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# **Topological Indices of Some New Graph Operations and Their Possible Applications**

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*This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.*

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# **Abstract**

A chemical graph theory is a fascinating branch of graph theory which has many applications related to chemistry. A topological index is a real number related to a graph, as its considered a structural invariant. It's found that there is a strong correlation between the properties of chemical compounds and their topological indices. In this paper, we introduce some new graph operations for the first Zagreb index, second Zagreb index and forgotten index "F-index". Furthermore, it was found some possible applications on some new graph operations such as roperties of molecular graphs that resulted by alkanes or cyclic alkanes.

*Keywords: New Graph operations; first Zagreb index; second Zagreb index; forgotten index.*

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#### **1 Introduction**

Chemical graphs are models of molecules, in which atoms are represented by vertices and chemical bonds by edges of a graph. The basic idea of chemical graph theory is the physicochemical properties of molecules can be studied by using the information in the mathematico-chemical literature [1],[2],[3],[4]. Throughout this paper, we consider a simple finite connected graph *G*. We respectively denote by *p* and *q* the cardinality of its vertices set  $V(G)$  and  $E(G)$ . The degree of the vertex *a* is the number of edges joined with this vertex denoted by  $\delta(a)$ . Graph operations produce new graphs from the initial ones. Some new graphs were found by new binary operations, which were introduced in [5]. In practical applications, Zagreb indices are among the best applications to recogni[ze](#page-13-0) t[h](#page-13-1)e [p](#page-13-2)h[ys](#page-13-3)ical properties and chemical reactions. First Zagreb index *M*1(*G*) and second Zagreb index  $M_2(G)$  were firstly considered by Gutman and Trinajstic in 1972 [6],[7] which are defined as:

$$
M_1(G) = \sum_{v \in V(G)} \delta_G^2(v) = \sum_{uv \in E(G)} [\delta_G(u) + \delta_G(v)], \qquad M_2(G) = \sum_{uv \in E(G)} \delta_G(u) \delta_G(v).
$$

Furtula and Gutman in 2015 was introduced forgotten index (F-index) [8],[9],[10],[11] which defined as:

$$
F(G) = \sum_{u \in V(G)} \delta_G^3(u) = \sum_{uv \in E(G)} (\delta_G^2(u) + \delta_G^2(v)).
$$

Furtula and Gutman raised that the predictive ability of forgotten inde[x](#page-13-5) is [a](#page-13-6)l[mos](#page-13-7)t [sim](#page-13-8)ilar to that of the first Zagreb index and for the acentric factor and entropy, and both of them obtain correlation coefficients larger than 0.95. This fact implies the reason why forgotten index is useful for testing the chemical and pharmacological properties of drug molecular structures and reported that this index can reinforce the physico-chemical flexibility of Zagreb indices [4]. Alameri in 2016 was introduced a new product operations on graphs which are classical of other binary operations, denoted *⊗i*, and *i ∈ {*1*,* 2*, ...,* 7*}* [5].

In this paper, we introduce some Zagreb Indices of new graph operations, we present some possible applications as special cases of chemical graph. Moreo[ve](#page-13-3)r, we have studied the correlation coefficient betw[ee](#page-13-4)n them to investigate the effectiveness of these indices in practical applications. We refer the interested reader to [12],[13],[2],[14],[15] for some recent results.

### **2 Preliminary Results**

In this section, we introduce defin[itio](#page-13-9)[ns a](#page-13-10)[nd](#page-13-1) s[om](#page-13-11)e [pr](#page-13-12)operties of graphs (resulted by the new binary operations introduced in [5]).

**Definitions 2.1:** Unary operations create a new graph from the old one, such as addition or deletion of a vertex or an edge or Complement graph.

**Definitions 2.2:** A bina[ry](#page-13-4) operation creates a new graph from two initial graphs, such as classic operations (tensor product, cartesian product, strong product, composition, disjunction and symmetric deference).

**Corollary 2.3:** Any classic operation can be deduced from our new product operations.

**Definitions 2.4:** The new binary operations on graphs [5] denoted  $\otimes_i$  where  $i \in \{1, 2, ..., 7\}$ , defined as follows:

If *G*<sup>1</sup> and *G*<sup>2</sup> are two graphs. Then, the vertex sets are defined as follows:

 $V(G_1 \otimes_i G_2) = V(G_2 \otimes_i G_1) = V(G_1) \times V(G_2)$ ,

Whereas, the edge sets are defined as follows:

 $E(G_1 \otimes_0 G_2) = \{(a, b)(c, d) : | ac \in E(G_1), bd \in E(G_2)|\},\$ 

 $E(G_1 \otimes_1 G_2) = \{(a, b)(c, d) : |ac \in E(G_1), b = d|\},\$ 

- (3)  $E(G_1 \otimes_2 G_2) = \{(a, b)(c, d) : [ac \in E(G_1), bd \in E(G_2^c)]\},\$
- $E(G_1 \otimes_3 G_2) = \{(a, b)(c, d) : |a = c, bd \in E(G_2)|\},\$
- (5)  $E(G_1 \otimes_4 G_2) = \{(a, b)(c, d) : [a = c, bd \in E(G_2^c)]\},\$
- $E(G_1 \otimes_S G_2) = \{(a, b)(c, d) : [ac \in E(G_1^c), bd \in E(G_2)]\},\$
- $E(G_1 \otimes_6 G_2) = \{(a, b)(c, d) : [ac \in E(G_1^c), b = d]\},\$
- $E(G_1 \otimes_7 G_2) = \{(a, b)(c, d) : [ac \in E(G_1^c), bd \in E(G_2^c)]\}.$

**Lemma 2.5:** Let two graphs  $G_1$  and  $G_2$  where;  $|V(G_1)| = p_1$ ,  $|V(G_2)| = p_2$ ,  $|E(G_1)| = q_1$  and  $|E(G_2)| = q_2$ . Then,

- $|E(G_1 \otimes_0 G_2)| = 2q_1q_2,$
- $|E(G_1 \otimes_1 G_2)| = q_1 p_2,$
- $|E(G_1 \otimes_2 G_2)| = 2q_1q_2^c = p_2^2q_1 p_2q_1 2q_1q_2,$
- $|E(G_1 \otimes_3 G_2)| = q_2 p_1$ ,
- $|E(G_1 \otimes_4 G_2)| = q_2^c p_1 = \frac{1}{2}(p_1 p_2^2 p_1 p_2 2p_1 q_2),$
- $|E(G_1 \otimes_5 G_2)| = 2q_1^c q_2 = p_1^2 q_2 p_1 q_2 2q_1 q_2,$
- $|E(G_1 \otimes_6 G_2)| = q_1^c p_2 = \frac{1}{2}(p_2 p_1^2 p_1 p_2 2p_2 q_1),$
- $|E(G_1 \otimes_7 G_2)| = 2q_1^c q_2^c = \frac{1}{2} [p_1(p_1 1) 2q_1][p_2(p_2 1) 2q_2].$

**Lemma 2.6:** If  $G_1$  and  $G_2$  are two graphs where;  $|V(G_1)| = p_1$ ,  $|V(G_2)| = p_2$ ,  $|E(G_1)| = q_1$  and  $|E(G_2)| = q_2$ , then

- $(1)$   $\delta_{G_1 \otimes_0 G_2}(u, v) = \delta_{G_1}(u) \delta_{G_2}(v),$
- $(2)$   $\delta_{G_1 \otimes_1 G_2}(u, v) = \delta_{G_1}(u),$
- (3)  $\delta_{G_1 \otimes_2 G_2}(u, v) = \delta_{G_1}(u) \, \delta_{G_2^c}(v),$
- $(4)$   $\delta_{G_1 \otimes_3 G_2}(u, v) = \delta_{G_2}(v),$
- $(5)$   $\delta_{G_1 \otimes_4 G_2}(u, v) = \delta_{G_2^c}(v),$
- $(6)$   $\delta_{G_1 \otimes_5 G_2}(u, v) = \delta_{G_1^c}(u) \, \delta_{G_2}(v),$
- $(7)$   $\delta_{G_1 \otimes_6 G_2}(u, v) = \delta_{G_1^c}(u),$
- (8)  $\delta_{G_1 \otimes_7 G_2}(u, v) = \delta_{G_1^c}(u) \, \delta_{G_2^c}(v)$ .

In the following sections we will create new relationships for some of topological indices for the operations introduced in [5].

# **3 First Zagreb Index of New Graph Operations**

In this section, we studied the first Zagreb Index of new graphs and some of its special cases.

**Theorem 3.1:** Let  $G_1^c$ ,  $G_2^c$  be complement graphs of  $G_1$  and  $G_2$  respectively, then

- $M_1(G_1 \otimes_0 G_2) = M_1(G_1)M_1(G_2),$
- $M_1(G_1 \otimes_1 G_2) = p_2 M_1(G_1),$
- (3)  $M_1(G_1 \otimes_2 G_2) = M_1(G_1)M_1(G_2^c),$
- $M_1(G_1 \otimes_3 G_2) = p_1 M_1(G_2),$
- (5)  $M_1(G_1 \otimes_4 G_2) = p_1 M_1(G_2^c),$
- (6)  $M_1(G_1 \otimes_5 G_2) = M_1(G_1^c)M_1(G_2),$
- $(M_1(G_1 \otimes_6 G_2) = p_2 M_1(G_1^c),$
- (8)  $M_1(G_1 \otimes_7 G_2) = M_1(G_1^c)M_1(G_2^c)$ *.*

**Proof:** By Lemma 2.5, Lemma 2.6 and through the definition of first Zagreb index, we get

$$
(1) \quad M_{1}(G_{1} \otimes_{0} G_{2}) = \sum_{(u,v) \in V(G_{1} \otimes_{0} G_{2})} \delta_{G_{1} \otimes_{0} G_{2}}^{2}(u,v)
$$
\n
$$
= \sum_{u \in V(G_{1})} \sum_{v \in V(G_{2})} \delta_{G_{1}}^{2}(u) \delta_{G_{2}}^{2}(v)
$$
\n
$$
= M_{1}(G_{1})M_{1}(G_{2}),
$$
\n
$$
(2) \quad M_{1}(G_{1} \otimes_{1} G_{2}) = \sum_{(u,v) \in V(G_{1} \otimes_{1} G_{2})} \delta_{G_{1} \otimes_{1} G_{2}}^{2}(u,v)
$$
\n
$$
= \sum_{u \in V(G_{1})} \delta_{G_{1}}^{2}(u) \sum_{v \in V(G_{2})} (1)
$$
\n
$$
= p_{2}M_{1}(G_{1}),
$$
\n
$$
(3) \quad M_{1}(G_{1} \otimes_{2} G_{2}) = \sum_{(u,v) \in V(G_{1} \otimes_{2} G_{2})} \delta_{G_{1} \otimes_{2} G_{2}}^{2}(u,v)
$$
\n
$$
= \sum_{u \in V(G_{1})} \sum_{v \in V(G_{2})} \delta_{G_{1}}^{2}(u) \delta_{G_{2}}^{2}(v)
$$
\n
$$
= M_{1}(G_{1})M_{1}(G_{2}^{c}),
$$
\n
$$
(4) \quad M_{1}(G_{1} \otimes_{3} G_{2}) = \sum_{(u,v) \in V(G_{1} \otimes_{3} G_{2})} \delta_{G_{1} \otimes_{3} G_{2}}^{2}(u,v)
$$
\n
$$
= \sum_{u \in V(G_{1})} \delta_{G_{1} \otimes_{3} G_{2}}^{2}(u,v)
$$
\n
$$
= \sum_{u \in V(G_{1})} (1) \sum_{v \in V(G_{2})} \delta_{G_{2}}^{2}(v)
$$

 $= p_1 M_1(G_2),$ 

(5) *M*1(*G*<sup>1</sup> *⊗*<sup>4</sup> *G*2) = ∑ (*u,v*)*∈V* (*G*1*⊗*4*G*2) *δ* 2 *G*1*⊗*4*G*<sup>2</sup> (*u, v*) = ∑ *u∈V* (*G*1) (1) ∑ *v∈V* (*G*2) *δ* 2 *G<sup>c</sup>* 2 (*v*) = *p*1*M*1(*G c* <sup>2</sup>)*,* (6) *M*1(*G*<sup>1</sup> *⊗*<sup>5</sup> *G*2) = ∑ (*u,v*)*∈V* (*G*1*⊗*5*G*2) *δ* 2 *G*1*⊗*5*G*<sup>2</sup> (*u, v*) = ∑ *u∈V* (*G*1) ∑ *v∈V* (*G*2) *δ* 2 *G<sup>c</sup>* 1 (*u*)*δ* 2 *G*2 (*v*) = *M*1(*G c* <sup>1</sup>)*M*1(*G*2)*,* (7) *M*1(*G*<sup>1</sup> *⊗*<sup>6</sup> *G*2) = ∑ (*u,v*)*∈V* (*G*1*⊗*6*G*2) *δ* 2 *G*1*⊗*6*G*<sup>2</sup> (*u, v*) = ∑ *u∈V* (*G*1) ∑ *v∈V* (*G*2) *δ* 2 *G<sup>c</sup>* 1 (*u*) = ∑ *u∈V* (*G*1) *δ* 2 *G<sup>c</sup>* 1 (*u*) ∑ *v∈V* (*G*2) (1) = *p*2*M*1(*G c* <sup>1</sup>)*,* (8) *M*1(*G*<sup>1</sup> *⊗*<sup>7</sup> *G*2) = ∑ (*u,v*)*∈V* (*G*1*⊗*7*G*2) *δ* 2 *G*1*⊗*7*G*<sup>2</sup> (*u, v*) = ∑ *u∈V* (*G*1) ∑ *v∈V* (*G*2) *δ* 2 *G<sup>c</sup>* 1 (*u*)*δ* 2 *G<sup>c</sup>* 2 (*v*) = *M*1(*G c* <sup>1</sup>)*M*1(*G c* <sup>2</sup>)*. ✷*

**Corollary 3.2** Let  $G_1 \simeq P_n$  be a path graph with *n* vertices and  $G_2 \simeq C_m$  be a cycle graph with *m* vertices, where

 $|V(P_n)| = n, |E(P_n)| = n - 1$  and  $|V(C_m)| = |E(C_m)| = m$ , then we have,

$$
M_1(P_n \otimes_0 C_m) = 8m(2n - 3),
$$
  
\n
$$
M_1(P_n \otimes_1 C_m) = 2m(2n - 3),
$$
  
\n
$$
M_1(P_n \otimes_2 C_m) = 2m(2n - 3)(m - 3)^2,
$$
  
\n
$$
M_1(P_n \otimes_3 C_m) = 4nm,
$$
  
\n
$$
M_1(P_n \otimes_4 C_m) = nm(m - 3)^2,
$$
  
\n
$$
M_1(P_n \otimes_5 C_m) = 4m(n - 2)(n^2 - 4n + 5),
$$
  
\n
$$
M_1(P_n \otimes_6 C_m) = m(n - 2)(n^2 - 4n + 5),
$$
  
\n
$$
M_1(P_n \otimes_7 C_m) = m(n - 2)(n^2 - 4n + 5)(m - 3)^2.
$$

**Proof:** By [16],[3];

$$
M_1(G^c) = M_1(G) + p(p-1)^2 - 4q(p-1).
$$

Where  $|V(G)| = p, |E(G)| = q$ 

From [9] we have  $M_1(P_n) = 4n - 6, M_1(C_m) = 4m$ 

Where  $|V(P_n)| = n, |E(P_n)| = n - 1$ 

and  $|V(C_m)| = |E(C_m)| = m$  $|V(C_m)| = |E(C_m)| = m$  $|V(C_m)| = |E(C_m)| = m$ .

Then,

$$
M_1(P_n^c) = (4n - 6) + n(n - 1)^2 - 4(n - 1)^2
$$
  
=  $(4n - 6) + (n - 4)(n - 1)^2$   
=  $(4n - 6) + (n - 4)(n^2 - 2n + 1)$   
=  $n^3 - 6n^2 + 13n - 10$   
=  $(n^3 - 4n^2 + 5n) - 2n^2 + 8n - 10$   
=  $n(n^2 - 4n + 5) - 2(n^2 - 4n + 5).$ 

Similarly;

$$
M_1(C_m^c) = 4m + m(m-1)^2 - 4m(m-1)
$$
  
=  $m(4 + m^2 - 2m + 1 - 4m + 4)$   
=  $m(m^2 - 6m + 9)$   
=  $m(m-3)^2$ .

By using Theorem 3.1, the proof was completed.  $\Box$ 

# **4 Second Zagreb Index of New Graph Operations**

In this section, we studied the second Zagreb Index of new graphs and some of its special cases.

**Theorem 4.1:** Suppose  $G_1^c, G_2^c$  be complements of  $G_1$  and  $G_2$  respectively, then

- $M_2(G_1 \otimes_0 G_2) = 2M_2(G_1)M_2(G_2),$
- $M_2(G_1 \otimes_1 G_2) = p_2 M_2(G_1),$
- (3)  $M_2(G_1 \otimes_2 G_2) = 2M_2(G_1)M_2(G_2^c),$
- (4)  $M_2(G_1 \otimes_3 G_2) = p_1 M_2(G_2),$
- (5)  $M_2(G_1 \otimes_4 G_2) = p_1 M_2(G_2^c),$
- (6)  $M_2(G_1 \otimes_5 G_2) = 2M_2(G_1^c)M_2(G_2),$
- $(M_2(G_1 \otimes_6 G_2) = p_2 M_2(G_1^c),$

(8)  $M_2(G_1 \otimes_7 G_2) = 2M_2(G_1^c)M_2(G_2^c)$ *.* 

**Proof:** By Lemma 2.5, Lemma 2.6 and definition of second Zagreb index, we get

$$
(1) \quad M_2(G_1 \otimes G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes G_2)} \delta_{G_1 \otimes G_2}(a,b) \delta_{G_1 \otimes G_2}(c,d)
$$
\n
$$
= 2 \sum_{a \in E(G_1)} \sum_{bd \in E(G_2)} \delta_{G_1 a} \delta_{G_2 b} \delta_{G_1 a} \delta_{G_2 d}
$$
\n
$$
= 2 \sum_{a \in E(G_1)} \delta_{G_1 a} \delta_{G_1 c} \sum_{bd \in E(G_2)} \delta_{G_2 b} \delta_{G_2 d}
$$
\n
$$
= 2 M_2(G_1) M_2(G_2),
$$
\n
$$
(2) \quad M_2(G_1 \otimes G_1 G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes G_1 G_2)} \delta_{G_1 \otimes G_1 G_2}(a,b) \delta_{G_1 \otimes G_1 G_2}(c,d)
$$
\n
$$
= \sum_{b=d=v \in V(G_2)} \sum_{a \in E(G_1)} \delta_{G_1 a} \delta_{G_1 c}
$$
\n
$$
= p_2 M_2(G_1),
$$
\n
$$
(3) \quad M_2(G_1 \otimes_2 G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes_2 G_2)} \delta_{G_1 a} \delta_{G_2 a} \delta_{G_1 a} \delta_{G_2 a} \delta_{G_2}(c,d)
$$
\n
$$
= 2 \sum_{a \in E(G_1)} \sum_{bd \in E(G_2^c)} \delta_{G_1 a} \delta_{G_2 a} \delta_{G_1 a} \delta_{G_2 a} \delta_{G_2 d}
$$
\n
$$
= 2 \sum_{a \in E(G_1)} \delta_{G_1 a} \delta_{G_1 c} \sum_{bd \in E(G_2^c)} \delta_{G_2^c b} \delta_{G_2^c d}
$$
\n
$$
= 2 M_2(G_1) M_2(G_2^c),
$$
\n
$$
(4) \quad M_2(G_1 \otimes_3 G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes_3 G_2)} \delta_{G_1 a} \delta_{G_2 a} \delta_{G_2 a} \delta_{G_2 a
$$

 $= p_1 M_2(G_2^c)$ 

(6) 
$$
M_2(G_1 \otimes_5 G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes_5 G_2)} \delta_{G_1 \otimes_5 G_2}(a,b) \delta_{G_1 \otimes_5 G_2}(c,d)
$$
  
\t
$$
= 2 \sum_{ac \in E(G_1^c) b d \in E(G_2)} \delta_{G_1^c} a \delta_{G_2} b \delta_{G_1^c} c \delta_{G_2} d
$$
  
\t
$$
= 2 \sum_{ac \in E(G_1^c)} \delta_{G_1^c} a \delta_{G_1^c} c \sum_{bd \in E(G_2)} \delta_{G_2} b \delta_{G_2} d
$$
  
\t
$$
= 2M_2(G_1^c) M_2(G_2),
$$
  
\t(7) 
$$
M_2(G_1 \otimes_6 G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes_6 G_2)} \delta_{G_1 \otimes_6 G_2}(a,b) \delta_{G_1 \otimes_6 G_2}(c,d)
$$
  
\t
$$
= \sum_{b=d=v \in V(G_2)} \sum_{ac \in E(G_1^c)} \delta_{G_1^c} a \delta_{G_1^c} c
$$
  
\t
$$
= \sum_{ac \in V(G_2)} \sum_{ac \in E(G_1^c)} \delta_{G_1^c} a \delta_{G_1^c} c
$$
  
\t
$$
= p_2 M_2(G_1^c),
$$
  
\t(8) 
$$
M_2(G_1 \otimes_7 G_2) = \sum_{(a,b)(c,d) \in E(G_1 \otimes_7 G_2)} \delta_{G_1^c} a \delta_{G_2^c} a \delta_{G_1^c} a \delta_{G_1^c} c \delta_{G_2^c} d
$$
  
\t
$$
= 2 \sum_{ac \in E(G_1^c) b d \in E(G_2^c)} \delta_{G_1^c} a \delta_{G_2^c} \delta_{G_1^c} a \delta_{G_2^c} d
$$
  
\t
$$
= 2 M_2(G_1^c) M_2(G_2^c).
$$

**Corollary 4.2** Let  $G_1 \simeq P_n$  is a path with *n* vertices and  $G_2 \simeq C_m$  is a cycle with *m* vertices, where:

$$
|V(P_n)| = n, |E(P_n)| = n - 1 \text{ and } |V(C_m)| = |E(C_m)| = m, \text{ then we have,}
$$
  
\n
$$
M_2(P_n \otimes_0 C_m) = 32m(n - 2),
$$
  
\n
$$
M_2(P_n \otimes_1 C_m) = 4m(n - 2),
$$
  
\n
$$
M_2(P_n \otimes_2 C_m) = 4m(n - 2)[4(3m - 5) + (m - 7)(m - 1)^2],
$$
  
\n
$$
M_2(P_n \otimes_3 C_m) = 4nm,
$$
  
\n
$$
M_2(P_n \otimes_4 C_m) = \frac{1}{2}nm[4(3m - 5) + (m - 7)(m - 1)^2],
$$
  
\n
$$
M_2(P_n \otimes_5 C_m) = 4m[(n - 5)(n - 2)(n - 1)^2 + 2(2n - 3)^2 - 8(n - 2)],
$$
  
\n
$$
M_2(P_n \otimes_6 C_m) = \frac{1}{2}m[(n - 5)(n - 2)(n - 1)^2 + 2(2n - 3)^2 - 8(n - 2)],
$$
  
\n
$$
M_2(P_n \otimes_7 C_m) = 2[\frac{1}{2}((n - 5)(n - 2)(n - 1)^2 + 2(2n - 3)^2 - 8(n - 2))],
$$
  
\n
$$
[\frac{1}{2}m(4(3m - 5) + (m - 7)(m - 1)^2)].
$$

**Proof:** By [16],[3];

$$
M_2(G^c) = \frac{1}{2}p(p-1)^3 - 3q(p-1)^2 + 2q^2 + \frac{2p-3}{2}M_1(G) - M_2(G).
$$

Where  $|V(G)| = p, |E(G)| = q$  $|V(G)| = p, |E(G)| = q$ 

From [9] we have  $M_2(P_n) = 4n - 8$ ,  $M_2(C_m) = 4m$ 

Where 
$$
|V(P_n)| = n, |E(P_n)| = n - 1
$$

and 
$$
|V(C_m)| = |E(C_m)| = m
$$
.

Then,

$$
M_2(P_n^c) = \frac{1}{2}n(n-1)^3 - 3(n-1)^3 + 2(n-1)^2 + \frac{2n-3}{2}(4n-6) - (4n-8)
$$
  
= 
$$
\frac{1}{2}[(n-1)^2(n^2 - n - 6n + 6 + 4) + 2(2n-3)^2 - 8(n-2)]
$$
  
= 
$$
\frac{1}{2}[(n-1)^2(n^2 - 7n + 10) + 2(2n-3)^2 - 8(n-2)]
$$
  
= 
$$
\frac{1}{2}[(n-1)^2(n-2)(n-5) + 2(2n-3)^2 - 8(n-2)].
$$

Similarly,

$$
M_2(C_m^c) = \frac{1}{2}m(m-1)^3 - 3m(m-1)^2 + 2m^2 + \frac{2m-3}{2}(4m) - 4m
$$
  
= 
$$
\frac{1}{2}m[(m-1)^2(m-1-6) + 4m + 8m - 12 - 8]
$$
  
= 
$$
\frac{1}{2}m[(m-1)^2(m-7) + 4(3m-5)].
$$

By using Theorem 4.1, the proof was completed.

# **5 Forgotten Zagreb Index of New Graph Operations**

In this section, we introduce forgotten Zagreb Index of new graphs and some of its special cases.

**Theorem 5.1** If  $G_1^c$ ,  $G_2^c$  be two complements of  $G_1$  and  $G_2$  respectively. Then

- (1)  $F(G_1 \otimes_0 G_2) = F(G_1)F(G_2),$
- $F(G_1 \otimes_1 G_2) = p_2 F(G_1),$
- (3)  $F(G_1 \otimes_2 G_2) = F(G_1)F(G_2^c),$
- (4)  $F(G_1 \otimes_3 G_2) = p_1 F(G_2),$
- (5)  $F(G_1 \otimes_4 G_2) = p_1 F(G_2^c),$
- (6)  $F(G_1 \otimes_5 G_2) = F(G_1^c)F(G_2),$
- $F(G_1 \otimes_6 G_2) = p_2 F(G_1^c),$
- (8)  $F(G_1 \otimes_7 G_2) = F(G_1^c)F(G_2^c)$ *.*

**Proof:** By Lemma 2.5, Lemma 2.6 and definition of F-index, we get

$$
(1) \quad F(G_1 \otimes_0 G_2) = \sum_{(u,v) \in V(G_1 \otimes_0 G_2)} \delta_{G_1 \otimes_0 G_2}^3(u,v)
$$
  

$$
= \sum_{(u,v) \in V(G_1 \otimes_0 G_2)} (\delta_{G_1}(u)\delta_{G_2}(v))^3
$$
  

$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1}^3(u)\delta_{G_2}^3(v)
$$
  

$$
= \sum_{u \in V(G_1)} \delta_{G_1}^3(u) \sum_{v \in V(G_2)} \delta_{G_2}^3(v)
$$
  

$$
= F(G_1)F(G_2),
$$

$$
(2) \quad F(G_1 \otimes_1 G_2) = \sum_{(u,v) \in V(G_1 \otimes_1 G_2)} \delta^3_{G_1 \otimes_1 G_2}(u,v)
$$
  

$$
= \sum_{(u,v) \in V(G_1 \otimes_1 G_2)} (\delta_{G_1}(u))^3
$$
  

$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta^3_{G_1}(u)
$$
  

$$
= \sum_{u \in V(G_1)} \delta^3_{G_1}(u) \sum_{v \in V(G_2)} (1)
$$
  

$$
= P_2F(G_1),
$$

$$
(3) \quad F(G_1 \otimes_2 G_2) = \sum_{(u,v) \in V(G_1 \otimes_2 G_2)} \delta^3_{G_1 \otimes_2 G_2}(u,v)
$$
  

$$
= \sum_{(u,v) \in V(G_1 \otimes_2 G_2)} (\delta_{G_1}(u) \delta_{G_2^c}(v))^3
$$
  

$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta^3_{G_1}(u) \delta^3_{G_2^c}(v)
$$
  

$$
= \sum_{u \in V(G_1)} \delta^3_{G_1}(u) \sum_{v \in V(G_2)} \delta^3_{G_2^c}(v)
$$
  

$$
= F(G_1)F(G_2^c),
$$

$$
(4) \quad F(G_1 \otimes_3 G_2) = \sum_{(u,v) \in V(G_1 \otimes_3 G_2)} \delta^3_{G_1 \otimes_3 G_2}(u,v)
$$
  
= 
$$
\sum_{u \in V(G_1)} (1) \sum_{v \in V(G_2)} \delta^3_{G_2}(v)
$$
  
= 
$$
p_1 F(G_2),
$$

$$
(5) \quad F(G_1 \otimes_4 G_2) = \sum_{(u,v) \in V(G_1 \otimes_4 G_2)} \delta_{G_1 \otimes_4 G_2}^3(u,v)
$$
  
\n
$$
= \sum_{u \in V(G_1)} (1) \sum_{v \in V(G_2)} \delta_{G_2}^3(v)
$$
  
\n
$$
= p_1 F(G_2^c),
$$
  
\n
$$
(6) \quad F(G_1 \otimes_5 G_2) = \sum_{(u,v) \in V(G_1 \otimes_5 G_2)} \delta_{G_1 \otimes_5 G_2}^3(u,v)
$$
  
\n
$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} (\delta_{G_1^c}(u) \delta_{G_2}(v))^3
$$
  
\n
$$
= \sum_{u \in V(G_1)} \delta_{G_1^c}(u) \sum_{v \in V(G_2)} \delta_{G_2}^3(v)
$$
  
\n
$$
= F(G_1^c) F(G_2),
$$
  
\n
$$
(7) \quad F(G_1 \otimes_6 G_2) = \sum_{(u,v) \in V(G_1 \otimes_6 G_2)} \delta_{G_1 \otimes_6 G_2}^3(u,v)
$$
  
\n
$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1^c}(u,v)
$$
  
\n
$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1^c}(u)
$$
  
\n
$$
= P_2 F(G_1^c),
$$
  
\n
$$
(8) \quad F(G_1 \otimes_7 G_2) = \sum_{(u,v) \in V(G_1 \otimes_7 G_2)} \delta_{G_1 \otimes_7 G_2}^3(u,v)
$$
  
\n
$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} (\delta_{G_1^c}(u) \delta_{G_2^c}(v))^3
$$
  
\n
$$
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \delta_{G_1^c}(v)
$$
  
\n
$$
= F(G_1^c) F(G_2^c).
$$

**Corollary 5.2** Let  $G_1 \simeq P_n$  be a path graph with *n* vertices and  $G_2 \simeq C_m$  be a cycle graph with *m* vertices, where

 $|V(P_n)| = n, |E(P_n)| = n - 1$  and  $|V(C_m)| = |E(C_m)| = m$ , then we have,  $F(P_n \otimes_0 C_m) = 16m(4n - 7)$ ,  $F(P_n \otimes_1 C_m) = 2m(4n - 7)$ ,  $F(P_n \otimes_2 C_m) = 2m(4n-7)[(m-7)(m-1)^2 + 4(3m-5)],$  $F(P_n \otimes_3 C_m) = 8nm,$  $F(P_n \otimes_4 C_m) = nm[(m-7)(m-1)^2 + 4(3m-5)],$ 

$$
F(P_n \otimes_5 C_m) = 8m[(n-1)^3(n-6) + 6(n-1)(2n-3) - 2(4n-7)],
$$
  
\n
$$
F(P_n \otimes_6 C_m) = m[(n-1)^3(n-6) + 6(n-1)(2n-3) - 2(4n-7)],
$$
  
\n
$$
F(P_n \otimes_7 C_m) = m[(m-7)(m-1)^2 + 4(3m-5)],
$$
  
\n
$$
[(n-1)^3(n-6) + 6(n-1)(2n-3) - 2(4n-7)].
$$

**Proof:** By [17], for a graph *G*, where  $|V(G)| = p$ ,  $|E(G)| = q$ 

$$
F(G^{c}) = p(p-1)^{3} - F(G) - 6q(p-1)^{2} + 3(p-1)M_{1}(G).
$$

Where  $|V(G)| = p, |E(G)| = q$ 

Where  $|V(P_n)| = n, |E(P_n)| = n - 1$  and  $|V(C_m)| = |E(C_m)| = m$ .

Then,

$$
F(P_n^c) = n(n-1)^3 - (8n - 14) - 6(n - 1)^3 + 3(n - 1)(4n - 6)
$$
  
=  $(n-1)^3(n-6) - 2(4n - 7) + 6(2n - 3)(n - 1).$ 

Similarly,

$$
F(C_m^c) = m(m-1)^3 - 8m - 6m(m-1)^2 + 3(m-1)(4m)
$$
  
=  $m(m-1)^2(m-7) - 4m(2-3m+3)$   
=  $m[(m-1)^2(m-7) + 4(3m-5)].$ 

By using Theorem 5.1, the proof was completed.  $\Box$ 

### **6 Possible Applications of New Graph Operations**

A chemical graph is a graph which vertices denote atoms and edges denote bonds between atoms of any underlying chemical structure. The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4 [18]. In this section, we give in (Table 1) some applications as special cases ( Zagreb Indices of graphs resulted by molecular structures as alkanes  $P_n$  and cyclic alkanes  $C_m$ ). In (Table 2) we compute the correlation coefficient between previous Zagreb Indices as shown in (Table 1).

In (Tab[le 2](#page-14-0)),  $r_i = r(P_n \otimes_i C_m)$  are correlation coefficients between Zagreb Indices of  $P_n \otimes_i C_m$ , where  $i \in \{0, 1, ..., 7\}$ . It is clear that Zagreb indices considered are perfect correlated since  $0.99 \le r \le 1$ . Therefore, we can use these indices to compare between properties of molecular graphs that resulted by  $P_n$  and  $C_m$ .

(n, m)	(4,4)	(4,5)	(4,6)	(5,4)	$^{(5,5)}$	$^{(5,6)}$	(6,4)	$\left( 6,5\right)$	(6, 6)
$M_1(P_n\otimes_0 C_m)$	40	50	240	224	280	336	288	360	432
$M_2(P_n\otimes_0 C_m)$	256	320	384	384	480	576	512	640	768
$F(P_n \otimes_0 C_m)$	576	720	864	832	1040	1248	1088	1360	1632
$M_1(P_n \otimes_1 C_m)$	40	50	60	56	70	84	72	90	108
$M_2(P_n\otimes_1 C_m)$	32	40	48	48	60	72	64	80	96
$F(P_n \otimes_1 C_m)$	72	90	108	104	130	156	136	170	204
$M_1(P_n \otimes_2 C_m)$	80	400	1080	112	560	1512	144	720	1944
$M_2(P_n\otimes_2 C_m)$	32	320	1296	48	480	1944	64	640	2592
$F(P_n \otimes_2 C_m)$	72	720	2916	104	1040	4212	136	1360	5508
$M_1(P_n \otimes_3 C_m)$	64	80	96	80	100	120	96	120	144
$M_2(P_n\otimes_3 C_m)$	64	80	96	80	100	120	96	120	144
$F(P_n \otimes_3 C_m)$	128	160	192	160	200	240	192	240	288
$M_1(P_n \otimes_4 C_m)$	16	80	216	20	100	270	24	120	324
$M_2(P_n \otimes_4 C_m)$	8	80	324	10	100	405	$\overline{12}$	120	486
$F(P_n \otimes_4 C_m)$	16	160	648	20	200	810	24	240	972
$\overline{M_1}(P_n \otimes_5 C_m)$	160	200	240	480	600	720	1088	1360	1632
$M_2(P_n\otimes_5 \overline{C_m})$	256	320	384	1184	1480	1776	3680	4600	5520
$F(P_n \otimes_5 C_m)$	576	720	864	2496	3120	3744	7552	9440	11328
$M_1(P_n\otimes_6 C_m)$	40	50	60	120	150	180	272	340	408
$M_2(P_n\otimes_6 C_m)$	32	40	48	148	185	222	460	575	690
$F(P_n \otimes_6 C_m)$	72	90	108	312	390	468	944	1180	1416
$M_1(P_n \otimes_7 C_m)$	40	200	540	120	600	1620	272	1360	3672
$M_2(P_n\otimes_7 C_m)$	64	640	2592	296	2960	11988	920	9200	37260
$F(P_n \otimes_7 C_m)$	$72\,$	720	2916	312	3120	12636	944	9440	38232

Table 1. Some Zagreb Indices of  $P_n \otimes_i C_m$ 

Table 2. Correlation coefficient between Zagreb Indices of  $P_n \otimes_i C_m$ 

$r_0$	$M_1$	$M_2$	$\overline{F}$	$r_1$	$M_1$	$M_2$	$\boldsymbol{F}$
$M_1$	1.000	0.998	0.999	$M_1$	1.000	0.998	0.999
$M_2$	0.998	1.000	0.999	$M_2$	0.998	1.000	0.999
$\overline{F}$	0.999	0.999	1.000	F	0.999	0.999	1.000
r <sub>2</sub>	$M_1$	$M_2$	$\overline{F}$	$r_3$	$M_1$	$M_2$	$\overline{F}$
$M_1$	1.000	0.995	0.995	$M_1$	1.000	1.000	1.000
$M_2$	0.995	1.000	1.000	$M_2$	1.000	1.000	1.000
$\overline{F}$	0.995	1.000	1.000	$\boldsymbol{F}$	1.000	1.000	1.000
$r_4$	$M_1$	$M_2$	$\overline{F}$	$r_5$	$M_1$	$M_2$	F
$M_1$	1.000	0.995	0.995	$M_1$	1.000	0.996	0.996
$M_2$	0.995	1.000	1.000	$M_2$	0.996	1.000	1.000
F	0.995	1.000	1.000	F	0.996	1.000	1.000
r <sub>6</sub>	$M_1$	$M_2$	F	r <sub>7</sub>	$M_1$	$M_2$	F
$M_1$	1.000	0.996	0.996	$M_1$	1.000	0.990	0.991
$M_2$	0.996	1.000	1.000	$M_2$	0.990	1.000	1.000

# **7 Concluding Remarks**

Several articles have studied the Zagreb indices of the different graph operations. In this article, we have studied some new graph operations for well-known degree-based topological indices such as the first Zagreb index, second Zagreb index and forgotten index "F-index". Moreover, our computed results have applied on some molecular structures as alkanes *P<sup>n</sup>* and cyclic alkanes *Cm*, and the strong correlation coefficients between them have been appeared.

### **Competing Interests**

Authors have declared that no competing interests exist.

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 $\mathcal{L}=\{1,2,3,4\}$  , we can consider the constant of  $\mathcal{L}=\{1,2,3,4\}$ 

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