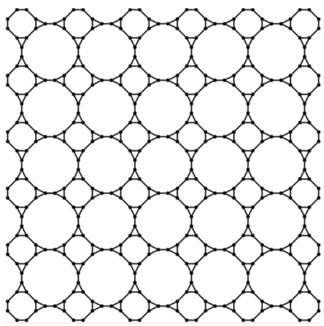
The line graph of the subdivision graph of Archimedean Lattice, $L_{4,8^2}$ is shown in Figure 2(a).

Theorem 2.1. *Let G be the line graph of the subdivision graph of Archimedean Lattice $L_{4,8^2}$. Then*

$$VLTI(G) = \frac{(4n+2)(48n^2-8n-1)}{(24n^2-4n-1)^2} + \frac{(108n^2-66n+6)(96n^2-16n-3)}{(48n^2-8n-3)^2} + \frac{(4n-2)(240n^2-40n-6)}{(24n^2-4n-1)(48n^2-8n-3)}.$$

Proof. The line graph of the subdivision graph of Archimedean Lattice, $L_{4,8^2}$ are shown in Fig. 2(a). The total number of vertices of G is $48n^2-8n$. The total number of edges of G is $72n^2-20n$. Therefore we get the edge partition based on the temperature of the vertices as shown in Table 1. Therefore, using Equation (1)

$$VLTI(G) = \frac{8n+4}{2}\left[\left(\frac{2}{48n^2-8n-2}+\frac{2}{48n^2-8n-2}+\frac{2}{48n^2-8n-2}.\frac{2}{48n^2-8n-2}\right)\right]$$
$$+\frac{72n^2-44n+4}{2}\left[\left(\frac{3}{48n^2-8n-3}+\frac{3}{48n^2-8n-3}+\frac{3}{48n^2-8n-3}.\frac{3}{48n^2-8n-3}\right)\right]$$
$$+\frac{16n-8}{2}\left[\left(\frac{2}{48n^2-8n-2}+\frac{3}{48n^2-8n-3}+\frac{2}{48n^2-8n-2}.\frac{3}{48n^2-8n-3}\right)\right]$$
$$=\frac{(4n+2)(48n^2-8n-1)}{(24n^2-4n-1)^2}+\frac{(108n^2-66n+6)(96n^2-16n-3)}{(48n^2-8n-3)^2}$$
$$+\frac{(4n-2)(240n^2-40n-6)}{(24n^2-4n-1)(48n^2-8n-3)}.$$



(a)

Figure 2: (a) Line graph of subdivision graph of $L_{4,8^2}$ Archimedean Lattice.

Table 1: The edge partition of the graph G

(T_u, T_v), where $uv \in E(G)$	Number of edges
$(\frac{2}{48n^2-8n-2}, \frac{2}{48n^2-8n-2})$	$8n+4$
$(\frac{3}{48n^2-8n-3}, \frac{3}{48n^2-8n-3})$	$72n^2-44n+4$
$(\frac{2}{48n^2-8n-2}, \frac{3}{48n^2-8n-3})$	$16n-8$

3. Result for Archimedean Lattice L_{4^4}

The line graph of the subdivision graph of Archimedean Lattice, L_{4^4} is shown in Figure 3(a).

Theorem 3.1. *Let G be the line graph of the subdivision graph of Archimedean*

Lattice L_{4^4}. Then

$$VLTI(G) = \frac{4n(16n^2-8n-1)}{(8n^2-4n-1)^2} + \frac{(4n-4)(80n^2-40n-6)}{(8n^2-4n-1)(16n^2-8n-3)} + \frac{(n-1)(112n^2-56n-12)}{(16n^2-8n-3)(4n^2-2n-1)} + \frac{(16n^2-34n+18)(8n^2-4n-1)}{(4n^2-2n-1)^2}.$$

Proof. The line graph of the subdivision graph of Archimedean Lattice, L_{4^4} are shown in Fig. 3(a). The total number of vertices of G is $16n^2-8n$. The total number of edges of G is $32n^2-36n+12$. Therefore we get the edge partition based on the temperature of the vertices as shown in Table 2. Therefore, using Equation (1)

$$\begin{aligned}VLTI(G) &= \frac{8n}{2}\left[\left(\frac{2}{16n^2-8n-2}+\frac{2}{16n^2-8n-2}+\frac{2}{16n^2-8n-2}.\frac{2}{16n^2-8n-2}\right)\right]\\ &+ \frac{16n-16}{2}\left[\left(\frac{2}{16n^2-8n-2}+\frac{3}{16n^2-8n-3}+\frac{2}{16n^2-8n-2}.\frac{3}{16n^2-8n-3}\right)\right]\\ &+ \frac{8n-8}{2}\left[\left(\frac{3}{16n^2-8n-3}+\frac{4}{16n^2-8n-4}+\frac{3}{16n^2-8n-3}.\frac{4}{16n^2-8n-4}\right)\right]\\ &+ \frac{32n^2-68n+36}{2}\left[\left(\frac{4}{16n^2-8n-4}+\frac{4}{16n^2-8n-4}+\frac{4}{16n^2-8n-4}.\frac{4}{16n^2-8n-4}\right)\right]\\ &= \frac{4n(16n^2-8n-1)}{(8n^2-4n-1)^2} + \frac{(4n-4)(80n^2-40n-6)}{(8n^2-4n-1)(16n^2-8n-3)} + \frac{(n-1)(112n^2-56n-12)}{(16n^2-8n-3)(4n^2-2n-1)}\\ &+ \frac{(16n^2-34n+18)(8n^2-4n-1)}{(4n^2-2n-1)^2}.\end{aligned}$$

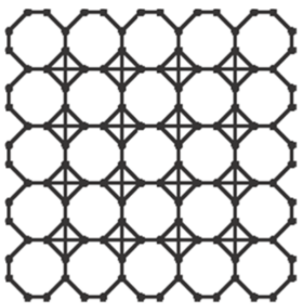

(a)

Figure 3: (a) Line graph of subdivision graph of L_{4^4} Archimedean Lattice.

Table 2: The edge partition of the graph G

(T_u, T_v), where $uv \in E(G)$	Number of edges
$(\frac{2}{16n^2-8n-2}, \frac{2}{16n^2-8n-2})$	$8n$
$(\frac{2}{16n^2-8n-2}, \frac{3}{16n^2-8n-3})$	$16n-16$
$(\frac{3}{16n^2-8n-3}, \frac{4}{16n^2-8n-4})$	$8n-8$
$(\frac{4}{16n^2-8n-4}, \frac{4}{16n^2-8n-4})$	$32n^2-68n+36$

4. Result for Archimedean Lattice L_{6^3}

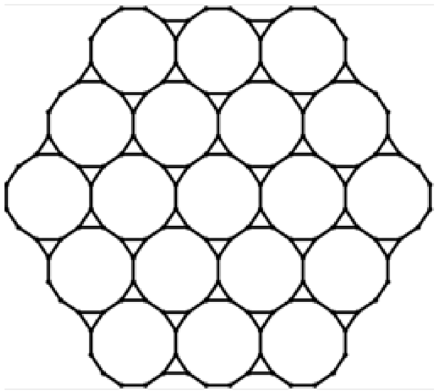
The line graph of the subdivision graph of Archimedean Lattice, L_{4^4} is shown in Figure 3(a).

Theorem 4.1. *Let G be the line graph of the subdivision graph of Archimedean Lattice L_{6^3}. Then*

$$VLTI(G) = \frac{(3n+3)(18n^2-6n-1)}{(9n^2-3n-1)^2} + \frac{(n-1)(90n^2-30n-6)}{(9n^2-3n-1)(6n^2-2n-1)} + \frac{(9n^2-11n+2)(36n^2-12n-3)}{2(6n^2-2n-1)^2}.$$

Proof. The line graph of the subdivision graph of Archimedean Lattice, L_{6^3} are shown in Fig. $4(a)$. The total number of vertices of G is $18n^2-6n$. The total number of edges of G is $27n^2-15n$. Therefore we get the edge partition based on the temperature of the vertices as shown in Table 3. Therefore, using Equation (1)

$$VLTI(G) = \frac{6n+6}{2}\left[\left(\frac{2}{18n^2-6n-2} + \frac{2}{18n^2-6n-2} + \frac{2}{18n^2-6n-2}.\frac{2}{18n^2-6n-2}\right)\right]$$
$$+ \frac{12n-12}{2}\left[\left(\frac{2}{18n^2-6n-2} + \frac{3}{18n^2-6n-3} + \frac{2}{18n^2-6n-2}.\frac{3}{18n^2-6n-3}\right)\right]$$
$$+ \frac{27n^2-33n+6}{2}\left[\left(\frac{3}{18n^2-6n-3} + \frac{3}{18n^2-6n-3} + \frac{3}{18n^2-6n-3}.\frac{3}{18n^2-6n-3}\right)\right]$$
$$= \frac{(3n+3)(18n^2-6n-1)}{(9n^2-3n-1)^2} + \frac{(n-1)(90n^2-30n-6)}{(9n^2-3n-1)(6n^2-2n-1)}$$
$$+ \frac{(9n^2-11n+2)(36n^2-12n-3)}{2(6n^2-2n-1)^2}.$$



(a)

Figure 4: (a) Line graph of subdivision graph of L_{6^3} Archimedean Lattice.

Table 3: The edge partition of the graph G

(T_u, T_v), where $uv \in E(G)$	Number of edges
$(\frac{2}{18n^2-6n-2}, \frac{2}{18n^2-6n-2})$	$6n+6$
$(\frac{2}{18n^2-6n-2}, \frac{3}{18n^2-6n-3})$	$12n-12$
$(\frac{3}{18n^2-6n-3}, \frac{3}{18n^2-6n-3})$	$27n^2-33n+6$

Note: The VL temperature index of L_{6^3} Archimedean lattice using line operation is same as the VL temperature index of $L_{3,12^2}$ Archimedean lattice without using line operation.

5. On Chemical Applicability of the VL Temperature Index

In this section we will discuss the regression analysis of Surface tension, Complexity and Heavy Atomic Count of Butane derivatives on the VL temperature index of the corresponding molecular graph. The productivity of $VLTI$ was tested using a data set of Butane derivatives, found at *http://www.moleculardescriptors .eu /dataset.htm.*

Fig. 5(a), 5(b), 5(c), 5(d), 5(e) shows the Scatter plot between Surface Tension, Complexity and Heavy Atomic Count, Density and Index of Refraction of Butane derivatives and VL temperature index respectively. The correlation coefficient (R) of the Surface Tension, Complexity and Heavy Atomic Count with VL temperature index is shown in Table 5.

Table 4: Correlation of $VLTI$ index and some properties of Butane derivatives:

Name of the Compound	Surface Tension	Complexity	H.A.C	Density	Index of Refraction	$VLTI$
1,4-butanedithiol	31.1	17.5	6	1.03	1.51	2.675
2-butanone	22.9	38.5	5	8.32	1.37	4.25
1,3-butanediol	34.9	28.7	6	9.96	1.44	3.425
butane dinitrile	40.7	92	6	1.01	1.42	2.675
butanediamide	53	96.6	8	1.18	1.49	3.1793
butane-1-sulfonamide	41.9	133	8	1.15	1.47	3.8015
1-butanethiol	24.8	13.1	5	8.5	1.44	2.8611
1,4-diaminobutane	35.8	17.5	6	8.65	1.46	2.675
butane-1,4-disulfonic acid	77.9	266	12	1.66	1.54	3.1465
butyraldehyde	23.1	24.8	5	8.18	1.37	2.8611
2,3-butanedione	27.3	71.5	6	9.75	1.38	4.3
butanedihydrazide	59	119	10	1.28	1.53	2.7812
1-butanesulfonyl chloride	36.4	133	8	1.26	1.45	3.8016

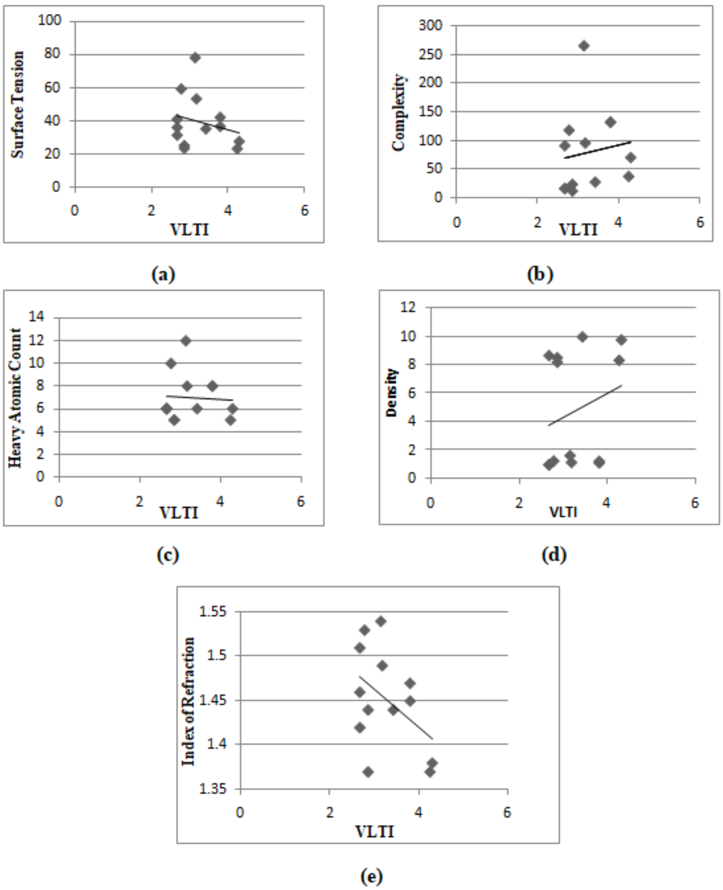


Figure 5: Correlation of $VLTI$ index with physico-chemical properties of Butane derivatives

Table 5: Pearson's Correlation Coefficient

	$VLTI$
Surface Tension	-0.2294
Complexity	0.1413
Heavy Atomic Count	-0.0551
Density	0.2532
Index of Refraction	-0.4466

The VL Temperature index is positively correlated with Complexity and Density except Surface Tension, Heavy Atomic Count and Index of Refraction. In table 5, one can easily verify that VL Temperature index shows not a good correlation with all Physical-Chemical properties (Surface Tension, Complexity, Heavy Atomic Count, Density and Index of Refraction) of Butane derivatives.

6. Conclusion

In this work, we propose a new index, called the VL temperature index and compute the VL temperature index of line graphs of subdivision graphs of Archimedean Lattices. Also, we study the correlation between Surface Tension, Complexity, Heavy Atomic Count, Density and Index of refraction of Butane derivatives with VL temperature index. Similar way, researchers can find VL temperature index of different Archimedean lattices and their dual leaves lattices using different graph operators.

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