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ON THE INDICES OF CERTAIN GRAPH PRODUCTS

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Abstract. Molecular descriptors are numerical graph invariants that are used to study the chemical structure of molecules. In this paper, we determine the upper bound of the Sombor index based on four operations involving the subdivision graph, semi-total point graph, semi-total line graph, and total graph related to the lexicographic and tensor product. The exact expressions of the first reformulated Zagreb index and the second hyper-Zagreb index of the tensor product are formulated on the basis of the four significant graphs. Further, the descriptors for certain standard graphs are obtained and the graphical comparison for the first reformulated Zagreb index has also been illustrated to understand the result better.

1. **Introduction**

Topology of a molecule is primarily a non-mathematical that reflects various features of a molecular network. Numerous quantitative molecular attributes are frequently represented by precise numerals. To analyze topological invariants, a chemical compound must be amended to a molecular graph, with the atoms in the molecule corresponding to vertices and the atomic connections represented as edges. The topological indices are beneficial in many fields, but degree-based invariants are notably essential in the arena of chemical graph theory.

$V(H)$ and $E(H)$ denotes the vertex and edge set for a molecular graph $H = (V, E)$, with their cardinality as p and q respectively. The degree of vertex z of H is denoted by $d(z)$ and $e = yz$ is a

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representation of the edge linking the nodes y and z. The line graph of H, $L(H)$ is the graph wherein the edges of H correspond to vertices of $L(H)$ and two edges of $L(H)$ are adjacent if and only if they are incident in H. δ_H and Δ_H indicates minimum and maximum degree for the graph,H respectively.

Initiated by Gutman[18, 17], the First (M_1) and the Second (M_2) Zagreb Index are the widely known degree based topological descriptors for the specification of π-electron energy of the molecules. The study on first general Zagreb index, M_α $(\alpha \in \mathbb{R},\ \alpha \neq 0, 1)$ was initiated by the implementation of particular generalizations by Xueliang Li and Jie Zheng [25].

$$M_\alpha(H) = \sum_{z \in V(H)} (d_H(z))^\alpha$$

The sum-connectivity index, χ was proposed by Bo Zhou and Nenad Trinajstić. Following that, several properties and discrete constraints for the associated invariant were determined in [40].

$$\chi(H) = \sum_{yz \in E(H)} (d_H(y) + d_H(z))^{-1/2}$$

On generalizing sum-connectivity index with the first Zagreb index laid the foundation of research on another invariant called the general sum-connectivity index, χ_α $(\alpha \in \mathbb{R})$[41]. Significant core concepts for the descriptor have also been investigated in regard to specific graph operations[1].

$$\chi_\alpha(H) = \sum_{yz \in E(H)} (d_H(y) + d_H(z))^\alpha$$

Detailed study on another descriptor, the forgotten topological index have also been acted upon in papers[12]. Various graph operational expressions have been determined with reference to the index [8].

$$\mathbf{F}(H) = \sum_{z \in V(H)} d_H(z)^3 \text{ or } \sum_{yz \in E(H)} \left(d_H(y)^2 + d_H(z)^2\right)$$

The study on first hyper Zagreb index (HM_1) was initiated in [34] and specific outcomes with reference to the mathematical graph operational procedures were obtained. In addition, the formulation of second hyper Zagreb index (HM_2) was proposed in [11] and computational techniques pertaining to various classes of graphs have been established [13].

$$HM_1(H) = \sum_{yz \in E(H)} (d_H(y) + d_H(z))^2 \text{ and } HM_2(H) = \sum_{yz \in E(H)} \left(d_H(y).d_H(z)\right)^2$$

In relation to the edge degrees, reformulations of the Zagreb indices have been identified in [29] as

$$EM_1(H) = \sum_{e \in E(H)} d_H(e)^2 \text{ and } EM_2(H) = \sum_{e \sim f \in E(H)} d_H(e) d_H(f)$$

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Lately, the theoretical implications of Sombor index(SO) was postulated by Gutman[14] and further work on the graph index has been acted upon[6, 15, 21, 37].

$$SO(H) = \sum_{yz \in E(H)} \sqrt{d_H(y)^2 + d_H(z)^2}$$

The analysis of Sombor index related to some graph operations have been resolved in [2, 23]. Also recently, reformulation of the Sombor index have been determined in terms of edge degrees in [19].

On a connected graph H, [10, 39, 32] defines the graphs related as:

(i) $S(H)$ or subdivision graph is generated by replacing every edge of the graph with a vertex of degree two, keeping the original vertices unchanged.

(ii) $R(H)$ or semi total point graph is the graph including the edges of $S(H)$ along with the edges of H.

(iii) $Q(H)$ or semi total line graph is the one including edges of $S(H)$ along with the edges of $L(H)$.

(iv) $T(H)$ or total graph includes edges of $S(H)$, $L(H)$ along with the edges of H.

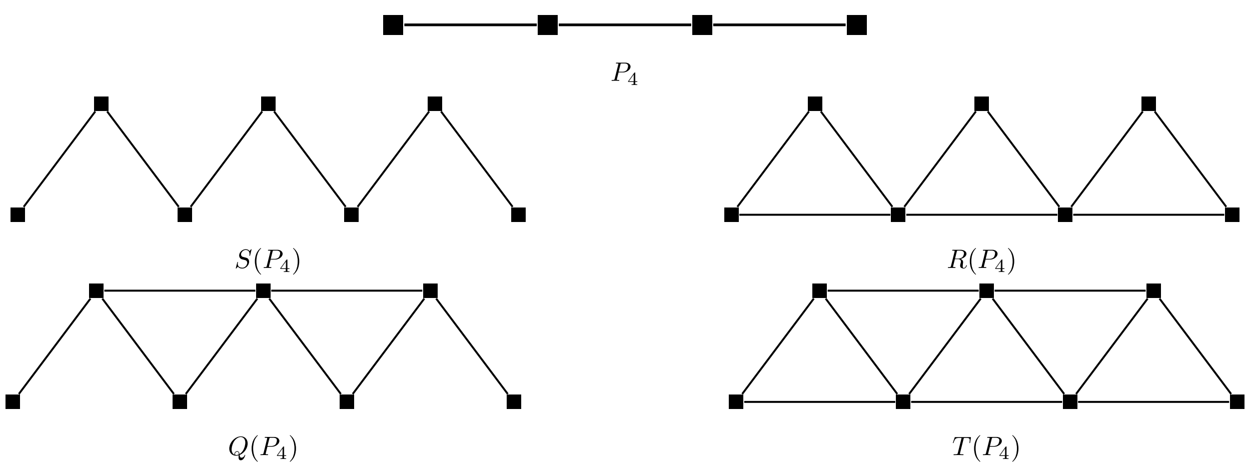

Figure 1. Base graph and some of its derived graphs

The lexicographic product of graphs H_1 and H_2, denoted as $H_1[H_2]$[38], is a graph wherein $V(H_1[H_2]) = V(H_1) \times V(H_2)$ and (y_1, z_1) is adjacent to (y_2, z_2) of $H_1[H_2]$ if and only if either $y_1 = y_2$ and z_1 is adjacent to z_2 or y_1 is adjacent to y_2. The tensor product $H_1 \otimes H_2$[22] for the graphs H_1 and H_2 possesses the vertex set as $V(H_1) \times V(H_2)$ wherein (y_1, z_1) is incident on (y_2, z_2) whenever in H_1, y_1 is adjacent to y_2 and in H_2, z_1 is adjacent to z_2. Works pertaining to the structure-invariants of the lexicographic and tensor products have been carried out[3, 36, 7, 31, 9, 5]. Works on various graph join and corona product variants have been established for SK indices in [28]. Also, findings related to other significant graph invariants of graph operations have also been investigated [27, 35, 20, 24, 16, 26, 30].

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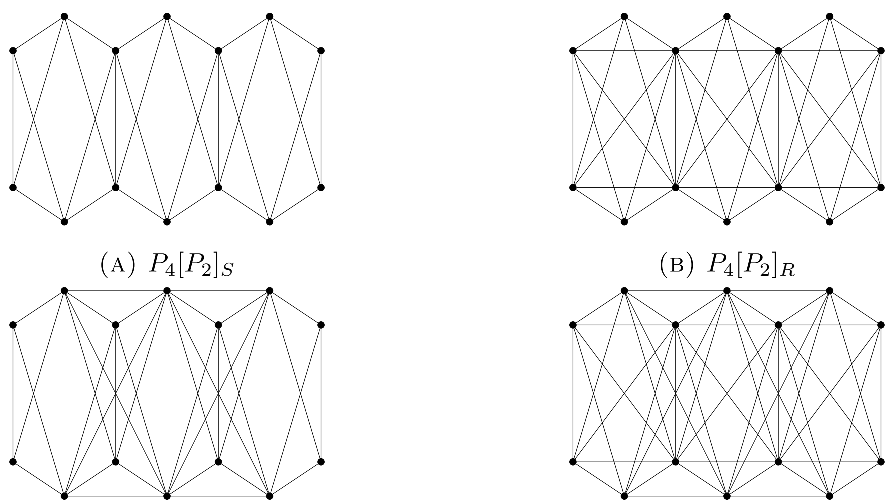
2. Methodology

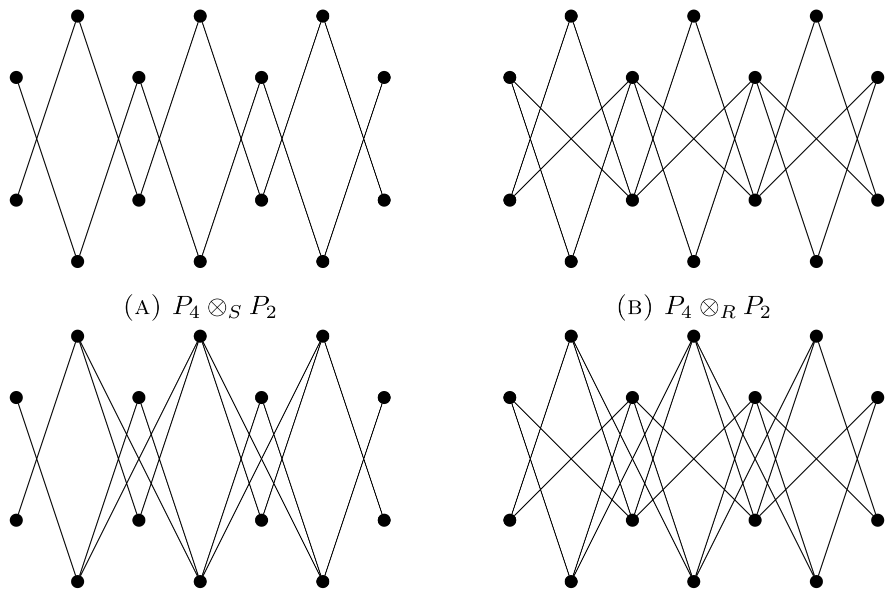
The notion of the graph operational products is to obtain many pairs of co-spectral graphs. The operational procedure begins with simple graph and results in complex network structures from the base graphs. The F-lexicographic product of H_1 and H_2 for $F \in \{S, R, Q, T\}$ denoted by $H_1[H_2]_F$[33] is a graph with $V(H_1[H_2]_F) = (V(H_1) \cup E(H_1)) \times V(H_2)$ and $u = (y_1, z_1)$ and $v = (y_2, z_2)$ of $H_1[H_2]$ are adjacent if and only if either $[y_1y_2 \in E(F(H_1))$ and $z_1, z_2 \in V(H_2)]$ or $[y_1 = y_2 \in V(H_1)$ and $z_1z_2 \in E(H_2)]$. Below we have representations of $P_4[P_2]_S$, $P_4[P_2]_R$, $P_4[P_2]_Q$ and $P_4[P_2]_T$ in the figure (2).



(A) $P_4[P_2]_S$ (B) $P_4[P_2]_R$ (C) $P_4[P_2]_Q$ (D) $P_4[P_2]_T$

FIGURE 2. $P_4[P_2]_F$

Assume F belongs to one among the symbols S, R, Q or T . The F-tensor product $H_1 \otimes_F H_2$[4] depicts a graph having $V(H_1 \otimes_F H_2) = (V(H_1) \cup E(H_1)) \times V(H_2)$ and vertices (y_1, z_1) and (y_2, z_2) of $H_1 \otimes_F H_2$ are adjacent if and only if y_1 is incident on y_2 in $E(F(H_1))$ and z_1 is incident on z_2 in H_2. Below we have representations of $P_4 \otimes_S P_2$, $P_4 \otimes_R P_2$, $P_4 \otimes_Q P_2$ and $P_4 \otimes_T P_2$ in the figure (3).



(A) $P_4 \otimes_S P_2$ (B) $P_4 \otimes_R P_2$

(C) $P_4 \otimes_Q P_2$ (D) $P_4 \otimes_T P_2$

FIGURE 3. $P_4 \otimes_F P_2$

2.1. **Sombor index based on four operations related to the lexicographic and tensor product.** In this section, we obtain the upper bounds of Sombor index based on the four operations related to the lexicographic and tensor product of two graphs. In addition, we have carried out the determination of the upper bound expressions for the descriptor of some standard graphs like path and cycle graphs.

Theorem 2.1. *Assume $H_1(p_1, q_1)$ and $H_2(p_2, q_2)$ be two arbitrary graphs. Then,*

$$\begin{aligned} SO(H_1[H_2]_S) \leq\ & p_2^3(M_1(H_1) + 4q_1) + p_1 SO(H_2) + (2p_2)^{1/2}\big(p_2 M_{3/2}(H_1) M_{1/2}(H_2) + M_{1/2}(H_1)\chi_{1/2}(H_2)\big) \\ & + 2^{3/2}(2^{1/2} + 1)p_2 q_1 q_2 \end{aligned}$$

Equality holds if and only if the components of the graph are isolated vertices.

Proof.

$$\begin{aligned} SO(H_1[H_2]_S) &= \sum_{(y_1,z_1)(y_2,z_2)\in E(H_1[H_2]_S)} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= \sum_{y_1=y_2\in V(H_1)} \sum_{z_1 z_2\in E(H_2)} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1 y_2\in E(S(H_1))} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= S_1 + S_2 \end{aligned}$$

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$$S_1 = \sum_{y_1=y_2\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}$$

$$= \sum_{y\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{(p_2d_{H_1}(y)+d_{H_2}(z_1))^2+(p_2d_{H_1}(y)+d_{H_2}(z_2))^2}$$

$$= \sum_{y\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{p_2^2d_{H_1}(y)^2+d_{H_2}(z_1)^2+2p_2d_{H_1}(y)d_{H_2}(z_1)+p_2^2d_{H_1}(y)^2+d_{H_2}(z_2)^2+2p_2d_{H_1}(y)d_{H_2}(z_2)}$$

$$\leq p_1SO(H_2)+(2p_2)^{1/2}M_{1/2}(H_1)\chi_{1/2}(H_2)+2^{3/2}p_2q_1q_2$$

$$S_2 = \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(S(H_1))} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}$$

$$= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y\in V(H_1)\\ a\in V(S(H_1))\setminus V(H_1)\\ y\sim a}} \sqrt{d(y,z_1)^2+d(a,z_2)^2}$$

$$= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y\in V(H_1)\\ a\in V(S(H_1))\setminus V(H_1)\\ y\sim a}} \sqrt{(p_2d_{H_1}(y)+d_{H_2}(z_1))^2+(2p_2)^2}$$

$$\leq p_2^3M_1(H_1)+(2p_2^3)^{1/2}M_{3/2}(H_1)M_{1/2}(H_2)+4p_2q_1q_2+4p_2^3q_1$$

From all the computations,

$$SO(H_1[H_2]_S) \leq p_2^3(M_1(H_1)+4q_1)+p_1SO(H_2)+(2p_2)^{1/2}\big(p_2M_{3/2}(H_1)M_{1/2}(H_2)+M_{1/2}(H_1)\chi_{1/2}(H_2)\big)$$
$$+2^{3/2}(2^{1/2}+1)p_2q_1q_2$$

Equality holds if and only if the components of the graph are isolated vertices. This concludes the result. □

Theorem 2.2. *Assume $H_1(p_1,q_1)$ and $H_2(p_2,q_2)$ be two arbitrary graphs. Then,*

$$SO(H_1[H_2]_R) \leq 2p_2^3(SO(H_1)+M_1(H_1))+p_1SO(H_2)+2p_2^{1/2}\Big[M_{1/2}(H_1)\chi_{1/2}(H_2)+p_2M_{3/2}(H_1)$$
$$M_{1/2}(H_2)\Big]+4(2)^{1/2}(2^{1/2}+1)p_2q_1q_2+4p_2^3q_1+(8p_2^5\Delta_{H_1}\Delta_{H_2})^{1/2}q_1$$

Equality holds if and only if the components of the graph are isolated vertices.

Proof.

$$SO(H_1[H_2]_R) = \sum_{(y_1,z_1)(y_2,z_2)\in E(H_1[H_2]_R)} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}$$

$$= \sum_{y_1=y_2\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}$$

$$+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(R(H_1))} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}$$

$$= R_1+R_2$$

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$$\begin{aligned}
R_1 &= \sum_{y_1=y_2\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= \sum_{y_1=y_2\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{(p_2d_{R(H_1)}(y_1)+d_{H_2}(z_1))^2+(p_2d_{R(H_1)}(y_1)+d_{H_2}(z_2))^2}\\
&= \sum_{y\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{(2p_2d_{H_1}(y)+d_{H_2}(z_1))^2+(2p_2d_{H_1}(y)+d_{H_2}(z_2))^2}\\
&\leq p_1SO(H_2)+2(p_2)^{1/2}M_{1/2}(H_1)\chi_{1/2}(H_2)+4(2)^{1/2}p_2q_1q_2
\end{aligned}$$

$$\begin{aligned}
R_2 &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(R(H_1))} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(H_1)} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(R(H_1))\\ y_1\in V(H_1)\\ y_2\in V(R(H_1))\setminus V(H_1)}} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= R_2^{'}+R_2^{''}
\end{aligned}$$

$$\begin{aligned}
R_2^{'} &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(H_1)} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(H_1)} \sqrt{(p_2d_{R(H_1)}(y_1)+d_{H_2}(z_1))^2+(p_2d_{R(H_1)}(y_2)+d_{H_2}(z_2))^2}\\
&= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(H_1)} \sqrt{(2p_2d_{H_1}(y_1)+d_{H_2}(z_1))^2+(2p_2d_{H_1}(y_2)+d_{H_2}(z_2))^2}\\
&\leq 2p_2^3SO(H_1)+(8p_2^5\Delta_{H_1}\Delta_{H_2})^{1/2}q_1+4p_2q_1q_2
\end{aligned}$$

$$\begin{aligned}
R_2^{''} &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(R(H_1))\\ y_1\in V(H_1)\\ y_2\in V(R(H_1))\setminus V(H_1)}} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(R(H_1))\\ y_1\in V(H_1)\\ y_2\in V(R(H_1))\setminus V(H_1)}} \sqrt{(p_2d_{R(H_1)}(y_1)+d_{H_2}(z_1))^2+(p_2d_{R(H_1)}(y_2))^2}\\
&= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(R(H_1))\\ y_1\in V(H_1)\\ y_2\in V(R(H_1))\setminus V(H_1)}} \sqrt{(2p_2d_{H_1}(y_1)+d_{H_2}(z_1))^2+(2p_2)^2}\\
&\leq 2p_2^3M_1(H_1)+2p_2^{3/2}M_{3/2}(H_1)M_{1/2}(H_2)+4p_2q_1q_2+4p_2^3q_1
\end{aligned}$$

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Hence from all the computations,

$$SO(H_1[H_2]_R) \leq 2p_2^3(SO(H_1) + M_1(H_1)) + p_1 SO(H_2) + 2p_2^{1/2}\Big[M_{1/2}(H_1)\chi_{1/2}(H_2) + p_2 M_{3/2}(H_1) \\ M_{1/2}(H_2)\Big] + 4(2)^{1/2}(2^{1/2}+1)p_2 q_1 q_2 + 4p_2^3 q_1 + (8p_2^5 \Delta_{H_1}\Delta_{H_2})^{1/2} q_1$$

Equality holds if and only if the components of the graph are isolated vertices. This concludes the result. □

Theorem 2.3. *Assume $H_1(p_1, q_1)$ and $H_2(p_2, q_2)$ be two arbitrary graphs. Then,*

$$SO(H_1[H_2]_Q) \leq p_2^3(SO(L(H_1)) + M_1(H_1)) + p_1 SO(H_2) + (2p_2)^{1/2}\Big[M_{1/2}(H_1)\chi_{1/2}(H_2) + p_2 M_{3/2}(H_1) \\ M_{1/2}(H_2)\Big] + 2^{3/2}(2^{1/2}+1)p_2 q_1 q_2 + p_2^2\Big[2\chi_{1/2}(H_1) + 2^{1/2}p_2\Big\{M_1(H_1) - 2q_1 + 2^{1/2}\chi_{1/2}(L(H_1))\Big\}\Big]$$

Proof.

$$\begin{aligned} SO(H_1[H_2]_Q) &= \sum_{(y_1,z_1)(y_2,z_2)\in E(H_1[H_2]_Q)} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= \sum_{y_1=y_2\in V(H_1)} \sum_{z_1 z_2 \in E(H_2)} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1 y_2\in E(Q(H_1))} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= Q_1 + Q_2 \end{aligned}$$

$$\begin{aligned} Q_1 &= \sum_{y_1=y_2\in V(H_1)} \sum_{z_1 z_2\in E(H_2)} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= \sum_{y\in V(H_1)} \sum_{z_1 z_2\in E(H_2)} \sqrt{(p_2 d_{Q(H_1)}(y) + d_{H_2}(z_1))^2 + (p_2 d_{Q(H_1)}(y) + d_{H_2}(z_2))^2} \\ &\leq p_1 SO(H_2) + (2p_2)^{1/2} M_{1/2}(H_1)\chi_{1/2}(H_2) + 2^{3/2} p_2 q_1 q_2 \end{aligned}$$

$$\begin{aligned} Q_2 &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1 y_2\in E(Q(H_1))} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1 y_2\in E(Q(H_1)) \\ y_1\in V(H_1) \\ y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1 y_2\in E(Q(H_1)) \\ y_1,y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{d(y_1,z_1)^2 + d(y_2,z_2)^2} \\ &= Q_2' + Q_2'' \end{aligned}$$

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$$\begin{aligned}
Q_2^{'} &= \sum_{z_1\in V(H_2)}\sum_{z_2\in V(H_2)}\sum_{\substack{y_1y_2\in E(Q(H_1))\\ y_1\in V(H_1)\\ y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= \sum_{z_1\in V(H_2)}\sum_{z_2\in V(H_2)}\sum_{\substack{y_1y_2\in E(Q(H_1))\\ y_1\in V(H_1)\\ y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{(p_2d_{Q(H_1)}(y_1)+d_{H_2}(z_1))^2+(p_2d_{Q(H_1)}(y_2))^2}\\
&= \sum_{z_1\in V(H_2)}\sum_{z_2\in V(H_2)}\sum_{\substack{y_1y_2\in E(Q(H_1))\\ y_1\in V(H_1)\\ y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{p_2^2d_{H_1}(y_1)^2+d_{H_2}(z_1)^2+2p_2d_{H_1}(y_1)d_{H_2}(z_1)+p_2^2d_{Q(H_1)}(y_2)^2}\\
&\leq p_2^3M_1(H_1)+(2q_2)p_2(2q_1)+(2p_2^3)^{1/2}M_{3/2}(H_1)M_{1/2}(H_2)+2p_2^2\chi_{1/2}(H_1)
\end{aligned}$$

$$\begin{aligned}
Q_2^{''} &= \sum_{z_1\in V(H_2)}\sum_{z_2\in V(H_2)}\sum_{\substack{y_1y_2\in E(Q(H_1))\\ y_1,y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{d(y_1,z_1)^2+d(y_2,z_2)^2}\\
&= \sum_{z_1\in V(H_2)}\sum_{z_2\in V(H_2)}\sum_{\substack{y_1y_2\in E(Q(H_1))\\ y_1,y_2\in V(Q(H_1))\setminus V(H_1)}} \sqrt{(p_2d_{Q(H_1)}(y_1))^2+(p_2d_{Q(H_1)}(y_2))^2}\\
&= \sum_{z_1\in V(H_2)}\sum_{z_2\in V(H_2)}\sum_{r_i,r_j,r_k\in E(H_1)} \sqrt{p_2^2[(d_{H_1}(r_i)+d_{H_1}(r_j))^2+(d_{H_1}(r_j)+d_{H_1}(r_k))^2]}\\
&= p_2^3\sum_{S_iS_j\in E(L(H_1))}\sqrt{(d_{L(H_1)}(S_i)+2)^2+(d_{L(H_1)}(S_j)+2)^2}\\
&\leq p_2^3[SO(L(H_1))+2^{3/2}(\frac{M_1(H_1)}{2}-q_1)+2\chi_{1/2}(L(H_1))]
\end{aligned}$$

From all the computations,

$$\begin{aligned}
SO(H_1[H_2]_Q) &\leq p_2^3(SO(L(H_1))+M_1(H_1))+p_1SO(H_2)+(2p_2)^{1/2}\Big[M_{1/2}(H_1)\chi_{1/2}(H_2)+p_2M_{3/2}(H_1)\\
&M_{1/2}(H_2)\Big]+2^{3/2}(2^{1/2}+1)p_2q_1q_2+p_2^2\Big[2\chi_{1/2}(H_1)+2^{1/2}p_2\Big\{M_1(H_1)-2q_1+2^{1/2}\chi_{1/2}(L(H_1))\Big\}\Big]
\end{aligned}$$

This concludes the result. □

Theorem 2.4. *Assume $H_1(p_1,q_1)$ and $H_2(p_2,q_2)$ be two arbitrary graphs. Then,*

$$\begin{aligned}
SO(H_1[H_2]_T) \leq\ & 2p_2^3(M_1(H_1)+SO(H_1))+p_1SO(H_2)+2(p_2)^{1/2}[M_{1/2}(H_1)\chi_{1/2}(H_2)+p_2M_{3/2}(H_1)\\
& M_{1/2}(H_2)]+p_2^2[2\chi_{1/2}(H_1)+p_2\{SO(L(H_1))+2^{1/2}(M_1(H_1)-2q_1)+2\chi_{1/2}(L(H_1))\}]\\
& +4(2)^{1/2}(2^{1/2}+1)p_2q_1q_2+(8p_2^5\Delta_{H_1}\Delta_{H_2})^{1/2}q_1
\end{aligned}$$

Proof.

$$
\begin{aligned}
SO(H_1[H_2]_T) &= \sum_{(y_1,z_1)(y_2,z_2)\in E(H_1[H_2]_T)} \sqrt{d_{H_1[H_2]_T}(y_1,z_1)^2 + d_{H_1[H_2]_T}(y_2,z_2)^2} \\
&= \sum_{y\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{d_{H_1[H_2]_T}(y,z_1)^2 + d_{H_1[H_2]_T}(y,z_2)^2} \\
&+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(T(H_1))} \sqrt{d_{H_1[H_2]_T}(y_1,z_1)^2 + d_{H_1[H_2]_T}(y_2,z_2)^2} \\
&= \sum_{y\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{d_{H_1[H_2]_R}(y,z_1)^2 + d_{H_1[H_2]_R}(y,z_2)^2} \\
&+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(H_1)} \sqrt{d_{H_1[H_2]_R}(y_1,z_1)^2 + d_{H_1[H_2]_R}(y_2,z_2)^2} \\
&+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(T(H_1))\\ y_1\in V(H_1)\\ y_2\in V(T(H_1))\setminus V(H_1)}} \sqrt{d_{H_1[H_2]_R}(y_1,z_1)^2 + d_{H_1[H_2]_Q}(y_2,z_2)^2} \\
&+ \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(T(H_1))\\ y_1,y_2\in V(T(H_1))\setminus V(H_1)}} \sqrt{d_{H_1[H_2]_Q}(y_1,z_1)^2 + d_{H_1[H_2]_Q}(y_2,z_2)^2} \\
&= T_1 + T_2 + T_3 + T_4
\end{aligned}
$$

From the theorems (2.1),(2.2),(2.3), we have

$$
\begin{aligned}
T_1 &= \sum_{y\in V(H_1)} \sum_{z_1z_2\in E(H_2)} \sqrt{d_{H_1[H_2]_R}(y,z_1)^2 + d_{H_1[H_2]_R}(y,z_2)^2} \\
&\leq p_1 SO(H_2) + 2(p_2)^{1/2} M_{1/2}(H_1)\chi_{1/2}(H_2) + 4(2)^{1/2} p_2 q_1 q_2
\end{aligned}
$$

$$
\begin{aligned}
T_2 &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{y_1y_2\in E(H_1)} \sqrt{d_{H_1[H_2]_R}(y_1,z_1)^2 + d_{H_1[H_2]_R}(y_2,z_2)^2} \\
&\leq 2p_2^3 SO(H_1) + 4p_2 q_1 q_2 + (8p_2^5 \Delta_{H_1}\Delta_{H_2})^{1/2} q_1
\end{aligned}
$$

$$
\begin{aligned}
T_3 &= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(T(H_1))\\ y_1\in V(H_1)\\ y_2\in V(T(H_1))\setminus V(H_1)}} \sqrt{d_{H_1[H_2]_R}(y_1,z_1)^2 + d_{H_1[H_2]_Q}(y_2,z_2)^2} \\
&= \sum_{z_1\in V(H_2)} \sum_{z_2\in V(H_2)} \sum_{\substack{y_1y_2\in E(T(H_1))\\ y_1\in V(H_1)\\ y_2\in V(T(H_1))\setminus V(H_1)}} \sqrt{(2p_2 d_{H_1}(y_1) + d_{H_1}(z_2))^2 + (p_2 d_{Q(H_1)}(y_2))^2} \\
&\leq 2p_2^2(p_2 M_1(H_1) + \chi_{1/2}(H_1)) + 2p_2^{3/2} M_{1/2}(H_2) M_{3/2}(H_1) + 4p_2 q_1 q_2
\end{aligned}
$$

$$T_4 = \sum_{z_1 \in V(H_2)} \sum_{z_2 \in V(H_2)} \sum_{\substack{y_1y_2 \in E(T(H_1)) \\ y_1, y_2 \in V(T(H_1)) \setminus V(H_1)}} \sqrt{d_{H_1[H_2]_Q}(y_1, z_1)^2 + d_{H_1[H_2]_Q}(y_2, z_2)^2}$$
$$\leq p_2^3 \Big[SO(L(H_1)) + 2^{1/2}(M_1(H_1) - 2q_1) + 2\chi_{1/2}(L(H_1)) \Big]$$

Hence from all the computations,

$$SO(H_1[H_2]_T) \leq 2p_2^3(M_1(H_1) + SO(H_1)) + p_1 SO(H_2) + 2(p_2)^{1/2}[M_{1/2}(H_1)\chi_{1/2}(H_2) + p_2 M_{3/2}(H_1)$$
$$M_{1/2}(H_2)] + p_2^2[2\chi_{1/2}(H_1) + p_2\{SO(L(H_1)) + 2^{1/2}(M_1(H_1) - 2q_1) + 2\chi_{1/2}(L(H_1))\}]$$
$$+ 4(2)^{1/2}(2^{1/2} + 1)p_2 q_1 q_2 + (8p_2^5 \Delta_{H_1} \Delta_{H_2})^{1/2} q_1$$

This concludes the result. □

Corollary 2.5. *The upper bound for the Sombor index of the lexicographic product versions of the path graphs is given as:*

- $SO(P_m[P_n]_S) \leq 8mn^3 + 6.83mn^2 - 10n^3 - 4mn - 6.83n^2 - 4.01m + 6.83n + n^{1/2}\Big(5.66mn^2 + 0.69mn - 7.31n^2 - 5.07m + 1.94n + 2.97\Big)$
- $SO(P_m[P_n]_R) \leq 17.66mn^3 + 13.66mn^2 - 24.03n^3 - 10.83mn - 13.66n^2 - 4.01m + 13.66n + n^{1/2}\Big(8mn^2 + 0.97mn - 10.34n^2 - 7.17m + 2.75n + 4.20\Big) + (32n^5)^{1/2}(m-1)$
- $SO(P_m[P_n]_Q) \leq 13.66mn^3 + 10.83mn^2 - 27.57n^3 - 4mn - 11.90n^2 - 4.01m + 6.83n + n^{1/2}\Big(5.66mn^2 + 0.69mn - 7.31n^2 - 5.07m + 1.94n + 2.97\Big)$
- $SO(P_m[P_n]_T) \leq 23.31mn^3 + 17.66mn^2 - 41.60n^3 - 10.83mn - 18.73n^2 - 4.01m + 13.66n + n^{1/2}\Big(8mn^2 + 0.97mn - 10.34n^2 - 7.17m + 2.75n + 4.20\Big) + (32n^5)^{1/2}(m-1)$

Corollary 2.6. *The upper bound for the Sombor index of the lexicographic product versions of the cycle graphs is given as:*

- $SO(C_m[C_n]_S) \leq 8mn^3 + 6.83mn^2 + 2.83mn + n^{1/2}(5.66mn^2 + 4mn)$
- $SO(C_m[C_n]_R) \leq 17.66mn^3 + 13.66mn^2 + 2.83mn + n^{1/2}\Big(8mn^2 + 5.66\Big) + (32n^5)^{1/2}m$
- $SO(C_m[C_n]_Q) \leq 13.66mn^3 + 10.83mn^2 + 2.83mn + n^{1/2}\Big(5.66mn^2 + 4mn\Big)$
- $SO(C_m[C_n]_T) \leq 23.31mn^3 + 17.66mn^2 + 2.83mn + n^{1/2}\Big(8mn^2 + 5.66mn\Big) + (32n^5)^{1/2}m$

Corollary 2.7. *The upper bound for the Sombor index of the lexicographic product versions involving path and cycle graphs is given as:*

- $SO(P_m[C_n]_S) \leq 8mn^3 + 6.83mn^2 - 10n^3 + 2.83mn - 6.83n^2 + n^{1/2}\Big(5.66n^3 - 3.31n^2 - 2.34n\Big)$
- $SO(P_m[C_n]_R) \leq 17.66mn^3 + 13.66mn^2 - 24.03n^3 + 2.83mn - 13.66n^2 + n^{1/2}\Big(13.66mn^2 + 5.66mn - 15.997n^2 - 3.31n\Big)$
- $SO(P_m[C_n]_Q) \leq 13.66mn^3 + 10.83mn^2 - 27.57n^3 + 2.83mn - 11.90n^2 + n^{1/2}\Big(5.66mn^2 + 4mn - 7.31n^2 - 2.34n\Big)$

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- $SO(P_m[C_n]_T) \leq 23.31mn^3+17.66mn^2-41.60n^3+2.83mn-18.73n^2+n^{1/2}\Big(13.66mn^2+5.66mn-16n^2-3.31n\Big)$

Corollary 2.8. *The upper bound for the Sombor index of the lexicographic product versions involving cycle and path graphs is given as:*

- $SO(C_n[P_m]_S) \leq 8m^3n + 6.83m^2n - 4mn - 4.01n + m^{1/2}\Big(5.66m^2n + 0.69mn - 5.07n\Big)$
- $SO(C_n[P_m]_R) \leq 17.66m^3n + 13.66m^2n - 10.83mn - 4.01n + m^{1/2}\Big(13.66m^2n + 0.97mn - 7.17n\Big)$
- $SO(C_n[P_m]_Q) \leq 13.66m^3n + 10.83m^2n - 4mn - 4.01n + m^{1/2}\Big(5.66m^2n + 0.68mn - 5.07n\Big)$
- $SO(C_n[P_m]_T) \leq 23.31m^3n + 17.65m^2n - 10.83mn - 4.01n + m^{1/2}\Big(13.66m^2n + 0.97mn - 7.17n\Big)$

Theorem 2.9. *Assume $H_1(p_1, q_1)$ and $H_2(p_2, q_2)$ be two arbitrary graphs. Then,*

- $SO(H_1 \otimes_S H_2) < (M_1(H_1) + 4q_1)M_1(H_2)$
- $SO(H_1 \otimes_R H_2) < 4(M_1(H_1) + q_1)M_1(H_2)$
- $SO(H_1 \otimes_Q H_2) < (M_1(H_1) + HM_1(H_1))M_1(H_2)$
- $SO(H_1 \otimes_T H_2) < (4M_1(H_1) + HM_1(H_1))M_1(H_2)$

Corollary 2.10. *The upper bound for the Sombor index of the tensor product versions of the path graphs is given as:*

- $SO(P_m \otimes_S P_n) < 4(4m-5)(2n-3)$
- $SO(P_m \otimes_R P_n) < 8(5m-7)(2n-3)$
- $SO(P_m \otimes_Q P_n) < 8(5m-9)(2n-3)$
- $SO(P_m \otimes_T P_n) < 4(16m-27)(2n-3)$

Corollary 2.11. *The upper bound for the Sombor index of the tensor product versions of the cycle graphs is given as:*

- $SO(C_m \otimes_S C_n) < 32mn$
- $SO(C_m \otimes_R C_n) < 80mn$
- $SO(C_m \otimes_Q C_n) < 80mn$
- $SO(C_m \otimes_T C_n) < 128mn$

2.2. **Second Hyper Zagreb Index and First Reformulated Zagreb Index based on four operations related to the tensor product.** In this section, we determine the evaluated expressions of the second hyper-Zagreb index and the first reformulated Zagreb index of the tensor products based on the four graphs and further, we also obtain the expression values for the standard path and cycle graphs.

Theorem 2.12. *Assume $H_1(p_1, q_1)$ and $H_2(p_2, q_2)$ be two arbitrary graphs and $F \in \{S, R, Q, T\}$. Then,*

$$HM_2(H_1 \otimes_F H_2) \quad = \quad 2HM_2(F(H_1))HM_2(H_2)$$

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Proof.

$$\begin{aligned} HM_2(H_1 \otimes_F H_2) &= \sum_{(y_1,z_1)(y_2,z_2)\in E(H_1\otimes_F H_2)} (d_{H_1\otimes_F H_2}(y_1,z_1).d_{H_1\otimes_F H_2}(y_2,z_2))^2 \\ &= 2\sum_{y_1y_2\in E(F(H_1))}\sum_{z_1z_2\in E(H_2)} \Big[(d_{F(H_1)}(y_1)d_{H_2}(z_1)).(d_{F(H_1)}(y_2)d_{H_2}(z_2))\Big]^2 \\ &= 2\sum_{y_1y_2\in E(F(H_1))} (d_{F(H_1)}(y_1).d_{F(H_1)}(y_2))^2 \sum_{z_1z_2\in E(H_2)} (d_{H_2}(z_1).d_{H_2}(z_2))^2 \\ &= 2HM_2(F(H_1))HM_2(H_2) \end{aligned}$$

□

Corollary 2.13. *Assume $H_1(p_1,q_1)$ and $H_2(p_2,q_2)$ be two arbitrary graphs and $F \in \{S,R,Q,T\}$. Then,*

- $HM_2(H_1 \otimes_S H_2) = 8F(H_1)HM_2(H_2)$
- $HM_2(H_1 \otimes_R H_2) = 32(HM_2(H_1) + F(H_1))HM_2(H_2)$
- $HM_2(H_1 \otimes_Q H_2) \leq 16\Delta^4_{H_1} M_1(H_1)HM_2(H_2)$
- $HM_2(H_1 \otimes_T H_2) \leq 16\Delta^4_{H_1} (M_1(H_1) + 4q_1)HM_2(H_2)$

Theorem 2.14. *Assume $H_1(p_1,q_1)$ and $H_2(p_2,q_2)$ be two arbitrary graphs. Then,*

- $EM_1(H_1 \otimes_S H_2) = (\mathbf{F}(H_1) + 8q_1)\mathbf{F}(H_2) + 8M_2(H_2)M_1(H_1) - 4M_1(H_2)(M_1(H_1) + 4q_1) + 16q_1q_2$
- $EM_1(H_1 \otimes_R H_2) = 8\mathbf{F}(H_2)\Big(\mathbf{F}(H_1) + q_1\Big) + 16M_2(H_2)\Big(M_1(H_1) + M_2(H_1)\Big) - 16(M_1(H_1) + q_1)M_1(H_2) + 24q_1q_2$
- $EM_1(H_1 \otimes_Q H_2) = \mathbf{F}(H_2)\Big(\mathbf{F}(H_1) + \chi_3(H_1)\Big) + 4q_2\Big(M_1(H_1) + 2q_1\Big) + 4\Big(2EM_1(H_1) + EM_2(H_1) + 2\Big\{M_1(H_1) + M_2(H_1)\Big\} + \mathbf{F}(H_1) - 4q_1\Big)M_2(H_2) - 4\Big(M_1(H_1) + HM_1(H_1)\Big)M_1(H_2)$
- $EM_1(H_1 \otimes_T H_2) = \mathbf{F}(H_2)\Big(8\mathbf{F}(H_1) + \chi_3(H_1)\Big) + 4\Big(2M_1(H_1) + 8M_2(H_1) + 2EM_1(H_1) + EM_2(H_1) + 2\mathbf{F}(H_1) - 4q_1\Big)M_2(H_2) - 4\Big(4M_1(H_1) + HM_1(H_1)\Big)M_1(H_2) + 4q_2\Big(M_1(H_1) + 4q_1\Big)$

Corollary 2.15. *The exact expressions for the first reformulated Zagreb index for the path graphs P_m, P_n are:*

- $EM_1(P_m \otimes_S P_n) = 144mn - 304m - 224n + 468$
- $EM_1(P_m \otimes_R P_n) = 792mn - 1576m - 1432n + 2824$
- $EM_1(P_m \otimes_Q P_n) = 792mn - 1576m - 1792n + 3536$
- $EM_1(P_m \otimes_T P_n) = 1568mn - 3104m - 3288n + 6468$

Corollary 2.16. *The exact expressions for the first reformulated Zagreb index for the cycle graphs C_m, C_n are:*

- $EM_1(C_m \otimes_S C_n) = 144mn$
- $EM_1(C_m \otimes_R C_n) = 792mn$
- $EM_1(C_m \otimes_Q C_n) = 792mn$

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- $EM_1(C_m \otimes_T C_n) \quad = \quad 800mn$

Corollary 2.17. *The exact expressions for the first reformulated Zagreb index of* $P_m \otimes_F C_n$ $(F \in \{S, R, Q, T\})$ *are:*

- $EM_1(P_m \otimes_S C_n) \quad = \quad 144mn - 224n$
- $EM_1(P_m \otimes_R C_n) \quad = \quad 792mn - 1432n$
- $EM_1(P_m \otimes_Q C_n) \quad = \quad \begin{cases} 536mn + 512n^2 - 2336n, & m = 2 \\ 280mn + 512n^2 - 1792n, & m \geq 3 \end{cases}$
- $EM_1(P_m \otimes_T C_n) \quad = \quad \begin{cases} 1824mn - 3832n, & m = 2 \\ 1568mn - 3288n, & m \geq 3 \end{cases}$

Corollary 2.18. *The exact expressions for the first reformulated Zagreb index of* $C_n \otimes_F P_m$ $(F \in \{S, R, Q, T\})$ *are:*

- $EM_1(C_n \otimes_S P_m) \quad = \quad 144mn - 304n$
- $EM_1(C_n \otimes_R P_m) \quad = \quad 792mn - 1576n$
- $EM_1(C_n \otimes_Q P_m) \quad = \quad 792mn - 1576n$
- $EM_1(C_n \otimes_T P_m) \quad = \quad 1568mn - 3104n$

2.3. **Graphical Illustration.** The graphical depiction of the evaluated expression of the First Reformulated Zagreb index for the $P_m \otimes_F P_n$ and $C_m \otimes_F C_n$ graph operation is shown in Figure 4 where $F \in \{S, R, Q, T\}$.

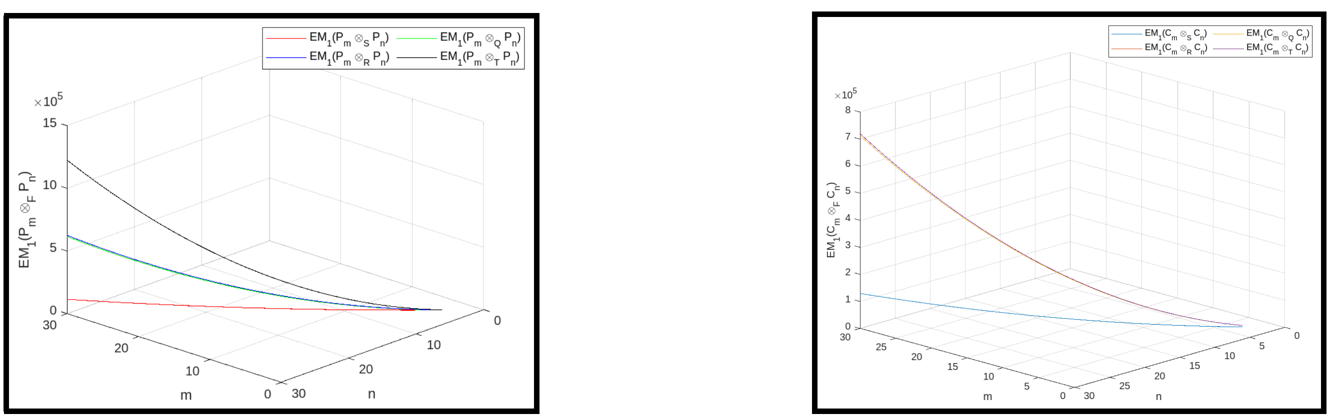

FIGURE 4. Graphical illustration of $EM_1(P_m \otimes_F P_n)$(left) and $EM_1(C_m \otimes_F C_n)$(right)

The graphical depiction of the evaluated expression of the First Reformulated Zagreb index for the $P_m \otimes_F C_n$ and $C_n \otimes_F P_m$ graph operation is shown in Figure (5) where $F \in \{S, R, Q, T\}$.

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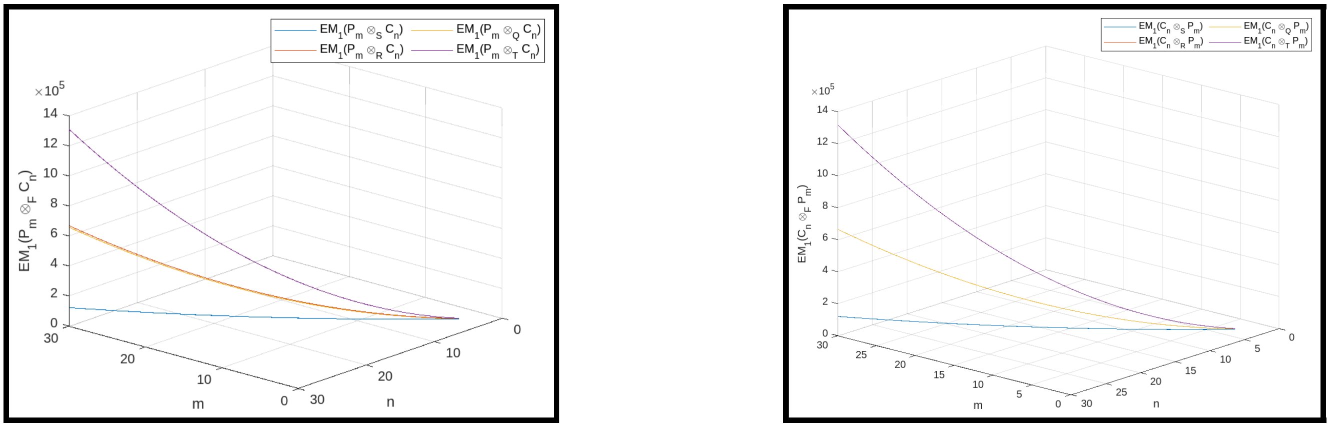

FIGURE 5. Graphical illustration of exact expression of $EM_1(P_m \otimes_F C_n)$(left) and $EM_1(C_n \otimes_F P_m)$(right)

From the figures 4 and 5, we can assert that the first reformulated Zagreb index for the tensor product graph operations involving the four derived graphs holds the greatest value for total graph product version in all the cases of path and cycle graphs.

3. Conclusion

Molecular descriptors have a considerable influence in the comprehension of medical techniques and social network theory. In this paper, we execute the determination of the upper bound expressions of the Sombor index of the lexicographic and tensor product of two graphs based on the four operations involving the subdivision graphs, semi-total point graphs, semi-total line graphs and the total graphs.

The formulation of the exact expressions for the second hyper Zagreb index and the first reformulated Zagreb index of the tensor products of the graphs based on the four graphical operations is carried out. Further, the descriptor bounds and values with respect to standard path and cycle graphs are obtained and for the proper illustration of the notion, the graphical comparison for the first reformulated Zagreb index has been depicted in the paper.

For the future scope of the study, one can look into the formulation of the indices for the generalized $F-$ lexicographic and $F-$ tensor product versions where $F \in \{S, R, Q, T\}$. The formulations of the topological index of the complex network structures which are of the forms of the resultant path and cycle graph lexicographic and tensor product graph combinations is obtained just with the knowledge of the base graph topological index computations. The results have strong significance towards wide and stringent investigation of bond-additive indices and graph transformed structural networks.

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