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VL INDEX AND BOUNDS FOR THE TENSOR PRODUCTS OF F -SUM GRAPHS

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ABSTRACT. In QSAR/QSPR study, topological indices are exploited to a presumption of the bioactivity of chemical compounds. Inspired by the work of Zagreb indices, we propound here a new topological index, namely *Veerabhadraiah Loksha* ($VL(G)$) index of a graph G . The $VL(G)$ index shows a good correlation with the physical properties of octane isomers and polychlorinated biphenyl (PCB). In this article, the bounds on graph operations of the tensor product are studied.

Keywords: VL index, graph operations, tensor product.

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

1. INTRODUCTION

The mathematical measure identify with chemical nature purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity is known as Topological index (grasping of oldest topological indices see in [8], [15]). In an explicit phrase, if Gr denotes the class of all finite graphs then a topological index is a function Top from Gr into real numbers with the property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are two basic parameters in topological indices. In recent decades, a large number of topological indices have been defined and utilized for chemical documentation, isomer discrimination, study of molecular complexity, chirality, similarity/dissimilarity, QSAR/QSPR (for more details refer [1],[3]), drug design and database selection, lead optimization, etc.

Chemical reactions cause changes in entropy and entropy plays an important role in determining in which direction a chemical reaction spontaneously proceeds.

The role of Enthalpy of Vaporization is to transform the quantity of a substance from a liquid into a gas at a given pressure. Furthermore physical properties of octane and Polychlorinated biphenyl (PCB) has their vital roles in the chemical application (details about structure-activity correlation assigned in [1], [16]).

Two of the most useful topological graph indices are the first and second Zagreb indices

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that have been introduced by Gutman and Trinajstić in [7]. They are denoted by $M_1(G)$ and $M_2(G)$ and were defined as

$$M_1(G) = \sum_{u \in V(G)} [d(u)]^2 = \sum_{uv \in E(G)} [d(u) + d(v)]$$

and

$$M_2(G) = \sum_{uv \in E(G)} d(u).d(v).$$

Alternatively, the first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying molecular graph G .

Bountiful of researchers are working on the Zagreb indices (some good work on Zagreb indices are noticed in [12],[13]). Their extended versions became the most interesting part of the research because of its applications in the field of chemical sciences.

Inspired by the works of Zagreb indices, the VL index 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 $d_f = (d_u \times d_v) - 2$, such that d_u and d_v are the degree vertices of u and v in G , respectively.

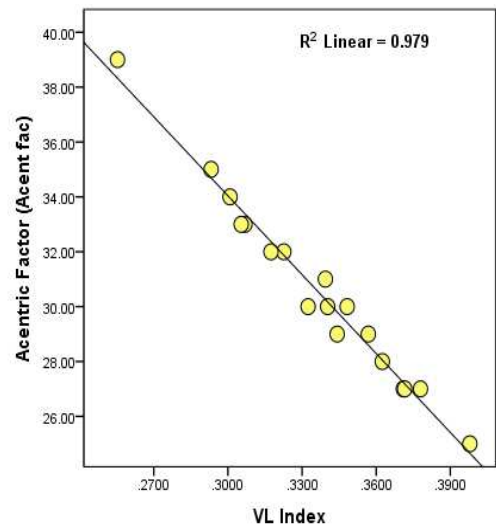
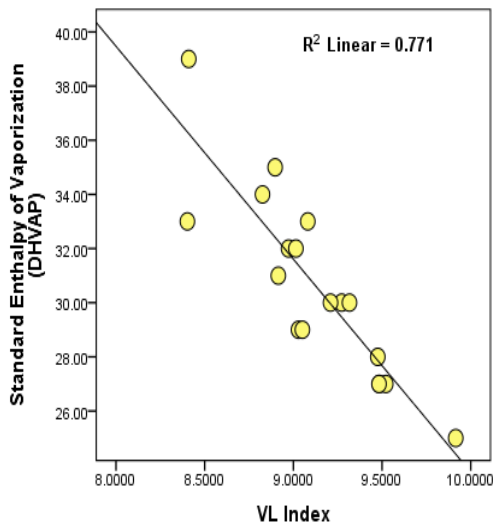
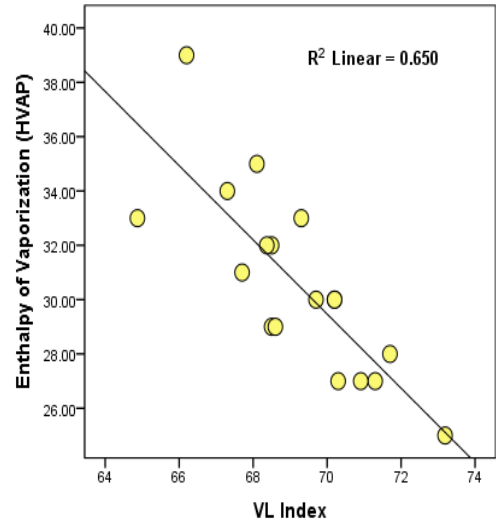
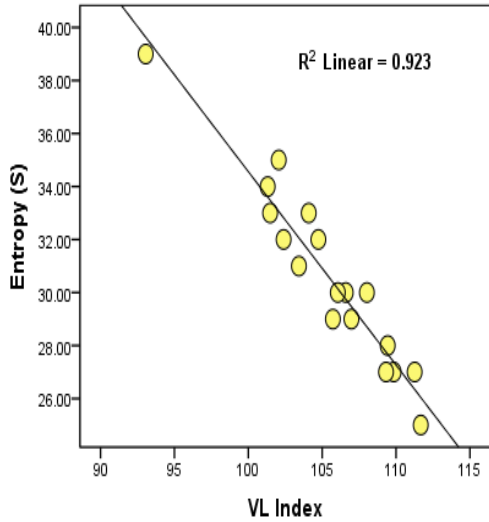
The target of this article is to introduce a new topological index named as *Veerabhadraiah Lokesha* ($VL(G)$) index and study bounds on tensor products of $VL(G)$ index of F -sum graph.

The following Table 1 shows the correlation between the physical properties of Octane isomers and PCB and VL index respectively. The correlation coefficient (R) is a measure of how strongly a pair of variables are related. More time on treadmill the calories burned can be given examples of this. It usually varies between -1 and $+1$ and if it's closer to 1 then variables are said to be highly linearly proportion and if close to -1 then highly linearly inversely proportional. If R is close to 0 , then there is no relation (as we can observe in Table 1, the physical properties of octane isomers with VL index is inversely proportional i.e., closer to -1 value).

TABLE 1. Correlation between isomers and topological indices

Physical Property of Octane isomers	R
Entropy Value (S)	-0.961
Enthalpy of Vaporization (HVAP)	-0.806
Standard Enthalpy of Vaporization (DHVAP)	-0.878
Acentric Factor (Acent Fac)	-0.99
Physical Property of PCB	R
Relative Retention Time (RRT)	0.946

The following Figure 1 shows the graph that variables coincident with each other. Here the coefficient of determination (R^2) is a measure of how variance in y (entropy) is explained by the regression model. Often if a model traces close to the actual values then Coefficient of Determination is high (0.85– ~ 0.9999) else the model needs to be improved upon. Below Figure 1 will help in understanding the case.



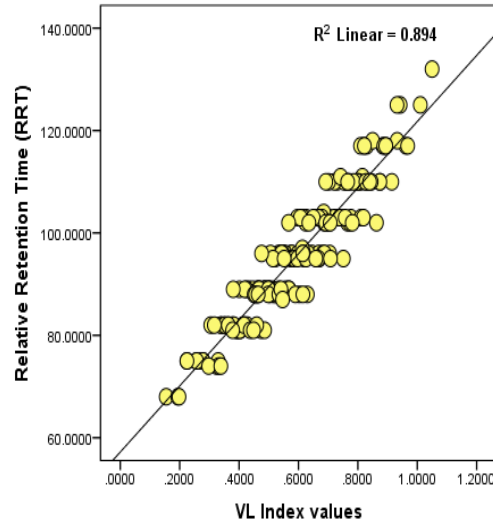


FIGURE 1. Correlation of physical properties with the VL index

2. SOME FUNDAMENTAL DEFINITIONS AND PROPERTIES

Throughout this paper G will denote a simple, connected and finite graph with vertex set $V(G) = \{u_1, u_2, u_3, \dots, u_n\}$, edge set $E(G) = \{e_1, e_2, e_3, \dots, e_m\}$ of order $|V(G)| = p$ and size of $|E(G)| = q$. An edge $e \in E(G)$ with end vertices u_i and u_j is denoted by $u_i u_j$. The vertices having an edge between them are called adjacent. The number of vertices adjacent to the vertex u is called the degree of u in G and is denoted by $d_G(u)$ or d_u . The minimum and maximum degrees of graph G is denoted by δ_G and Δ_G , respectively.

Definition 1: [10] The tensor product $G \otimes H$ of graphs G and H is the graph with the vertex set $V(G) \times V(H)$, two vertices (u_i, v_j) and (u_k, v_l) being adjacent in $G \times H$ if and only if $u_i u_k \in E(G)$ and $v_j v_l \in E(H)$. The tensor product of P_3 and C_5 is illustrated in below Figure 2.

The tensor product was introduced by Alfred North Whitehead and Bertrand Russell in (1912). It is also equivalent to the Kronecker product of the adjacency matrices of the graphs [6]. The cross symbol shows visually the two edges resulting from the tensor product of two edges [2]. The tensor product is also known as direct product, categorical product, cardinal product, relational product, Kronecker product, weak direct product, or conjunction.

For a connected graph G , let us define four related graphs $S(G), R(G), Q(G)$ and $T(G)$ (see [9]-[13]) as follows:

- $S(G)$ (subdivision graph) is the graph acquired by including an additional vertex in each edge of G . Equivalently, each edge of G is replaced by a path of length 2.
- $R(G)$ is obtained from G by appending a new vertex corresponding to each edge of G , and then joining each new vertex to the end vertices of the corresponding edge.
- $Q(G)$ is obtained from G by inserting a new vertex in to each edge of G , and then joining with edges those pairs of new vertices on adjacent edges of G .
- $T(G)$ (total graph) has as its vertices the edges and vertices of G . Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of G .

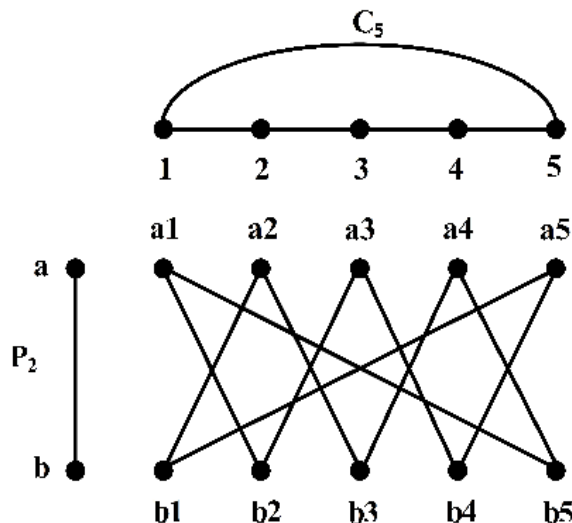


FIGURE 2. The tensor product of $P_2 \otimes C_5$

It is clear from the above definitions that,

$$\begin{aligned} V(S(G)) &= V(R(G)) = V(Q(G)) = V(T(G)) = V(G) \cup E(G), \\ E(R(G)) &= E(G) \cup E(S(G)), \\ E(Q(G)) &= E(L(G)) \cup E(S(G)), \\ E(T(G)) &= E(G) \cup E(L(G)) \cup E(S(G)), \end{aligned}$$

where $E(G)$, $E(L(G))$, $E(S(G))$ are mutually disjoint.

The four operations on graph $S(G), R(G), Q(G), T(G)$ are illustrated in below Figure 3.

Definition 2: [4, 5] F -sum graph $G +_F H$ for $F \in \{S, R, Q, T\}$ define as

$$\begin{aligned} V(G +_F H) &= (V_1 \cup E_1) \times V_2 \\ E(G +_F H) &= a_{ij}a_{kl} : i = k \text{ and } v_jv_l \in E_2 \vee j = l \text{ and } u_iu_k \in E(F(G)) \\ &\cup b_{ij}b_{kj} : e_ie_k \in E(F(H)) \cup b_{ij}a_{kj} : e_iu_k \in E(F(G)), \end{aligned}$$

where $a_{ij} = (u_i, v_j)$ and $b_{ij} = (e_i, v_j)$ (refer to a_{ij} as a black vertices and b_{ij} as a white vertices).

Suppose that G and H are two connected graphs. Based on these above operations, four new operations on the graphs $C_4 +_F C_5$ are shown in Figure 4.

Lemma 2.1. [10] *Let G_1 and G_2 be graphs of order p_1 and p_2 and size q_1 and q_2 , respectively. Then we have*

- (i) $|V(G_1 \otimes G_2)| = |V(G_1)| \cdot |V(G_2)|$ and $|E(G_1 \otimes G_2)| = 2|E(G_1)| \cdot |E(G_2)|$.
- (ii) $d_{G_1 \otimes G_2}(u, v) = d_{G_1}(u) \cdot d_{G_2}(v)$.
- (iii) *The tensor product is commutative and associative.*

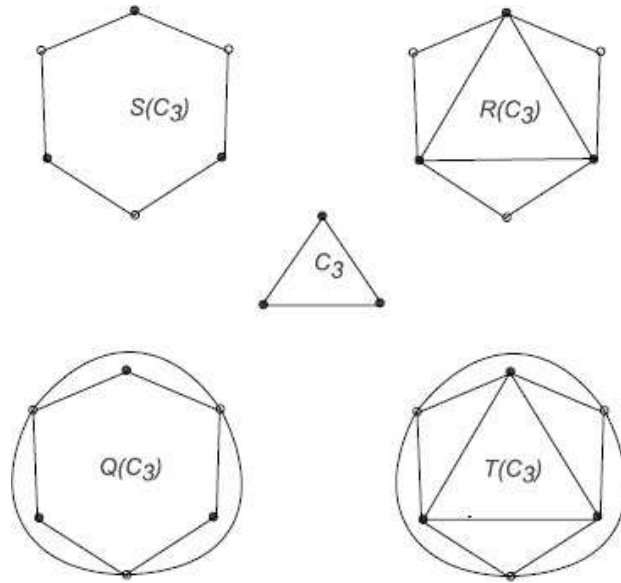


FIGURE 3. The graphs $G = C_3, S(G), R(G), Q(G)$ and $T(G)$

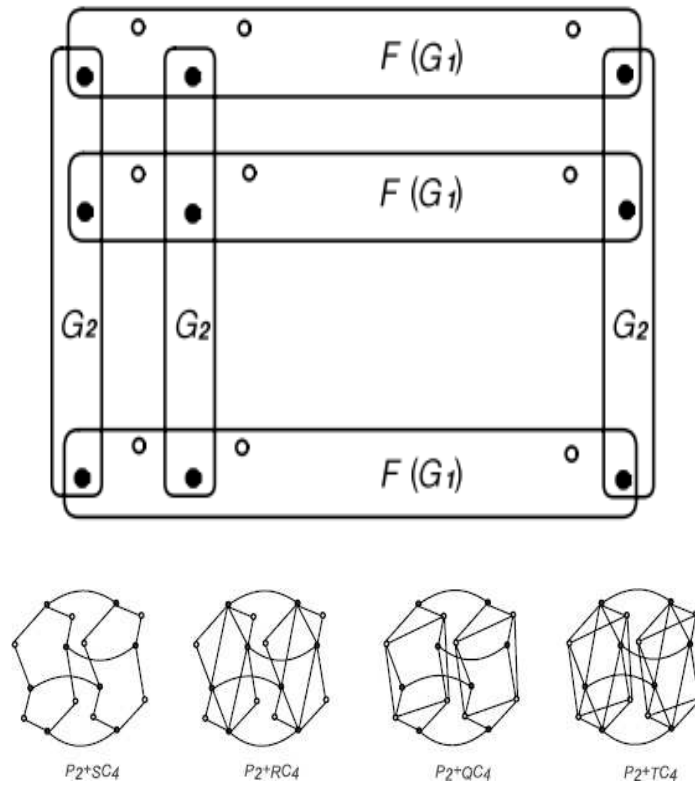


FIGURE 4. The graphs $P_2 +_S C_4, P_2 +_R C_4, P_2 +_Q C_4$ and $P_2 +_T C_4$

Lemma 2.2. Let G be a graph. Then the VL index is defined as

$$\frac{q}{2}[3d_{max} + 2] \leq VL(G) \leq \frac{q}{2}[3d_{min} + 2]$$

such that equality holds iff G is regular graph.

Proof. Let G be a graph with $|V(G)| = p$ and $|E(G)| = q$. Then

$$\begin{aligned} VL(G) &= \sum_{uv \in E(G)} \frac{d_u + d_v + 4}{2} \\ &= \frac{1}{2} (\sum_{uv \in E(G)} d_u + d_v + d_u d_v) \\ &= \frac{1}{2} [\sum_{uv \in E(G)} (d_u + d_v) + \sum_{uv \in E(G)} (d_u d_v)] \\ &\leq \frac{1}{2} [q(d_{max} + 2) + 2qd_{max}] \\ &\leq \frac{q}{2} [3d_{max} + 2]. \end{aligned}$$

Using similar arguments, we have

$$VL(G) \geq \frac{q}{2} [3d_{min} + 2].$$

□

3. BOUNDS ON NEW TOPOLOGICAL INDICES OF TENSOR PRODUCT OF GRAPH OPERATIONS

In this section, we will determine bounds for the VL index of tensor products of the F -sum on graphs in terms of their factor graphs. Let W, X, Y, Z be simple, connected graphs such that $|V(W)| = p_1$, $|V(X)| = p_2$, $|V(Y)| = p_3$, $|V(Z)| = p_4$, $|E(W)| = q_1$, $|E(X)| = q_2$, $|E(Y)| = q_3$, $|E(Z)| = q_4$.

In the following theorem, we will compute the lower and upper bounds for the VL index of tensor products of F -sum on graphs for $F = S, R, Q, T$.

Theorem 3.1. *Let $G = W +_S X$ and $H = Y +_S Z$. Then $\alpha_1 \leq VL(G \otimes H) \leq \beta_1$, where*

$$\begin{aligned} \alpha_1 &= (q_1 p_2 + 2p_1 q_2)(q_3 p_4 + 2p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\ &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4] \end{aligned}$$

and

$$\begin{aligned} \beta_1 &= (q_1 p_2 + 2p_1 q_2)(q_3 p_4 + 2p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{e(Y)} + \Delta_{e(Z)}) \\ &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4]. \end{aligned}$$

Proof. The vertex sets of G and H are $\{a_1, a_2, a_3, \dots, a_{p_1(p_2+q_2)}\}$ and $\{b_1, b_2, b_3, \dots, b_{p_3(p_4+q_4)}\}$, respectively. Then by definition, we have

$$\begin{aligned} VL(G \otimes H) &= \frac{1}{2} \sum_{(a_i, b_j), (a_k, b_l) \in E(G \otimes H)} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\ &= \frac{1}{2} \sum_{(a_i, b_j), (a_k, b_l) \in E(G \otimes H), i \neq k, j \neq l} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4]. \quad \rightarrow (1) \end{aligned}$$

Since, by Lemma 2.1 part (ii),

$$d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4 = d_{e(G)}(a_i) \cdot d_{e(H)}(b_j) + d_{f(G)}(a_k) \cdot d_{f(H)}(b_l) + 4.$$

Since, for a graph G , for all $a \in V(G)$, $d_G(a) \leq \Delta_G$ and $d_G(a) \geq \delta_G$. Therefore, using these facts, we have

$$d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4 \leq \Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4. \quad \rightarrow (2)$$

Using inequality (2), in Equation (1), we have

$$\begin{aligned} VL(G \otimes H) &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H), i \neq k, j \neq l} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\ &= \frac{1}{2} \sum_{a_i a_k \in E(G)} \sum_{b_j b_l \in E(H)} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\ &\leq E(G) \cdot E(H) [\Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4]. \end{aligned}$$

Since $|E(G)| = q_1 p_2 + 2 p_1 q_2$, $|E(H)| = q_2 p_4 + 2 p_3 q_4$, and $\Delta_{e(G)} = \Delta_{e(W)} + \Delta_{e(X)}$, $\Delta_H = \Delta_{f(Y)} + \Delta_{f(Z)}$.

$$\begin{aligned} VL(G \otimes H) &\leq (q_1 p_2 + 2 p_1 q_2)(q_2 p_4 + 2 p_3 q_4) [\Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4] \\ &\leq (q_1 p_2 + 2 p_1 q_2)(q_2 p_4 + 2 p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{f(Y)} + \Delta_{e(Z)}) \\ &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4]. \end{aligned}$$

Using similar arguments with $\Delta_G \geq \delta_G$,

$$\begin{aligned} VL(G \otimes H) &\geq (q_1 p_2 + 2 p_1 q_2)(q_2 p_4 + 2 p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\ &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4]. \end{aligned}$$

□

Theorem 3.2. Let $G = W +_Q X$ and $H = Y +_Q Z$. Then $\alpha_3 \leq VL(G \otimes H) \leq \beta_3$, where

$$\begin{aligned} \alpha_3 &= 4(q_1 p_2 + p_1 q_2)(q_3 p_4 + p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\ &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4] \end{aligned}$$

and

$$\begin{aligned} \beta_3 &= 4(q_1 p_2 + p_1 q_2)(q_3 p_4 + p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{e(Y)} + \Delta_{e(Z)}) \\ &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4]. \end{aligned}$$

Proof. The vertex sets of G and H are $\{a_1, a_2, a_3, \dots, a_{p_1(p_2+q_2)}\}$ and $\{b_1, b_2, b_3, \dots, b_{p_3(p_4+q_4)}\}$, respectively. Then by definition, we have

$$\begin{aligned} VL(G \otimes H) &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H)} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\ &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H), i \neq k, j \neq l} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4]. \quad \rightarrow (1) \end{aligned}$$

Since, by Lemma 2.1 part (ii),

$$d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4 = d_{e(G)}(a_i) \cdot d_{e(H)}(b_j) + d_{f(G)}(a_k) \cdot d_{f(H)}(b_l) + 4.$$

Since, for a graph G , for all $a \in V(G)$, $d_G(a) \leq \Delta_G$ and $d_G(a) \geq \delta_G$. Therefore, using these facts, we have

$$d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4 \leq \Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4. \quad \rightarrow (2)$$

Using inequality (2), in Eq. (1), we have

$$\begin{aligned}
 VL(G \otimes H) &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H), i \neq k, j \neq l} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\
 &= \frac{1}{2} \sum_{a_i a_k \in E(G)} \sum_{b_j b_l \in E(H)} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\
 &\leq E(G) \cdot E(H) [\Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4].
 \end{aligned}$$

Since $|E(G)| = 2(q_1 p_2 + p_1 q_2)$, $|E(H)| = 2(q_3 p_4 + p_3 q_4)$, and $\Delta_{e(G)} = \Delta_{e(W)} + \Delta_{e(X)}$, $\Delta_H = \Delta_{f(Y)} + \Delta_{f(Z)}$.

$$\begin{aligned}
 VL(G \otimes H) &\leq 4(q_1 p_2 + p_1 q_2)(q_3 p_4 + p_3 q_4) [\Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4] \\
 &\leq 4(q_1 p_2 + p_1 q_2)(q_3 p_4 + p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{f(Y)} + \Delta_{e(Z)}) \\
 &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4].
 \end{aligned}$$

Using similar arguments with $\Delta_G \geq \delta_G$,

$$\begin{aligned}
 VL(G \otimes H) &\geq 4(q_1 p_2 + p_1 q_2)(q_3 p_4 + p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\
 &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4].
 \end{aligned}$$

□

Theorem 3.3. *Let $G = W +_T X$ and $H = Y +_T Z$. Then $\alpha_4 \leq VL(G \otimes H) \leq \beta_4$, where*

$$\begin{aligned}
 \alpha_4 &= (q_1 p_2 + 4p_1 q_2)(q_3 p_4 + 4p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\
 &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4]
 \end{aligned}$$

and

$$\begin{aligned}
 \beta_4 &= (q_1 p_2 + 4p_1 q_2)(q_3 p_4 + 4p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{e(Y)} + \Delta_{e(Z)}) \\
 &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4].
 \end{aligned}$$

Proof. The vertex sets of G and H are $\{a_1, a_2, a_3, \dots, a_{p_1(p_2+q_2)}\}$ and $\{b_1, b_2, b_3, \dots, b_{p_3(p_4+q_4)}\}$, respectively. Then by definition, we have

$$\begin{aligned}
 VL(G \otimes H) &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H)} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\
 &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H), i \neq k, j \neq l} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4]. \quad \rightarrow (1)
 \end{aligned}$$

Since, by Lemma 2.1 part (ii),

$$d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4 = d_{e(G)}(a_i) \cdot d_{e(H)}(b_j) + d_{f(G)}(a_k) \cdot d_{f(H)}(b_l) + 4$$

Since, for a graph G , $d_G(a) \leq \Delta_G$ and $\Delta_G \geq \delta_G$ for all $a \in V(G)$. Therefore, using these facts, we have

$$d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4 \leq \Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4. \quad \rightarrow (2)$$

Using inequality (2), in Eq. (1), we have

$$\begin{aligned} VL(G \otimes H) &= \frac{1}{2} \sum_{(a_i, b_j)(a_k, b_l) \in E(G \otimes H), i \neq k, j \neq l} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\ &= \frac{1}{2} \sum_{a_i a_k \in E(G)} \sum_{b_j b_l \in E(H)} [d_{e(G \otimes H)}(a_i, b_j) + d_{f(G \otimes H)}(a_k, b_l) + 4] \\ &\leq E(G) \cdot E(H) [\Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4]. \end{aligned}$$

Since $|E(G)| = q_1 p_2 + 4 p_1 q_2$, $|E(H)| = q_3 p_4 + 4 p_3 q_4$, and $\Delta_{e(G)} = \Delta_{e(W)} + \Delta_{e(X)}$, $\Delta_H = \Delta_{f(Y)} + \Delta_{f(Z)}$.

$$\begin{aligned} VL(G \otimes H) &\leq (q_1 p_2 + 4 p_1 q_2)(q_3 p_4 + 4 p_3 q_4) [\Delta_{e(G)} \cdot \Delta_{e(H)} + \Delta_{f(G)} \cdot \Delta_{f(H)} + 4] \\ &\leq (q_1 p_2 + 4 p_1 q_2)(q_3 p_4 + 4 p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{f(Y)} + \Delta_{e(Z)}) \\ &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4]. \end{aligned}$$

Using similar arguments with $\Delta_G \geq \delta_G$,

$$\begin{aligned} VL(G \otimes H) &\geq (q_1 p_2 + 4 p_1 q_2)(q_3 p_4 + 4 p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\ &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4]. \end{aligned}$$

□

The ensuing Corollary 3.1 results intending to path and cycle graphs of tensor product of graph operations and in Corollary 3.2 results applicable to the applications in nanostructures.

Corollary 3.1. *Let C_n, C_m, P_n and P_m be the cycles and paths. Then,*

$$\begin{aligned} VL(C_n \otimes C_m) &= 24mn. \\ VL(P_n \otimes P_m) &= 24mn - 20(m + n) + 18. \\ VL(C_n \otimes P_m) &= 4n(6m - 5). \end{aligned}$$

Corollary 3.2. *Let N_1 and N_2 are the nanotube and nanotorus of TUC_4C_8 molecular graph. Then the VL index of tensor product of two molecular graphs is given by*

$$VL(N_1 \otimes N_2) = 18(A - 5p)(A + p) + (B - 21p)(B + 9p),$$

where $A = 6pq + q$ and $B = 54 + 9q$.

4. BOUNDS ON NEW TOPOLOGICAL INDICES OF TENSOR PRODUCT OF F- SUM ON GRAPHS FOR $F = \{SQ, ST, RQ, RT, QT\}$

The below consecutive theorems, the proof execution are analogous to preceding Section 3.

Theorem 4.1. *Let $G = W +_S X$ and $H = Y +_Q Z$. Then $\alpha_5 \leq T(G \times H) \leq \beta_5$, where*

$$\begin{aligned} \alpha_5 &= 2(q_1 p_2 + 2 p_1 q_2)(q_3 p_4 + p_3 q_4) [(\delta_{e(W)} + \delta_{e(X)}) \cdot (\delta_{e(Y)} + \delta_{e(Z)}) \\ &\quad + (\delta_{f(W)} + \delta_{f(X)}) \cdot (\delta_{f(Y)} + \delta_{f(Z)}) + 4] \end{aligned}$$

and

$$\begin{aligned} \beta_5 &= 2(q_1 p_2 + 2 p_1 q_2)(q_3 p_4 + p_3 q_4) [(\Delta_{e(W)} + \Delta_{e(X)}) \cdot (\Delta_{e(Y)} + \Delta_{e(Z)}) \\ &\quad + (\Delta_{f(W)} + \Delta_{f(X)}) \cdot (\Delta_{f(Y)} + \Delta_{f(Z)}) + 4]. \end{aligned}$$

Theorem 4.2. Let $G = W +_S X$ and $H = Y +_T Z$. Then $\alpha_6 \leq T(G \times H) \leq \beta_6$, where

$$\alpha_6 = (q_1p_2 + 2p_1q_2)(q_3p_4 + 4p_3q_4)[(\delta_e(W) + \delta_e(X)) \cdot (\delta_e(Y) + \delta_e(Z)) \\ + (\delta_f(W) + \delta_f(X)) \cdot (\delta_f(Y) + \delta_f(Z)) + 4]$$

and

$$\beta_6 = (q_1p_2 + 2p_1q_2)(q_3p_4 + 4p_3q_4)[(\Delta_e(W) + \Delta_e(X)) \cdot (\Delta_e(Y) + \Delta_e(Z)) \\ + (\Delta_f(W) + \Delta_f(X)) \cdot (\Delta_f(Y) + \Delta_f(Z)) + 4].$$

Theorem 4.3. Let $G = W +_R X$ and $H = Y +_Q Z$. Then $\alpha_7 \leq T(G \times H) \leq \beta_7$, where

$$\alpha_7 = 2(q_1p_2 + 3p_1q_2)(q_3p_4 + p_3q_4)\{(\delta_W + \delta_X)^2(\delta_Y + \delta_Z)^2 \\ + 2[(\delta_W + \delta_X)(\delta_Y + \delta_Z)]\}$$

and

$$\beta_7 = 2(q_1p_2 + 3p_1q_2)(q_3p_4 + p_3q_4)\{(\Delta_W + \Delta_X)^2(\Delta_Y + \Delta_Z)^2 \\ + 2[(\Delta_W + \Delta_X)(\Delta_Y + \Delta_Z)]\}.$$

Theorem 4.4. Let $G = W +_R X$ and $H = Y +_T Z$. Then $\alpha_8 \leq T(G \times H) \leq \beta_8$, where

$$\alpha_8 = (q_1p_2 + 3p_1q_2)(q_3p_4 + 4p_3q_4)\{(\delta_W + \delta_X)^2(\delta_Y + \delta_Z)^2 \\ + 2[(\delta_W + \delta_X)(\delta_Y + \delta_Z)]\}$$

and

$$\beta_8 = (q_1p_2 + 3p_1q_2)(q_3p_4 + 4p_3q_4)\{(\Delta_W + \Delta_X)^2(\Delta_Y + \Delta_Z)^2 \\ + 2[(\Delta_W + \Delta_X)(\Delta_Y + \Delta_Z)]\}.$$

Theorem 4.5. Let $G = W +_Q X$ and $H = Y +_T Z$. Then $\alpha_9 \leq T(G \times H) \leq \beta_9$, where

$$\alpha_9 = 2(q_1p_2 + p_1q_2)(q_3p_4 + 4p_3q_4)\{(\delta_W + \delta_X)^2(\delta_Y + \delta_Z)^2 \\ + 2[(\delta_W + \delta_X)(\delta_Y + \delta_Z)]\}$$

and

$$\beta_9 = 2(q_1p_2 + p_1q_2)(q_3p_4 + 4p_3q_4)\{(\Delta_W + \Delta_X)^2(\Delta_Y + \Delta_Z)^2 \\ + 2[(\Delta_W + \Delta_X)(\Delta_Y + \Delta_Z)]\}.$$

5. CONCLUSION

In this paper, the molecular structure data set of 18 octane isomers and 209 PCB were given by the International Academy of Mathematical Chemistry (IAMC), using this it is shown good correlation with the newly proposed index name as VL index this is highly correlated with physical properties of 18 octane isomers such as entropy, enthalpy, standard enthalpy of vaporization and Acentric factor and physical property of 209 PCB chemical structure such as relative retention time as shown in Table 1 and Figure 1. Further, we determined the bounds for tensor product of F - sum of graphs.

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