

## ZAGREB INDICES OF SOME CHEMICAL STRUCTURES USING NEW PRODUCTS OF GRAPHS

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**ABSTRACT.** Zagreb indices are one of the most extensively studied degree-based structural descriptors for analyzing various physico-chemical properties of chemical compounds. In this paper, we define four new products of graphs based on adjacency relations and compute their Zagreb indices. Using these expressions we compute the Zagreb indices of various chemical compounds such as linear polyacene, a class of nanotubes  $NA_m^{2n}$ , toroidal fullerene  $NC_{2m}^{2n}(\mathbb{H}_{2m}^{2n})$  and hexagonal lattice.

**Key Words:** first Zagreb index ( $M_1(G)$ ), second Zagreb index ( $M_2(G)$ ), Fullerenes

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### 1. INTRODUCTION

Topological indices, since their inception in 1947 by H. Wiener [29] has been subjected to an extensive study in analysing the structure-property relationship of compounds. In 1972, Gutman and Trinajstić defined the first and second Zagreb indices as an easier approximation in the computation of  $\pi$ -electron energy of hydrocarbons [22]. Let  $G$  be any connected graph with vertex set  $V(G)$  and edge set  $E(G)$ . The

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first Zagreb index  $M_1(G)$  and the second Zagreb index  $M_2(G)$  [21] are defined as

$$M_1(G) = \sum_{u \in V(G)} d(u)^2$$
$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

where  $d(u)$  denotes the degree of the vertex  $u$  in  $G$ . Through the years, several mathematical properties and structure activity relationships of Zagreb indices have been extensively studied. For a detailed literature on Zagreb indices and other topological indices, see [1, 5, 13, 16, 20, 23, 24].

The determination of topological indices of chemical graphs is an important research problem for the past several years [9, 10]. The computation of topological indices of complex chemical structures is a challenging problem which requires polynomial time. Graph operations generalize various classes of graphs thus making the computation of topological indices easier for larger classes of graphs. Graovac and Pisanski were the first ones to study the topological indices of graph operations. They computed the Wiener index of the Cartesian product of graphs [19]. Klavžar [26] determined the closed expressions for the Szeged index of the Cartesian product of graphs. In [25], Khalifeh *et al.* determined the exact expressions for Zagreb indices of Cartesian product and some chemical structures. In 2009, Eliasi and Taeri defined  $F$ -sums, a new set of operations on graphs and computed the Wiener index of the sums [17]. In [28], Metsidik *et al.* determined the hyper Wiener index and reverse Wiener index of  $F$ -sums. In 2016, Deng *et al.* gave the explicit expressions for the Zagreb indices of  $F$ -sums of graphs [14]. Akhtar and Imran computed the Forgotten index of  $F$ -sums [2]. Basavanagoud *et al.* introduced sixty new operations related to  $F$ -sums and computed Zagreb indices and Forgotten index of the operations [11]. In 2019, Liu *et al.* introduced the generalized form of subdivisions and  $F_k$ -sums. They also computed the Zagreb indices of the  $F_k$ -sums [27]. Awais *et al.* determined the exact expression for generalized  $F_k$ -sums of Forgotten index [8]. Numerous graph operations have been defined, and in-depth research has been done on computing various topological indices on various graph operations [3, 4, 7, 6, 12]. Although there are lots of graph operations which produce larger classes of graphs, most of them does not include large class of chemical structures. In this paper,

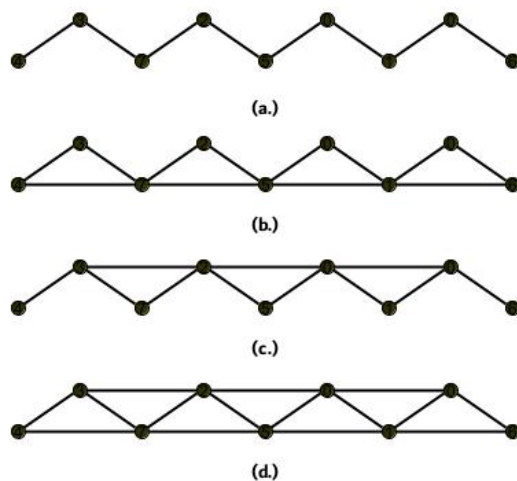


FIGURE 1. (a.)  $S(P_5)$ , (b.)  $R(P_5)$ , (c.)  $Q(P_5)$ , (d.)  $T(P_5)$

we define a new graph operation called adjacency product or A-product which generalizes the structure of some chemical compounds and compute the Zagreb indices of adjacency products.

## 2. FOUR NEW ADJACENCY BASED GRAPH PRODUCTS

Let  $G$  be a connected graph, then the four subdivision graphs  $S(G)$ ,  $R(G)$ ,  $Q(G)$  and  $T(G)$  associated with  $G$  are [17]

- Subdivision graph  $S(G)$  of a graph  $G$  is obtained from  $G$  by replacing each of its edges by a path of length 2, or equivalently, by inserting an additional vertex into each edge of  $G$ .
- $R(G)$  of a graph  $G$  is obtained from  $G$  by inserting an additional vertex into each edge of  $G$  and keeping every edge of  $G$ .
- $Q(G)$  of a graph  $G$  is obtained from  $G$  by inserting an additional vertex into each edge of  $G$ , then joining every pair of new vertices whose corresponding edges are adjacent in  $G$ .
- Total graph  $T(G)$  of a graph  $G$  is obtained from  $G$  by inserting an additional vertex into each edge of  $G$  and keeping every edge of  $G$  and joining every pair of new vertices whose corresponding edges are adjacent in  $G$ .

For example, the subdivision graphs of path  $P_5$  is plotted in Figure 1.

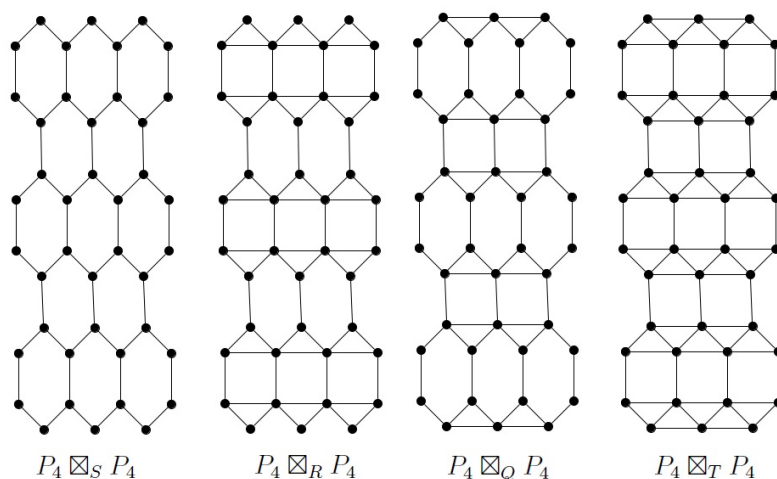


FIGURE 2. The Adjacency Products of two  $P_4$ 's.

For convenience, in  $F(G)$  where  $F = \{S, R, Q, T\}$  we call newly introduced vertices as white vertices and the vertices of  $G$  as black vertices. Let  $V_1 = \{u_1, u_2, \dots, u_n\}$ ,  $V_2 = \{v_1, v_2, \dots, v_m\}$  denotes the vertex sets and  $E_1 = \{e_1, e_2, \dots, e_t\}$ ,  $E_2 = \{f_1, f_2, \dots, f_s\}$  denotes the edge sets of the graphs  $G_1$  and  $G_2$  respectively. Associated with each edge  $f_j = v_p v_q \in G_2$ , define a set  $V_{f_j} = \{v_{pj}, v_{qj}\}$  of vertices and their union be  $A(G_2) = \cup_{j=1}^s V_{f_j}$ . Every vertex of  $A(G_2)$  is of the form  $v_{ij}$  where the vertex  $v_{ij}$  denote the copy of the vertex  $v_i$  in  $G_2$  corresponding to the edge  $f_j$ .

**Definition 2.1.** Let  $F$  be one among the four symbols  $S, R, Q, T$ , we define the adjacency product or A- product of  $G_1$  and  $G_2$  denoted by  $G_1 \boxtimes_F G_2$  is the graph with vertex set  $V(G_1 \boxtimes_F G_2) = (V_1 \cup E_1) \times (A(G_2))$  and edge set  $E(G_1 \boxtimes_F G_2)$  consist of edges  $(u_i, v_{jk})(u_p, v_{qr})$  if and only if either  $u_i u_p \in E(F(G))$  and  $v_{jk} = v_{qr}$  or  $u_i = u_p$  with  $v_j v_q \in E_2$  and  $k = r$  or  $u_i = u_p$  with  $f_k f_r \in L(G_2)$  and  $j = q$  where  $f_k, f_r \in E_2$ .

In other words, corresponding to each vertex  $v \in G_2$  we take  $d(v)$  copies of  $F(G_1)$  and pairwise join the corresponding black vertices of copies  $F(G_1)$  whenever the corresponding vertices are adjacent in  $G_2$  and the corresponding white vertices of each pair will be adjacent to another pair whenever the corresponding edges are adjacent in  $G_2$ . Throughout this paper we consider generalized Zagreb index as  $M_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha$ ,

$\alpha \geq 3$  is a natural number. When  $\alpha = 3$  it is called Forgotten index [18]. Figure 2 is an example of A - product with  $G_1, G_2 = P_4$ . Based on these subdivisions we have the following preliminary result from [14].

**Lemma 2.2.** [14] *Let  $G_1$  be a simple connected graph with vertex set  $V_1$  and edges set  $E_1$  and  $F(G_1)$  be the subdivision graph of  $G_1$  with  $F = Q$  or  $T$ . If  $u, x \in E_1$  with  $u = u_i u_j$  and  $x = u_j u_k$  where  $u_i, u_j, u_k \in V_1$ . Then*

(a).

$$\sum_{ux \in E(F(G_1)), u, x \in E_1} (d_{F(G_1)}(u) + d_{F(G_1)}(x)) = M_3(G_1) + 2M_2(G_1) - 2M_1(G_1)$$

(b.)

$$\begin{aligned} \sum_{ux \in E(F(G_1)), u, x \in E_1} d_{F(G_1)}(u) d_{F(G_1)}(x) &= \frac{1}{2} M_4(G_1) - \frac{1}{2} M_3(G_1) \\ + \sum_{u_i, u_j \in V_1} r_{ij} d_{G_1}(u_i) d_{G_1}(u_j) &+ \sum_{u_j \in V_1} d_{G_1}(u_j)^2 \sum_{u_i \in V_1, u_i u_j \in E_1} d_{G_1}(u_i) - 2M_2(G_1) \end{aligned}$$

$r_{ij}$  denotes the number of neighbouring vertices common to both  $u_i, u_j$ .

Fullerene is an all carbon skeleton of a molecule in which the atoms are arranged by means of pentagons and hexagons. Michel Deza [15] extended this fullerene structure onto other closed surfaces such as sphere, torus, Klein bottle and projective plane. Let  $L$  be a regular hexagonal lattice and  $P_n^m$  be an  $mn$  quadrilateral section cut from the regular hexagonal lattice. When  $n = 1$ , the structure is known as a linear hexagonal chain. When  $n \geq 2$ , if we identify the two lateral end sections of the hexagonal lattice and then identify the top and bottom sides of the lattice  $P_n^m$ , the resulting structure is known as toroidal fullerene with  $mn$  hexagons [10].

### 3. MAIN RESULTS

In this section we obtain the expression for the first and second Zagreb indices of the adjacency product or A - product in terms of the constituent graphs.

**Theorem 3.1.** *Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two simple connected graphs. Then*

$$\text{a. } M_1(G_1 \boxtimes_S G_2) = 2|E_2|(M_1(G_1) + 2|E_1|M_1(G_2) + |E_1|M_3(G_2) + 10|E_1||E_2| + 2|E_2||V_1|)$$

$$\begin{aligned} \text{b. } M_2(G_1 \boxtimes_S G_2) &= \frac{1}{2}|E_1|(M_4(G_2) + M_3(G_2)) + M_1(G_1)M_1(G_2) + \\ & 3|E_2|M_1(G_1) + \frac{3}{2}|E_1|M_1(G_2) + 7|E_1||E_2| + |E_2||V_1| \end{aligned}$$

*Proof.* From the definition of first Zagreb index, we have

$$\begin{aligned} M_1(G_1 \boxtimes_S G_2) &= \sum_{(u,v) \in V(G_1 \boxtimes_S G_2)} d_{(G_1 \boxtimes_S G_2)}^2(u, v) \\ &= \sum_{(u_i, v_{jk})(u_p, v_{qr}) \in E(G_1 \boxtimes_S G_2)} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_S G_2)}(u_p, v_{qr})) \\ &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_j) + d_{(G_1 \boxtimes_S G_2)}(u_i, v_q)) \\ &+ \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_S G_2)}(u_i, v_{qr})) \\ &+ \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_S G_2)}(u_p, v_{jk})) \\ &= A_1 + B_1 + C_1 \end{aligned}$$

Now we separately find the values of each parts of the sum.

$$\begin{aligned} A_1 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_j) + d_{(G_1 \boxtimes_S G_2)}(u_i, v_q)) \\ &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} [d_{G_1}(u_i) + 1 + d_{G_1}(u_i) + 1] \\ &= 2|E_2|(2|E_1| + |V_1|) \end{aligned}$$

The second part is,

$$\begin{aligned} B_1 &= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_S G_2)}(u_i, v_{qr})) \\ &= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} [d_{G_2}(v_j) + 1 + d_{G_2}(v_j) + 1] \\ &= \sum_{u_i \in E_1} \sum_{v_j \in V_2, d(v_j) \neq 1} d(v_j)(d(v_j)^2 - 1) \\ &= |E_1|(M_3(G_2) - 2|E_2|) \end{aligned}$$

The third part is,

$$\begin{aligned}
 C_1 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_S G_2)}(u_p, v_{jk})) \\
 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{G_1}(u_i) + 1 + d_{G_2}(v_j) + 1) \\
 &= \sum_{v_{jk} \in V_2} (M_1(G_1) + 4|E_1| + 2|E_1|d_{G_2}(v_j)) \\
 &= 2|E_2|(M_1(G_1) + 2|E_1|M_1(G_2) + 8|E_1||E_2|)
 \end{aligned}$$

From the expressions, we obtain

$$\begin{aligned}
 M_1(G_1 \boxtimes_S G_2) &= 2|E_2|(M_1(G_1) + 2|E_1|M_1(G_2) + |E_1|M_3(G_2)) \\
 &\quad + 10|E_1||E_2| + 2|E_2||V_1|
 \end{aligned}$$

Next Consider

$$\begin{aligned}
 M_2(G_1 \boxtimes_S G_2) &= \sum_{(u_i, v_{jk})(u_p, v_{qr}) \in E(G_1 \boxtimes_S G_2)} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk})d_{(G_1 \boxtimes_S G_2)}(u_p, v_{qr})) \\
 &= \sum_{u_i \in V_1} \sum_{\substack{v_j v_q \in E_2 \\ k=r}} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_j)d_{(G_1 \boxtimes_S G_2)}(u_i, v_q)) \\
 &\quad + \sum_{u_i \in E_1} \sum_{\substack{f_k f_r \in E(L(G_2)) \\ j=q}} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk})d_{(G_1 \boxtimes_S G_2)}(u_i, v_{qr})) \\
 &\quad + \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk})d_{(G_1 \boxtimes_S G_2)}(u_p, v_{jk})) \\
 &= A_2 + B_2 + C_2
 \end{aligned}$$

First part of the sum is

$$\begin{aligned}
 A_2 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_j)d_{(G_1 \boxtimes_S G_2)}(u_i, v_q)) \\
 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{G_1}(u_i) + 1)(d_{G_1}(u_i) + 1) \\
 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{G_1}(u_i)^2 + 2(d_{G_1}(u_i) + 1)) \\
 &= |E_2|(M_1(G_1) + 4|E_1| + |V_1|)
 \end{aligned}$$

The second part is,

$$\begin{aligned}
B_2 &= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_S G_2)}(u_i, v_{qr})) \\
&= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} (d_{G_2}(v_j) + 1)(d_{G_2}(v_j) + 1) \\
&= \frac{1}{2} \sum_{u_i \in E_1} \sum_{v_j \in V_2, d(v_j) \neq 1} d(v_j)(d(v_j)^2 - 1)(d(v_j) + 1) \\
&= \frac{1}{2} \sum_{u_i \in E_1} \sum_{v_j \in V_2} (d(v_j)^4 + d(v_j)^3 - d(v_j)^2 - d(v_j)) \\
&= \frac{1}{2} |E_1| (M_4(G_2) + M_3(G_2) - M_1(G_2) - 2|E_2|)
\end{aligned}$$

The third part is,

$$\begin{aligned}
C_2 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{(G_1 \boxtimes_S G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_S G_2)}(u_p, v_{jk})) \\
&= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{G_1}(u_i) + 1)(d_{G_2}(v_j) + 1) \\
&= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(S(G_1))} (d_{G_1}(u_i) d_{G_2}(v_j) + d_{G_1}(u_i) + d_{G_2}(v_j) + 1) \\
&= M_1(G_1) M_1(G_2) + 2|E_2| M_1(G_1) + 2|E_1| M_1(G_2) + 4|E_1| |E_2|
\end{aligned}$$

Thus we obtain,  $M_2(G_1 \boxtimes_S G_2) = A_2 + B_2 + C_2$ ,

$$\begin{aligned}
M_2(G_1 \boxtimes_S G_2) &= \frac{1}{2} |E_1| (M_4(G_2) + M_3(G_2)) + M_1(G_1) M_1(G_2) \\
&\quad + 3|E_2| M_1(G_1) + \frac{3}{2} |E_1| M_1(G_2) + 7|E_1| |E_2| + |E_2| |V_1|
\end{aligned}$$

□

**Theorem 3.2.** Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two simple connected graphs. Then

- a.  $M_1(G_1 \boxtimes_R G_2) = |E_1| M_3(G_2) + 8|E_2| M_1(G_1) + 2|E_1| M_1(G_2) + 18|E_1| |E_2| + 2|E_2| |V_1|$
- b.  $M_2(G_1 \boxtimes_R G_2) = \frac{1}{2} |E_1| (M_4(G_2) + M_3(G_2)) + 2M_1(G_1) M_1(G_2) + 12|E_2| M_1(G_1) + \frac{3}{2} |E_1| M_1(G_2) + 8|E_2| M_2(G_1) + 13|E_1| |E_2| + |E_2| |V_1|$



*Proof.* We have

$$\begin{aligned}
 M_1(G_1 \boxtimes_R G_2) &= \sum_{(u,v) \in V(G_1 \boxtimes_R G_2)} d_{(G_1 \boxtimes_R G_2)}^2(u, v) \\
 &= \sum_{(u_i, v_{jk})(u_p, v_{qr}) \in E(G_1 \boxtimes_R G_2)} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_R G_2)}(u_p, v_{qr})) \\
 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_j) + d_{(G_1 \boxtimes_R G_2)}(u_i, v_q)) \\
 &+ \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_R G_2)}(u_i, v_{qr})) \\
 &+ \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(R(G_1))} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_R G_2)}(u_p, v_{jk})) \\
 &= A_1 + B_1 + C_1
 \end{aligned}$$

Now we separately find the values of each parts of the sum

$$\begin{aligned}
 A_1 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_j) + d_{(G_1 \boxtimes_R G_2)}(u_i, v_q)) \\
 &= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} [2d_{G_1}(u_i) + 1 + 2d_{G_1}(u_i) + 1] \\
 &= 2|E_2|(4|E_1| + |V_1|)
 \end{aligned}$$

The second part of the sum is same as the second part of  $M_1(G_1 \boxtimes_S G_2)$ .

That is  $B_1 = |E_1|(M_3(G_2) - 2|E_2|)$ .

The third part is,

$$\begin{aligned}
 C_1 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(R(G_1))} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_R G_2)}(u_p, v_{jk})) \\
 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(R(G_1)), u_p \in E_1} (2d_{G_1}(u_i) + 1 + d_{G_2}(v_j) + 1) \\
 &+ \sum_{v_{jk} \in V_2} \sum_{\substack{u_i u_p \in E(R(G_1)) \\ u_i, u_p \in V_1}} (2d_{G_1}(u_i) + 1 + 2d_{G_1}(u_p) + 1) \\
 &= \sum_{v_{jk} \in V_2} (2M_1(G_1) + 4|E_1| + 2|E_1|d_{G_2}(v_j)) + \sum_{v_{jk} \in V_2} 2M_1(G_1) + 2|E_1| \\
 &= 8|E_2|M_1(G_1) + 2|E_1|M_1(G_2) + 12|E_1||E_2|
 \end{aligned}$$

Thus,

$$M_1(G_1 \boxtimes_R G_2) = |E_1|M_3(G_2) + 8|E_2|M_1(G_1) + 2|E_1|M_1(G_2) \\ + 18|E_1||E_2| + 2|E_2||V_1|$$

Similarly,

$$M_2(G_1 \boxtimes_R G_2) = \sum_{(u_i, v_{jk})(u_p, v_{qr}) \in E(G_1 \boxtimes_R G_2)} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk})d_{(G_1 \boxtimes_R G_2)}(u_p, v_{qr})) \\ = \sum_{u_i \in V_1} \sum_{\substack{v_j v_q \in E_2 \\ k=r}} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_j)d_{(G_1 \boxtimes_R G_2)}(u_i, v_q)) \\ + \sum_{u_i \in E_1} \sum_{\substack{f_k f_r \in E(L(G_2)) \\ j=q}} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk})d_{(G_1 \boxtimes_R G_2)}(u_i, v_{qr})) \\ + \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(R(G_1))} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk})d_{(G_1 \boxtimes_R G_2)}(u_p, v_{jk})) \\ = A_2 + B_2 + C_2$$

First part of the sum is

$$A_2 = \sum_{u_i \in V_1} \sum_{\substack{v_j v_q \in E_2 \\ k=r}} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_j)d_{(G_1 \boxtimes_R G_2)}(u_i, v_q)) \\ = \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (2d_{G_1}(u_i) + 1)(2d_{G_1}(u_i) + 1) \\ = \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} (4d_{G_1}(u_i)^2 + 4(d_{G_1}(u_i)) + 1) \\ = |E_2|(4M_1(G_1) + 8|E_1| + |V_1|)$$

The second part of the sum in both cases are same. i.e,

$$B_2 = \frac{1}{2}|E_1|(M_4(G_2) + M_3(G_2) - M_1(G_2) - 2|E_2|)$$

The third part is,

$$\begin{aligned}
C_2 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(R(G_1))} (d_{(G_1 \boxtimes_R G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_R G_2)}(u_p, v_{jk})) \\
&= \sum_{v_{jk} \in V_2} \sum_{\substack{u_i u_p \in E(R(G_1)) \\ u_p \in E_1}} (2d_{G_1}(u_i) + 1)(d_{G_2}(v_j) + 1) \\
&\quad + \sum_{v_{jk} \in V_2} \sum_{\substack{u_i u_p \in E(R(G_1)) \\ u_i, u_p \in V_1}} (2d_{G_1}(u_i) + 1)(2d_{G_2}(u_p) + 1) \\
&= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(R(G_1))} (2d_{G_1}(u_i) d_{G_2}(v_j) + 2d_{G_1}(u_i) + d_{G_2}(v_j) + 1) \\
&\quad + \sum_{v_{jk} \in V_2} \sum_{\substack{u_i u_p \in E(R(G_1)) \\ u_i, u_p \in V_1}} (4d_{G_1}(u_i) d_{G_2}(u_p) + 2(d_{G_1}(u_i) + d_{G_2}(u_p)) + 1) \\
&= 2M_1(G_1)M_1(G_2) + 4|E_2|M_1(G_1) + 2|E_1|M_1(G_2) \\
&\quad + 4|E_1||E_2| + 8|E_2|M_2(G_1) + 4|E_2|M_1(G_1) + 2|E_1||E_2|
\end{aligned}$$

Thus we obtain,  $M_2(G_1 \boxtimes_R G_2) = A_2 + B_2 + C_2$ ,

$$\begin{aligned}
M_2(G_1 \boxtimes_R G_2) &= \frac{1}{2}|E_1|(M_4(G_2) + M_3(G_2)) + 2M_1(G_1)M_1(G_2) \\
&\quad + 12|E_2|M_1(G_1) + \frac{3}{2}|E_1|M_1(G_2) \\
&\quad + 8|E_2|M_2(G_1) + 13|E_1||E_2| + |E_2||V_1|
\end{aligned}$$

□

**Theorem 3.3.** Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two simple connected graphs, then

- $M_1(G_1 \boxtimes_Q G_2) = 2|E_2|M_3(G_1) + |E_1|M_3(G_2) + 2M_1(G_1)M_1(G_2) + 4|E_2|M_2(G_1) - 2|E_2|M_1(G_1) - 2|E_1|M_1(G_2) + 10|E_1||E_2| + 2|E_2||V_1|$
- $M_2(G_1 \boxtimes_Q G_2) = |E_2|M_4(G_1) + \frac{1}{2}|E_1|(M_4(G_2) + \frac{3}{2}M_3(G_1)M_1(G_2) + \frac{3}{2}M_3(G_2)M_1(G_1) - 4|E_2|M_3(G_1) - \frac{5}{2}|E_1|M_3(G_2)) + 3M_1(G_2)M_2(G_1) - 5M_1(G_1)M_1(G_2) + 8|E_2|M_1(G_1) - 10|E_2|M_2(G_1) + \frac{7}{2}|E_1|M_1(G_2) - |E_1||E_2| + |E_2||V_1| + 2|E_2| \left( \sum_{x,y \in V_1} r_{xy} d_{G_1}(x) d_{G_1}(y) + \sum_{y \in V_1} d_{G_1}(y)^2 \sum_{x \in V_1, xy \in E_1} d_{G_1}(x) \right)$

where  $r_{xy}$  denote the number of common neighbours to the vertices  $x$  and  $y$  in  $G_1$

*Proof.* Using the definition,

$$\begin{aligned}
M_1(G_1 \boxtimes_Q G_2) &= \sum_{(u,v) \in V(G_1 \boxtimes_Q G_2)} d_{(G_1 \boxtimes_Q G_2)}^2(u, v) \\
&= \sum_{(u_i, v_{jk})(u_p, v_{qr}) \in E(G_1 \boxtimes_Q G_2)} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_Q G_2)}(u_p, v_{qr}) \right) \\
&= \sum_{u_i \in V_1} \sum_{v_j v_q \in E_2, k=r} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_j) + d_{(G_1 \boxtimes_Q G_2)}(u_i, v_q) \right) \\
&\quad + \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{qr}) \right) \\
&\quad + \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(Q(G_1))} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_Q G_2)}(u_p, v_{jk}) \right) \\
&= A_1 + B_1 + C_1
\end{aligned}$$

Now we separately find the values of the each parts of the sum. The first part of the sum is same as in Theorem 3.1, so  $A_1 = 2|E_2|(2|E_1| + |V_1|)$ . The second part is,

$$\begin{aligned}
B_1 &= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{qr}) \right) \\
&= 2 \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} [d_{Q(G_1)}(u_i) + d_{G_2}(v_j) - 1] \\
&= \sum_{u_i \in E_1} \sum_{v_j \in E_2, d(v_j) \neq 1} d(v_j)(d(v_j) - 1)(d_{Q(G_1)}(u_i)) \\
&\quad + \sum_{u_i \in E_1} \sum_{v_j \in E_2, d(v_j) \neq 1} d(v_j)(d(v_j) - 1)^2 \\
&= \sum_{u_i \in E_1} (M_1(G_2) - 2|E_2|)(d_{Q(G_1)}(u_i)) + \sum_{u_i \in E_1} (M_3(G_2) - 2M_1(G_2) + 2|E_2|)
\end{aligned}$$

Also,  $d_{Q(G_1)}(u_i) = d_{G_1}(x) + d_{G_1}(y)$  where  $u_i$  is the vertex inserted corresponding to the edge  $xy \in E_1$ . So the sum becomes

$$B_1 = M_1(G_1)(M_1(G_2) - 2|E_2|) + |E_1|(M_3(G_2) - 2M_1(G_2) + 2|E_2|)$$

The third part of the sum is,

$$\begin{aligned}
C_1 &= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(Q(G_1))} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) + d_{(G_1 \boxtimes_Q G_2)}(u_p, v_{jk}) \right) \\
&= \sum_{v_{jk} \in V_2} \sum_{u_i u_p \in E(Q(G_1)), u_p \in E_1} (d_{G_1}(u_i) + 1 + d_{Q(G_1)}(u_p) + d_{G_2}(v_j) - 1) \\
&\quad + \sum_{v_{jk} \in V_2} \sum_{\substack{u_i u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} (d_{Q(G_1)}(u_i) + d_{G_2}(v_j) - 1 + d_{Q(G_1)}(u_p) + d_{G_2}(v_j) - 1) \\
&= C_{11} + C_{12}
\end{aligned}$$

Also if  $u_i$  is the vertex corresponding to edge  $xy$  and  $u_p$  is the vertex corresponding to the edge  $yz$ , then

$$\sum_{u_i u_p \in E(Q(G_1)), u_i \in V_1, u_p \in E_1} d_{Q(G_1)}(u_p) = 2 \sum_{yz \in E_1} (d(y) + d(z)) = 2M_1(G_1)$$

By using Lemma 2.2,

$$\begin{aligned}
C_{11} &= \sum_{v_{jk} \in V_2} (M_1(G_1) + 2M_1(G_1) + 2|E_1|d_{G_2}(v_j)) \\
&= 6|E_2|M_1(G_1) + 2|E_1|M_1(G_2) \\
C_{12} &= \sum_{v_{jk} \in V_2} \sum_{\substack{u_i u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} (d_{Q(G_1)}(u_i) + d_{G_2}(v_j) - 1 + d_{Q(G_1)}(u_p) + d_{G_2}(v_j) - 1) \\
&= 2|E_2|(M_3(G_1) + 2M_2(G_1) - 2M_1(G_1)) \\
&\quad + \sum_{v_{jk} \in V_2} (M_1(G_1) - 2|E_1|)(d_{G_2}(v_j) - 1) \\
&= 2|E_2|(M_3(G_1) + 2M_2(G_1) - 2M_1(G_1)) + M_1(G_1)M_1(G_2) \\
&\quad - 2|E_1|M_1(G_2) - 2|E_2|M_1(G_2) + 4|E_1||E_2|
\end{aligned}$$

Thus we obtain,

$$\begin{aligned}
M_1(G_1 \boxtimes_Q G_2) &= 2|E_2|M_3(G_1) + |E_1|M_3(G_2) + 2M_1(G_1)M_1(G_2) \\
&\quad + 4|E_2|M_2(G_1) - 2|E_2|M_1(G_1) - 2|E_1|M_1(G_2) \\
&\quad + 10|E_1||E_2| + 2|E_2||V_1|
\end{aligned}$$

Next Consider

$$\begin{aligned}
M_2(G_1 \boxtimes_Q G_2) &= \sum_{(u_i, v_{jk})(u_p, v_{qr}) \in E(G_1 \boxtimes_Q G_2)} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_Q G_2)}(u_p, v_{qr}) \right) \\
&= \sum_{u_i \in V_1} \sum_{v_j, v_q \in E_2, k=r} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_j) d_{(G_1 \boxtimes_Q G_2)}(u_i, v_q) \right) \\
&+ \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{qr}) \right) \\
&+ \sum_{v_{jk} \in V_2} \sum_{u_i, u_p \in E(Q(G_1))} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_Q G_2)}(u_p, v_{jk}) \right) \\
&= A_2 + B_2 + C_2
\end{aligned}$$

First part of the sum is the same as in the proof of Theorem 3.1,  $A_2 = |E_2|(M_1(G_1) + 4|E_1| + |V_1|)$ .

The second part is,

$$\begin{aligned}
B_2 &= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{qr}) \right) \\
&= \sum_{u_i \in E_1} \sum_{f_k f_r \in E(L(G_2)), j=q} \left( d_{Q(G_1)}(u_i) + d_{G_2}(v_j) - 1 \right)^2 \\
&= \frac{1}{2} \sum_{u_i \in E_1} \sum_{\substack{v_j \in V_2 \\ d(v_j) \neq 1}} d(v_j)(d(v_j) - 1) \left( d_{Q(G_1)}(u_i)^2 + 2d_{Q(G_1)}(u_i)(d(v_j) - 1) + (d(v_j) - 1)^2 \right) \\
&= \frac{1}{2} \sum_{u_i \in E_1} \left( M_1(G_2) - 2|E_2| \right) d_{Q(G_1)}(u_i)^2 + \sum_{u_i \in E_1} \left( M_3(G_2) - 2M_1(G_2) + 2|E_2| \right) d_{Q(G_1)}(u_i) \\
&+ \frac{1}{2} \sum_{u_i \in E_1} \sum_{v_j \in V_2, d(v_j) \neq 1} \left( d(v_j)^4 - 3d(v_j)^3 + 3d(v_j)^2 - d(v_j) \right) \\
&= \frac{1}{2} \left( M_1(G_2) - 2|E_2| \right) \left( M_3(G_1) + 2M_2(G_1) \right) + \left( M_3(G_2) - 2M_1(G_2) + 2|E_2| \right) M_1(G_1) \\
&+ \frac{|E_1|}{2} \left( M_4(G_2) - 3M_3(G_2) + 3M_1(G_2) - 2|E_2| \right)
\end{aligned}$$

The third part is,

$$\begin{aligned}
C_2 &= \sum_{v_{jk} \in V_2} \sum_{\substack{u_i, u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} \left( d_{(G_1 \boxtimes_Q G_2)}(u_i, v_{jk}) d_{(G_1 \boxtimes_Q G_2)}(u_p, v_{jk}) \right) \\
&= \sum_{v_{jk} \in V_2} \sum_{\substack{u_i, u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} (d_{Q(G_1)}(u_i) + d_{G_2}(v_j) - 1)(d_{Q(G_1)}(u_p) + d_{G_2}(v_j) - 1) \\
&= \sum_{v_{jk} \in V_2} \sum_{\substack{u_i, u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} d_{Q(G_1)}(u_i) d_{Q(G_1)}(u_p) \\
&\quad + \sum_{v_{jk} \in V_2} \sum_{\substack{u_i, u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} (d_{Q(G_1)}(u_i) + d_{Q(G_1)}(u_p))(d_{G_2}(v_j) - 1) \\
&\quad + \sum_{v_{jk} \in V_2} \sum_{\substack{u_i, u_p \in E(Q(G_1)) \\ u_i, u_p \in E_1}} (d_{G_2}(v_j) - 1)^2 \\
&= 2|E_2| \left( \frac{1}{2} M_4(G_1) - \frac{1}{2} M_3(G_1) + \sum_{x, y \in V_1} r_{xy} d_{G_1}(x) d_{G_1}(y) \right) \\
&\quad + 2|E_2| \left( \sum_{y \in V_1} d_{G_1}(y)^2 \sum_{x \in V_1, xy \in E_1} d_{G_1}(x) - 2M_2(G_1) \right) \\
&\quad + M_1(G_2) (M_3(G_1) + 2M_2(G_1) - 2M_1(G_1)) - 2|E_2| (M_3(G_1) + 2M_2(G_1) - 2M_1(G_1)) \\
&\quad + \frac{1}{2} (M_1(G_1) - 2|E_1|) (M_3(G_2) - 2M_1(G_2) + 2|E_2|)
\end{aligned}$$

Thus we obtain,

$$\begin{aligned}
M_2(G_1 \boxtimes_Q G_2) &= |E_2| M_4(G_1) + \frac{1}{2} |E_1| (M_4(G_2) + \frac{3}{2} M_3(G_1) M_1(G_2)) \\
&\quad + \frac{3}{2} M_3(G_2) M_1(G_1) - 4|E_2| M_3(G_1) - \frac{5}{2} |E_1| M_3(G_2) \\
&\quad + 3M_1(G_2) M_2(G_1) - 5M_1(G_1) M_1(G_2) + 8|E_2| M_1(G_1) \\
&\quad - 10|E_2| M_2(G_1) + \frac{7}{2} |E_1| M_1(G_2) - |E_1| |E_2| + |E_2| |V_1| \\
&\quad + 2|E_2| \left( \sum_{x, y \in V_1} r_{xy} d_{G_1}(x) d_{G_1}(y) + \sum_{y \in V_1} d_{G_1}(y)^2 \sum_{x \in V_1, xy \in E_1} d_{G_1}(x) \right)
\end{aligned}$$

where  $r_{xy}$  denote the number of common neighbours to the vertices  $x$  and  $y$  in  $G_1$   $\square$

Using Theorem 3.2, 3.3 along with the fact  $d_{(G_1 \boxtimes_T G_2)}(x, y) = d_{(G_1 \boxtimes_Q G_2)}(x, y)$  for  $x \in V_1$  and  $y \in E_1$  or  $x, y \in E_1$  and  $d_{(G_1 \boxtimes_T G_2)}(x, y) = d_{(G_1 \boxtimes_R G_2)}(x, y)$  whenever  $x, y \in V_1$ . We can state the following theorem.

**Theorem 3.4.** *Let  $G_1$  and  $G_2$  be two simple connected graphs, then*

- a.  $M_1(G_1 \boxtimes_T G_2) = 2|E_2|M_3(G_1) + |E_1|M_3(G_2) + 2M_1(G_1)M_1(G_2) + 4|E_2|M_2(G_1) + 2|E_2|M_1(G_1) - 2|E_1|M_1(G_2) + 14|E_1||E_2| + 2|E_2||V_1|$
- b.  $M_2(G_1 \boxtimes_T G_2) = |E_2|M_4(G_1) + \frac{1}{2}|E_1|(M_4(G_2) + \frac{3}{2}M_3(G_1)M_1(G_2) + \frac{3}{2}M_3(G_2)M_1(G_1) - 4|E_2|M_3(G_1) - \frac{5}{2}|E_1|M_3(G_2)) + 3M_1(G_2)M_2(G_1) - 5M_1(G_1)M_1(G_2) + 12|E_2|M_1(G_1) - 2|E_2|M_2(G_1) + \frac{7}{2}|E_1|M_1(G_2) + |E_1||E_2| + |E_2||V_1| + 2|E_2| \left( \sum_{x,y \in V_1} r_{xy} d_{G_1}(x) d_{G_1}(y) + \sum_{y \in V_1} d_{G_1}(y)^2 \sum_{x \in V_1, xy \in E_1} d_{G_1}(x) \right)$   
*where  $r_{xy}$  denote the number of common neighbours to the vertices  $x$  and  $y$  in  $G_1$*

**Corollary 3.5.** *Let  $n > 3$  be any positive integer, the Zagreb indices of linear hexagonal chain  $L_n$*

- a.  $M_1(L_n) = 26n - 2$
- b.  $M_2(L_n) = 33n - 9$

*Proof.* Use the fact that  $L_n = P_{n+1} \boxtimes_S P_2$  and by Theorem 3.1.  $\square$

Let  $P_n^m$  denote the hexagonal lattice, then using the results we can obtain

**Corollary 3.6.** *Let  $n > 3, m > 2$  be positive integers, the Zagreb indices of linear hexagonal lattice  $P_{n+1}^{2m-1}$*

- a.  $M_1(P_{n+1}^{2m-1}) = 36mn - 10n - 38m + 10$
- b.  $M_2(P_{n+1}^{2m-1}) = 54mn - 21n - 67m + 25$

*Proof.* Use the fact that  $P_{n+1}^{2m-1} = P_n \boxtimes_S P_m$  and by Theorem 3.1.  $\square$

Using these results we can compute the Zagreb indices of certain fullerene nanotubes  $NA_m^{2n}, NC_{2m}^{2n}(\mathbb{H}_{2m}^{2n})$  [9, 10].



**Corollary 3.7.** *Let  $n, m > 3$  be positive integers, the Zagreb indices of the fullerene nanotubes  $NA_m^{2n}$  are*

- a.  $M_1(NA_m^{2n}) = 36mn - 46m$
- b.  $M_2(NA_m^{2n}) = 54mn - 75m$

*Proof.* Use  $NA_m^{2n} = C_m \boxtimes_S P_n$  and use Theorem 3.1. □

*Example 3.8.* When  $G_1 = C_m$ ,  $G_2 = C_n$ ,  $n, m > 3$ , using the Theorem 3.1

- a.  $M_1(C_m \boxtimes_S C_n) = 36mn$
- b.  $M_2(C_m \boxtimes_S C_n) = 54mn$
- c.  $M_1(C_m \boxtimes_R C_n) = 68mn$
- d.  $M_2(C_m \boxtimes_R C_n) = 144mn$
- e.  $M_1(C_m \boxtimes_Q C_n) = 68mn$
- f.  $M_2(C_m \boxtimes_Q C_n) = 144mn$
- g.  $M_1(C_m \boxtimes_T C_n) = 100mn$
- h.  $M_2(C_m \boxtimes_T C_n) = 250mn$

Also  $NC_{2m}^{2n} = C_m \boxtimes_S C_n$  which is computed in Example 3.8.

#### 4. SUMMARY AND CONCLUSION

We have defined the Adjacency product or A - product in terms of the Cartesian product of graphs and computed some degree-based topological indices of A- products. These products generalize the structure of various chemical compounds such as graphene, linear polyacene, toroidal fullerene, and some fullerene nanotubes  $NC_{2m}^{2n}$  ( $H_{2m}^{2n}$ ),  $NA_m^{2n}$ . These sums can be defined in terms of other graph products and computation of various other topological indices on A - products are also a problem for further research.

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