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The first general Zagreb coindex of graph operations

Melaku Berhe Belay<sup>1,2</sup><sup>†</sup>, Chunxiang Wang<sup>1‡</sup>

<sup>1</sup>Faculty of Mathematics and Statistics, Central China Normal University, Wuhan 430079, P.R. China

<sup>2</sup>Department of Mathematics, Addis Ababa Science and Technology University, Addis Ababa 16417, Ethiopia

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## Abstract

Many chemically important graphs can be obtained from simpler graphs by applying different graph operations. Graph operations such as union, sum, Cartesian product, composition and tensor product of graphs are among the important ones. In this paper, we introduce a new invariant which is named as the first general Zagreb coindex and defined as  $\overline{M}_1^{\alpha}(G) = \sum_{uv \in E(\overline{G})} [d_G(u)^{\alpha} + d_G(v)^{\alpha}]$ , where  $\alpha \in \mathbb{R}, \alpha \neq 0$ . Here, we study the basic properties of the newly introduced invariant and its behavior under some graph operations such as union, sum, Cartesian product, composition and tensor product of graphs and hence apply the results to find the first general Zagreb coindex of different important nano-structures and molecular graphs.

**Keywords:** Topological index, first general Zagreb index, first general Zagreb coindex, Graph operation. **AMS 2010 codes:** 05C76, 05C07, and 05C90.

# **1** Introduction

The branch of mathematical chemistry which deals in the study of chemical graphs is called chemical graph theory. Chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by the edges of the graph. Chemical graph theory is useful to study various physico-chemical properties of molecules by using the information encoded in their corresponding chemical graphs. The study is achieved by considering various graph-theoretical invariants of molecular graphs (also known as topological indices or molecular descriptors). Topological indices are mathematical procedures which transforms chemical information encoded within a symbolic representation of a molecular properties and also predicts some interesting property of other molecules.

<sup>†</sup>Corresponding author.

<sup>‡</sup>E-mail address: wcxiang@mail.ccnu.edu.cn



Email address: melaku.berhe@aastu.edu.et

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Here, we introduce an invariant, the first general Zagreb coindex. The formal definition of the first generale Zagreb coindex, basic properties and main results are given in sections 2,3 and 4 respectively.

#### 2 Definitions and preliminaries

For convenience of our discussion, we first recall some relevant terminology and notations. In this paper, all the graphs are simple and finite. For any concepts and terms not defined here we recommend the reader to any standard monographs such as [1,2]. Let *G* be a finite simple graph on *n* vertices and *m* edges. The vertex set and edge set of *G* are denoted respectively by V(G) and E(G). The complement of a graph *G* which is denoted by  $\overline{G}$  is the simple graph with the same vertex set V(G) and any two vertices  $uv \in E(\overline{G})$  if and only if  $uv \notin E(G)$ . Since  $E(\overline{G}) \cup E(G) = E(K_n)$ , we have that  $\overline{m} = n(n-1)/2 - m$ , where  $\overline{m} = |E(\overline{G})|$ . The degree of a vertex *v* in *G* is denoted by  $d_G(v)$  and the degree of the same vertex *v* in  $\overline{G}$  is then given by  $d_{\overline{G}}(v) = n - 1 - d_G(v)$ . We next list the definitions of some topological indices with which we are particularly concerned in this paper.

The first  $(M_1)$  and second  $(M_2)$  Zagreb indices are the oldest and most thoroughly studied degree based topological indices. These indices were introduced in (1972) by Gutman and Trinajstić [8] with in a study of the structure-dependency of the total  $\pi$ -electron energy ( $\varepsilon$ ) where approximate formulas for the total  $\pi$ -electron energy ( $\varepsilon$ ) were obtained. These indices provide a measure of branching of the carbon-atom skeleton. These quantities are defined as

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

and

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

In [8] another degree based topological index which is also a measure of branching was also introduced but it was not studied further. After more than 40 years, Furtula and Gutman [9] re-initiated and establish some basic properties of it. This index is denoted by F(G) and named as forgotten topological index or *F*-index. It is defined as

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

Li and Zheng [10] introduced the concept of the first general Zagreb index  $M_1^{\alpha}(G)$  of G as follows:

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_G(u)^{\alpha}$$

where,  $\alpha \neq 0, 1$  and  $\alpha \in \mathbb{R}$ . Obviously, when  $\alpha = 2$  it gives first Zagreb index and when  $\alpha = 3$  we obtain *F*-index. If *G* has *n* vertices and *m* edges, then it is known that  $M_1^0(G) = n$  and  $M_1^1(G) = 2m$  (hand shaking lemma.)

By taking the contributions of non adjacent pairs of vertices into consideration, the first  $(\overline{M}_1)$  and second  $(\overline{M}_2)$ Zagreb coindices were introduced by Došlic [11] while computing weighted Winner Polynomial of some composite graphs. In this case the sum runs over the edges of the complement of *G*. They are defined as

$$\overline{M}_1(G) = \sum_{uv \in E(\overline{G})} (d_G(u) + d_G(v))$$

and

$$\overline{M}_2(G) = \sum_{uv \in E(\overline{G})} (d_G(u)d_G(v))$$

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De et al. [19] introduced the *F*-coindex of a graph *G*, denoted by  $\overline{F}$ , and testifying that *F*-coindex can predict the logarithm of octanol-water partition coefficient (log(P)) values with high accuracy. It is defined as

$$\overline{F}(G) = \sum_{uv \in E(\overline{G})} [d_G(u)^2 + d_G(v)^2]$$

Motivated by the first Zagreb coindex and F-coindex, we introduce a coindex in a more general form, called the first general Zagreb coindex and defined as follows:

$$\overline{M}_{1}^{\alpha}(G) = \sum_{uv \in E(\overline{G})} [d_{G}(u)^{\alpha} + d_{G}(v)^{\alpha}], \text{ where } \alpha \in \mathbb{R}, \alpha \neq 0.$$
(2.1)

The reader should note that the defining sums in (2.1) run over  $E(\overline{G})$  but the degrees are with respect to *G*. Clearly, when  $\alpha = 1$  it gives first Zagreb coindex  $(\overline{M}_1)$  and when  $\alpha = 2$  it gives *F*-coindex  $(\overline{F})$ . Obviously, if  $\alpha = 0$  then  $\overline{M}_1^0(G) = 2\overline{m}$ .

There are many chemically important graphs which are obtained from simpler graphs by applying different graph operations. To mention a few, the Cartesian product of a path and a cycle produces a  $C_4$  nanotube, the Cartesian product of two cycles produce the  $C_4$  nanotorus and using the products of two paths we obtain rectangular grids, composition of a path and cycle with  $K_2$  produces open and closed fences respectively etc... Hence, it is vital to understand how certain invariants of such composite graphs are related to their corresponding invariants as well as with other related invariants.

So far, several studies on different graph invariants under different graph operations have been studied. Graovac and Pisanski [13] derived exact formula for the Wiener index of the Cartesian product of graphs. Khalifeh et al. [14] computed some exact formulae for computing first and second Zagreb indices under some graph operations. Azari and Iranmanesh [15] presented explicit formulas for computing the eccentric-distance sum of different graph operations. De et al. presented the reformulated Zagreb index of graph operations in [7] and the F-index of some graph operations in [12]. Many other results concerning various topological indices under different graph operations are available in the literature and for details we refer the reader to see [3–6,16,21–23]. Beside to this, there are few studies on the coindex version of invariants under different graph operations. In [17] Ashrafi et al. derived some explicit formulae of Zagreb coindices under some graph operations. De et al. [19] presented the F-coindex of some graph operation and Basavanagoud and Patil [20] computed hyper Zagreb coindex of some graph operations. Here, we continue this line of research by exploring the behavior of the newly introduced first general Zagreb coindex under some important graph operations such as union, sum, Cartesian product, tensor product and composition.

## **3** Basic properties

**Proposition 1.** Let G be a connected graph of order n with degree sequence  $\pi = (d_1, d_2, \dots, d_n)$ , then  $\overline{M}_1^{\alpha}(G)$  can be expressed as  $\overline{M}_1^{\alpha}(G) = \sum_{i=1}^n (n-1-d_i)d_i^{\alpha}$ .

*Proof.* Since every vertex  $d_i$  (i = 1, 2, ..., n) has  $(n - 1 - d_i)$  non adjacent vertices, the result follows immediately.

**Proposition 2.** Let G be a simple graph of order n and size m. Then  $\overline{M}_1^{\alpha}(G) + M_1^{\alpha+1}(G) = (n-1)M_1^{\alpha}(G).$ 

*Proof.* By proposition 1,

$$\begin{split} \overline{M}_{1}^{\alpha}(G) &= \sum_{u \in V(G)} [n - 1 - d_{G}(u)] d_{G}(u)^{\alpha} \\ &= (n - 1) \sum_{u \in V(G)} d_{G}(u)^{\alpha} - \sum_{u \in V(G)} d_{G}(u)^{\alpha + 1} \\ &= (n - 1) M_{1}^{\alpha}(G) - M_{1}^{\alpha + 1}(G). \end{split}$$

From the definition (2.1) or proposition 1, the first general Zagreb coindex acheive the smallest possible value of 0 on the complete and on the empty graphs. In case of complete graph, all the degrees are n - 1 and in the case of empty graphs, all the degrees are zero.

**Proposition 3.** For any complete graph and empty graph of order n, we have

$$\overline{M}_1^{\alpha}(K_n) = 0.$$
$$\overline{M}_1^{\alpha}(\overline{K}_n) = 0.$$

The following results for paths and cycles on *n* vertices can be easily obtained by using direct calculations.

**Proposition 4.** For any path and cycle of order n we have

$$\overline{M}_1^{\alpha}(P_n) = (n-2)[2^{\alpha}(n-3)+2].$$
  
$$\overline{M}_1^{\alpha}(C_n) = n(n-3)2^{\alpha}.$$

## 4 Main results

In this section, we study the first general Zagreb coindex of some graph operations such as union, sum, Cartesian product, composition, and tensor product of graphs. For more information on composite graphs we refer the reader to monograph [18]. All considered graph operations are binary. For a given graph  $G_i$ , we use the notations  $V(G_i)$  for the set of vertex,  $E(G_i)$  for the set of edge,  $n_i$  for the cardinality of  $V(G_i)$ ,  $m_i$  for the cardinality of  $E(G_i)$  and  $\overline{m}_i$  for the cardinality of edges in the graph  $\overline{G}_i$ . When more than two graphs can be combined using a given operation, the values of subscripts will vary accordingly. Here, we consider five operations and each of them is treated in a separate subsection.

#### 4.1 Union

The union of two graphs  $G_1$  and  $G_2$  is the graph denoted by  $G_1 \cup G_2$  with vertex set  $V(G_1) \cup V(G_2)$  and edge set  $E(G_1) \cup E(G_2)$ . Here we assume that  $V(G_1)$  and  $V(G_2)$  are disjoint. Obviously,  $|V(G_1 \cup G_2)| = n_1 + n_2$  and  $|E(G_1 \cup G_2)| = m_1 + m_2$ .

**Proposition 5.** Let  $G_i$  (i = 1, 2) be simple graph with order  $n_i$  (i = 1, 2). Then  $\overline{M}_1^{\alpha}(G_1 \cup G_2) = \overline{M}_1^{\alpha}(G_1) + \overline{M}_1^{\alpha}(G_2) + n_2 M_1^{\alpha}(G_1) + n_1 M_1^{\alpha}(G_2)$ .

*Proof.* The degree of a vertex u of  $G_1 \cup G_2$  is equal to the degree of the component  $G_i$  (i = 1, 2) that contains it. So  $\forall u \in V(G_1 \cup G_2)$ , we have

$$d_{G_1 \cup G_2}(u) = \begin{cases} d_{G_1}(u), & \text{if } u \in V(G_1) \\ d_{G_2}(u), & \text{if } u \in V(G_2). \end{cases}$$

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So, by using proposition 1,

$$\overline{M}_{1}^{\alpha}(G_{1}\cup G_{2}) = \sum_{u\in V(G_{1}\cup G_{2})} [(n_{1}+n_{2})-1-d_{G_{1}\cup G_{2}}(u)]d_{G_{1}\cup G_{2}}(u)^{\alpha}$$

$$= \sum_{u\in V(G_{1})} [n_{1}-1-d_{G_{1}}(u)]d_{G_{1}}(u)^{\alpha}+n_{2}\sum_{u\in V(G_{1})} d_{G_{1}}(u)^{\alpha}$$

$$+ \sum_{u\in V(G_{2})} [n_{2}-1-d_{G_{2}}(u)]d_{G_{2}}(u)^{\alpha}+n_{1}\sum_{u\in V(G_{2})} d_{G_{2}}(u)^{\alpha}$$

$$= \overline{M}_{1}^{\alpha}(G_{1})+\overline{M}_{1}^{\alpha}(G_{2})+n_{2}M_{1}^{\alpha}(G_{1})+n_{1}M_{1}^{\alpha}(G_{2}).$$

The union operation can be extended inductively to more than two graphs in an obvious way. Let  $G_i$  (i = 1, 2, ..., p) be graphs with vertex sets  $V_i$  and edge sets  $E_i$  of cardinality  $n_i$  and  $m_i$ , respectively. Their union is a graph  $G_1 \cup G_2 \cup ... \cup G_p$  on the vertex set  $V_1 \cup ... \cup V_p$  and the edge set  $E_1 \cup E_2 \cup ... \cup E_p$ . By starting from Proposition 5, deduce induction on p, we can obtain the following result for the first general Zagreb coindex of the union of several graphs.

**Corollary 4.1.** Let  $G_i$  ( $i = 1, 2, \dots, p$ ) be p disjoint graph of order  $n_i$ . Then

$$\overline{M}_{1}^{\alpha}(\bigcup_{i=1}^{p}G_{i}) = \sum_{i=1}^{p}\overline{M}_{1}^{\alpha}(G_{i}) + \sum_{i=1}^{p}[M_{1}^{\alpha}(G_{i})(\sum_{j=1}^{p}n_{j}-n_{i})].$$

## 4.2 Sum

The sum of two graphs with disjoint vertex sets  $V_1$  and  $V_2$  is the graph denoted by  $G_1 + G_2$  with the vertex set  $V(G_1) \cup V(G_2)$  and edge set  $E(G_1) \cup E(G_2) \cup \{u_1u_2 : u_1 \in V_1, u_2 \in V_2\}$ . Thus, the sum of two graphs is obtained by connecting each vertex of one graph to each vertex of the other graph, while keeping all the edges of both graphs. Here also,  $|V(G_1 \cup G_2)| = n_1 + n_2$ .

**Proposition 6.** Let  $G_i(i = 1, 2)$  be simple graphs and  $\alpha \in \mathbb{N}$ . Then,

$$\overline{M}_1^{\alpha}(G_1+G_2) = \overline{M}_1^{\alpha}(G_1) + \overline{M}_1^{\alpha}(G_2) + \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} \left[ \overline{M}_1^{\alpha-i}(G_1)n_2^i + \overline{M}_1^{\alpha-i}(G_2)n_1^i \right] \\ + 2(\overline{m}_1n_2^{\alpha} + \overline{m}_2n_1^{\alpha}).$$

*Proof.* From the definition of sum of two graphs, the degree of a vertex u of  $G_1 + G_2$  is given by

$$d_{G_1+G_2}(u) = \begin{cases} d_{G_1}(u) + n_2, & \text{if } u \in V(G_1) \\ d_{G_2}(u) + n_1, & \text{if } u \in V(G_2). \end{cases}$$

By using proposition 1,

$$\begin{split} \overline{M}_1^{\alpha}(G_1+G_2) &= \sum_{u \in V(G_1+G_2)} \left[ (n_1+n_2) - 1 - d_{G_1+G_2}(u) \right] \left[ d_{G_1+G_2}(u) \right]^{\alpha} \\ &= \sum_{u \in V(G_1)} \left[ n_1 - 1 - d_{G_1}(u) \right] (d_{G_1}(u) + n_2)^{\alpha} \\ &+ \sum_{u \in V(G_2)} \left[ n_2 - 1 - d_{G_2}(u) \right] (d_{G_2}(u) + n_1)^{\alpha} = A + B. \end{split}$$

Now,

$$\begin{split} A &= \sum_{u \in V(G_1)} [n_1 - 1 - d_{G_1}(u)] [d_{G_1}(u) + n_2]^{\alpha} \\ &= \sum_{u \in V(G_1)} [n_1 - 1 - d_{G_1}(u)] [d_{G_1}(u)^{\alpha} + \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} d_{G_1}(u)^{\alpha-i} n_2^i + n_2^{\alpha}] \\ &= \overline{M}_1^{\alpha}(G_1) + \sum_{u \in V(G_1)} \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} [n_1 - 1 - d_{G_1}(u)] d_{G_1}(u)^{\alpha-i} n_2^i + \sum_{u \in V(\overline{G}_1)} d_{\overline{G}_1}(u) n_2^{\alpha} \\ &= \overline{M}_1^{\alpha}(G_1) + \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} \overline{M}_1^{\alpha-i}(G_1) n_2^i + 2\overline{m}_1 n_2^{\alpha}. \end{split}$$

Similarly, we get

$$B = \overline{M}_1^{\alpha}(G_2) + \sum_{i=1}^{\alpha-1} {\alpha \choose i} \overline{M}_1^{\alpha-i}(G_2) n_1^i + 2\overline{m}_2 n_1^{\alpha}.$$

Combining A and B, we get the desired result.

The complete bipartite graph  $K_{p,q}$   $(p,q \ge 2)$  is sum of two empty graphs  $\overline{K}_p$  and  $\overline{K}_q$ . Thus, by using proposition 6 and result in proposition 3 (ii) we give an explicit formulae below.

#### **Corollary 4.2.**

$$\overline{M}_1^{\alpha}(K_{p,q}) = pq[q^{\alpha-1}(p-1) + p^{\alpha-1}(q-1)].$$

The suspension graph of G is defined as sum of G with  $K_1$ . Thus, from proposition 6, we obtain the following result.

Corollary 4.3. The first general Zagreb coindex of suspension of G is given by

$$\overline{M}_{1}^{\alpha}(G+K_{1}) = \overline{M}_{1}^{\alpha}(G) + \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} \overline{M}_{1}^{\alpha-i}(G) + 2\overline{m}_{1}^{\alpha-i}(G)$$

For example, the wheel graph  $W_n$  on (n+1) vertices, the fan graph  $F_n$  on (n+1) vertices and the star graph  $S_n$  on *n* vertices are suspensions of the graphs  $C_n$ ,  $P_n$  and  $\overline{K}_{n-1}$  respectively. Thus, by using corollary 3 we get the following results in Example 1.

Example 1:  $\overline{M}_{1}^{\alpha}(W_{n}) = n(n-3)3^{\alpha}.$   $\overline{M}_{1}^{\alpha}(F_{n}) = (n-2)[2^{\alpha+1} + (n-3)3^{\alpha}].$  $\overline{M}_{1}^{\alpha}(S_{n}) = (n-1)(n-2).$ 

The sum operation can also be extended to more than two graphs. Let  $G_i$  (i = 1, 2, ..., p) be graphs with vertex sets  $V_i$  and edge sets  $E_i$  of cardinality  $n_i$  and  $m_i$ , respectively. Their sum is a graph  $\sum_{i=1}^p G_i = G_1 + G_2 + ... + G_p$  on the vertex set  $(\bigcup_{i=1}^p V(G_i))$  and edge set  $(\bigcup_{i=1}^p E(G_i)) \cup \{u_i v_j : u_i \in V_i, v_j \in V_j, i \neq j\}$ . Therefore, for  $\alpha \in \mathbb{N}$ , the first general Zagreb coindex of the sums of graphs  $\sum_{i=1}^p G_i$  is given as in the following proposition.

**Proposition 7.** Let  $G_i$  (i = 1, 2, ..., p) be simple graphs and  $\alpha \in \mathbb{N}$ . Then,

$$\overline{M}_1^{\alpha}(\sum_{i=1}^p G_i) = \sum_{i=1}^p \overline{M}_1^{\alpha}(G_i) + \sum_{i=1}^p \sum_{k=1}^{\alpha-1} \binom{\alpha}{k} \overline{M}_1^{\alpha-k}(G_i)(\sum_{j=1,j\neq i}^p n_j)^k] + 2\sum_{i=1}^p \overline{m}_i(\sum_{j=1,j\neq i}^p n_j)^{\alpha}.$$

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*Proof.* The degree of a vertex u in  $\sum_{i=1}^{p} G_i$  is given by  $d_{\sum_{i=1}^{p} G_i}(u) = d_{G_i}(u) + \sum_{j=1, j \neq i}^{p} n_j$ . By proposition 1,

$$\begin{split} \overline{M}_{1}^{\alpha}(\sum_{i=1}^{p}G_{i}) &= \sum_{u \in V(\sum_{i=1}^{p}G_{i})} [(\sum_{i=1}^{p}n_{i}) - 1 - d_{\sum_{i=1}^{p}G_{i}}(u)][d_{\sum_{i=1}^{p}G_{i}}(u)]^{\alpha} \\ &= \sum_{i=1}^{p}\sum_{u \in V(G_{i})} [n_{i} - 1 - d_{G_{i}}(u)][d_{G_{i}}(u) + \sum_{j=1, j \neq i}^{p}n_{j})^{\alpha} \\ &= \sum_{i=1}^{p}\sum_{u \in V(G_{i})} [n_{i} - 1 - d_{G_{i}}(u)][d_{G_{i}}(u)^{\alpha} + \sum_{k=1}^{\alpha-1} \binom{\alpha}{k} d_{G_{i}}(u)^{\alpha-k} (\sum_{j=1, j \neq i}^{p}n_{j})^{k} + (\sum_{j=1, j \neq i}^{p}n_{j})^{\alpha} ] \\ &= \sum_{i=1}^{p}\overline{M}_{1}^{\alpha}(G_{i}) + \sum_{i=1}^{p} (\sum_{u \in V(G_{1})} \sum_{k=1}^{\alpha-1} \binom{\alpha}{k} [n_{i} - 1 - d_{G_{i}}(u)]d_{G_{i}}(u)^{\alpha-k} (\sum_{j=1, j \neq i}^{p}n_{j})^{k} ) \\ &+ \sum_{i=1}^{p}\sum_{u \in V(\overline{G}_{i})} d_{\overline{G}_{i}}(u) (\sum_{j=1, j \neq i}^{p}n_{j})^{\alpha} \\ &= \sum_{i=1}^{p}\overline{M}_{1}^{\alpha}(G_{i}) + \sum_{i=1}^{p} [\sum_{k=1}^{\alpha-1} \binom{\alpha}{k} \overline{M}_{1}^{\alpha-k}(G_{i}) (\sum_{j=1, j \neq i}^{p}n_{j})^{k}] + 2\sum_{i=1}^{p} \overline{m}_{i} (\sum_{j=1, j \neq i}^{p}n_{j})^{\alpha}. \end{split}$$

The complete *p*-partite graph  $K_{n_1,\dots,n_p}$  with partition classes of size  $n_i$  is a sum of *p* empty graphs  $\overline{K}_{n_i}(i = 1,\dots,p)$ . So by proposition 7, we obtain a formula for  $\overline{M}_1^{\alpha}(K_{n_1,\dots,n_p})$ .

**Corollary 4.4.** Let  $G_i$  (i = 1, 2, ..., p) be empyt graph of order  $n_i$  and  $\alpha \in \mathbb{N}$ . Then,

$$\overline{M}_1^{\alpha}(K_{n_1,\cdots,n_p}) = \sum_{i=1}^p \left[ (n_i^2 - n_i) \left( \sum_{j=1}^p n_j - n_i \right)^{\alpha} \right].$$

In particular when all classes are of equal size, say q, i.e in the case of balanced complete p-partite graph on  $p \cdot q$  vertices, its first general Zagreb coindex is given by

$$\overline{M}_1^{\alpha}(K_{q,\cdots,q}) = 2p.\binom{q}{2}(pq-q)^{\alpha}.$$

## 4.3 Cartesian product

The Cartesian product of two graphs  $G_1$  and  $G_2$  which is denoted by  $G_1 \times G_2$ , is the graph with vertex set  $V(G_1) \times V(G_2)$  and any two vertices  $(u_1, u_2)$  and  $(v_1, v_2)$  are adjacent if and only if  $[u_1 = v_1 \in V(G_1)$  and  $u_2v_2 \in E(G_2)]$  or  $[u_2 = v_2 \in V(G_2)$  and  $u_1v_1 \in E(G_1)]$ . Obviously,  $|V(G_1 \times G_2)| = n_1n_2$  and  $|E(G_1 \times G_2)| = n_1m_2 + n_2m_1$ .

Obviously,  $|V(G_1 \times G_2)| = n_1 n_2$  and  $|E(G_1 \times G_2)| = n_1 m_2 + n_2 m_1$ 

**Proposition 8.** Let  $G_i(i = 1, 2)$  be simple graph and  $\alpha \in \mathbb{N}$ . Then

$$\overline{M}_{1}^{\alpha}(G_{1} \times G_{2}) = (n_{1}n_{2} - 1)[n_{2}M_{1}^{\alpha}(G_{1}) + \sum_{i=1}^{\alpha-1} {\alpha \choose i} M_{1}^{\alpha-i}(G_{1})M_{1}^{i}(G_{2}) + n_{1}M_{1}^{\alpha}(G_{2})] - [n_{2}M_{1}^{\alpha+1}(G_{1}) + \sum_{i=1}^{\alpha} {\alpha+1 \choose i} M_{1}^{\alpha+1-i}(G_{1})M_{1}^{i}(G_{2}) + n_{1}M_{1}^{\alpha+1}(G_{2})]$$

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*Proof.* From the definition of Cartesian product, the degree of vertex (a,b) of  $G_1 \times G_2$  is given by  $d_{G_1 \times G_2}(a,b) = d_{G_1}(a) + d_{G_2}(b)$ .

By using proposition 1, we have

$$\overline{M}_{1}^{\alpha}(G_{1} \times G_{2}) = \sum_{a \in V(G_{1})} \sum_{b \in V(G_{2})} [n_{1}n_{2} - 1 - (d_{G_{1}}(a) + d_{G_{2}}(b))](d_{G_{1}}(a) + d_{G_{2}}(b))^{\alpha}$$

$$= \sum_{a \in V(G_{1})} \sum_{b \in V(G_{2})} [(n_{1}n_{2} - 1)(d_{G_{1}}(a) + d_{G_{2}}(b))^{\alpha}]$$

$$- \sum_{a \in V(G_{1})} \sum_{b \in V(G_{2})} (d_{G_{1}}(a) + d_{G_{2}}(b))^{\alpha+1}$$

$$= A - B.$$

Now,

$$\begin{split} A &= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} \left[ (n_1 n_2 - 1) \left( d_{G_1}(a) + d_{G_2}(b) \right)^{\alpha} \right] \\ &= (n_1 n_2 - 1) \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} \left[ d_{G_1}(a)^{\alpha} + \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} d_{G_1}(a)^{\alpha-i} d_{G_2}(b)^i + d_{G_2}(b)^{\alpha} \right] \\ &= (n_1 n_2 - 1) \left[ n_2 M_1^{\alpha}(G_1) + \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} d_{G_1}(a)^{\alpha-i} d_{G_2}(b)^i + n_1 M_1^{\alpha}(G_2) \right] \\ &= (n_1 n_2 - 1) \left[ n_2 M_1^{\alpha}(G_1) + \sum_{i=1}^{\alpha-1} \binom{\alpha}{i} M_1^{\alpha-i}(G_1) M_1^i(G_2) + n_1 M_1^{\alpha}(G_2) \right]. \end{split}$$

Similarly, we obtain

$$B = n_2 M_1^{\alpha+1}(G_1) + \sum_{i=1}^{\alpha} {\alpha+1 \choose i} M_1^{\alpha+1-i}(G_1) M_1^i(G_2) + n_1 M_1^{\alpha+1}(G_2).$$

Subtracting B from A, we get the desired result.

The rectangular grid, the  $C_4$  nanotube  $(TUC_4(r,q))$  and the  $C_4$  nanotorus  $(TC_4(r,q))$  are isomorphic to the Cartesian products  $(P_r \times P_q)$ ,  $(P_r \times C_q)$ , and  $(C_r \times C_q)$  respectively. Thus, as an application we present formulae for the first general Zagreb coindx of these structures and obtained from proposition 8 after certain steps of simplifications.

#### Corollary 4.5.

$$\begin{split} \overline{M}_1^{\alpha}(P_r \times P_q) &= (rq-3)2^{\alpha+2} + (rq-4)(2r+2q-8)3^{\alpha} + (rq-5)(r-2)(q-2)4^{\alpha}.\\ \overline{M}_1^{\alpha}(TUC_4(r,q)) &= q \big[ 2(rq-4)3^{\alpha} + (rq-5)(r-2)4^{\alpha} \big].\\ \overline{M}_1^{\alpha}(TC_4(r,q)) &= 4^{\alpha}rq[rq-5]. \end{split}$$

## 4.4 Tensor product

The tensor product of two graphs  $G_1$  and  $G_2$  is denoted by  $G_1 \otimes G_2$  is the graph with vertex set  $V(G_1) \times V(G_2)$  and any two vertices  $(u_1, u_2)$  and  $(v_1, v_2)$  are adjacent if and only if  $u_1v_1 \in E(G_1)$  and  $u_2v_2 \in E(G_2)$ . Here,  $|V(G_1 \otimes G_2)| = n_1n_2$ .

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**Proposition 9.** Let  $G_i$  (i = 1, 2) be simple graph and  $\alpha \in \mathbb{R}$ . Then

$$\overline{M}_1^{\alpha}(G_1 \otimes G_2) = (n_1 n_2 - 1) M_1^{\alpha}(G_1) M_1^{\alpha}(G_2) - M_1^{\alpha+1}(G_1) M_1^{\alpha+1}(G_2).$$

*Proof.* From the definition of tensor product, the degree of vertex (a,b) of  $G_1 \otimes G_2$  is given by  $d_{G_1 \otimes G_2}(a,b) = d_{G_1}(a)d_{G_2}(b)$ .

By using proposition 1, we have

$$\begin{split} \overline{M}_{1}^{\alpha}(G_{1}\otimes G_{2}) &= \sum_{(a,b)\in V(G_{1}\otimes G_{2})} [n_{1}n_{2}-1-d_{G_{1}\otimes G_{2}}(a,b)]d_{G_{1}\otimes G_{2}}(a,b)^{\alpha} \\ &= \sum_{a\in V(G_{1})} \sum_{b\in V(G_{2})} [n_{1}n_{2}-1-d_{G_{1}}(a)d_{G_{2}}(b)][d_{G_{1}}(a)d_{G_{2}}(b)]^{\alpha} \\ &= \sum_{a\in V(G_{1})} \sum_{b\in V(G_{2})} [(n_{1}n_{2}-1)[d_{G_{1}}(a)d_{G_{2}}(b)]^{\alpha} - [d_{G_{1}}(a)d_{G_{2}}(b)]^{\alpha+1}] \\ &= (n_{1}n_{2}-1) \sum_{a\in V(G_{1})} \sum_{b\in V(G_{2})} [d_{G_{1}}(a)d_{G_{2}}(b)]^{\alpha} - \sum_{a\in V(G_{1})} \sum_{b\in V(G_{2})} [d_{G_{1}}(a)d_{G_{2}}(b)]^{\alpha+1} \\ &= (n_{1}n_{2}-1)M_{1}^{\alpha}(G_{1})M_{1}^{\alpha}(G_{2}) - M_{1}^{\alpha+1}(G_{1})M_{1}^{\alpha+1}(G_{2}). \end{split}$$

Example 2:  $\overline{M}_{1}^{\alpha}(K_{n} \otimes K_{m}) = nm(n-1)^{\alpha}(m-1)^{\alpha}(n+m-2).$   $\overline{M}_{1}^{\alpha}(C_{n} \otimes C_{m}) = nm(nm-5)2^{2\alpha}.$   $\overline{M}_{1}^{\alpha}(C_{n} \otimes K_{m}) = nm(2m-2)^{\alpha}(nm-2m+1).$   $\overline{M}_{1}^{\alpha}(P_{n} \otimes P_{m}) = 4(nm-1)(1+(n-2)2^{k})(1+(m-2)2^{k}) - 4(1+(n-2)^{k+1})(1+(m-2)^{k+1}).$ 

## 4.5 Composition

The composition  $G_1[G_2]$  of graphs  $G_1$  and  $G_2$  with disjoint vertex sets and edge sets is also a graph on the vertex set  $V(G_1) \times V(G_2)$  in which  $u = (u_1, u_2)$  is adjacent with  $v = (v_1, v_2)$  whenever  $[u_1$  is adjacent with  $v_1]$  or  $[u_1 = v_1$  and  $u_2$  is adjacent with  $v_2]$ . The composition is not commutative. The degree of a vertex  $(u_1, u_2)$  of  $G_1[G_2]$  is given by  $d_{G_1[G_2]}(u_1, u_2) = n_2 d_{G_1}(u_1) + d_{G_2}(u_2)$  and it has  $n_1 m_2 + m_1 n_2^2$  number of edges.

**Proposition 10.** Let  $G_i$  (i = 1, 2) be simple graph and  $\alpha \in \mathbb{N}$ . Then

$$\overline{M}_{1}^{\alpha}(G_{1}[G_{2}]) = (n_{1}n_{2}-1)[n_{2}^{\alpha+1}M_{1}^{\alpha}(G_{1}) + \sum_{i=1}^{\alpha-1} {\alpha \choose i} n_{2}^{\alpha-i}M_{1}^{\alpha-i}(G_{1})M_{1}^{i}(G_{2}) + n_{1}M_{1}^{\alpha}(G_{2})] - [n_{2}^{\alpha+2}M_{1}^{\alpha+1}(G_{1}) + \sum_{i=1}^{\alpha} {\alpha+1 \choose i} n_{2}^{\alpha+1-i}M_{1}^{\alpha+1-i}(G_{1})M_{1}^{i}(G_{2}) + n_{1}M_{1}^{\alpha+1}(G_{2})].$$

*Proof.* The proof follows in similar way as in proposition 8 case and we omit it.

As an application we present formulae for the first general Zagreb coindx of open and closed fences,  $P_n[K_2]$  and  $C_n[K_2]$ .

# Corollary 4.6.

$$\overline{M}_{1}^{\alpha}(P_{n}[K_{2}]) = (2n-4)[4 \cdot 3^{\alpha} + (2n-6)5^{\alpha}]$$
$$\overline{M}_{1}^{\alpha}(C_{n}[K_{2}]) = 2n(2n-6)5^{\alpha}.$$

In proposition 18 of [17], the following proposition is stated.

## **Proposition 11.**

$$\overline{M}_1(G_1[G_2]) = 2n_1n_2(n_1m_2 + n_2^2m_1) - 2m_1(n_1 + n_2^2) - 8n_2m_1m_2 - n_2^3M_1(G_1) - n_1M_1(G_2).$$

However, in the above proposition 11, the expression is incorrect. Consider figure below as a counter example.



By proposition 11,  $\overline{M}_1(P_2[P_3]) = 20$ . Where as by definition (2.1) or proposition 1, we obtain  $\overline{M}_1(P_2[P_3]) = 16$  (as it is the first Zagreb coindex we use  $\alpha = 1$ ). Clearly they are not equal. The following corollary gives the correct version of proposition 11 and obtained by substituting  $\alpha = 1$  in proposition 10.

# Corollary 4.7.

$$\overline{M}_{1}^{1}(G_{1}[G_{2}]) = (n_{1}n_{2} - 1)(2n_{2}^{2}m_{1} + 2m_{2}n_{1}) - 8n_{2}m_{1}m_{2} - n_{2}^{3}M_{1}(G_{1}) - n_{1}M_{1}(G_{2}) - n_{2}M_{1}(G_{1}) - n_{1}M_{1}(G_{2}) - n_$$

The following corollary corrects some errors in Corollary 19 of [17].

#### **Corollary 4.8.**

$$\overline{M}_1^1(P_n[K_2]) = 20n^2 - 76n + 72;$$
  
$$\overline{M}_1^1(C_n[K_2]) = 10n(2n - 6).$$

#### **5** Conclusion

In this paper, we have introduced an invariant called the first general Zagreb coindex and studied its basic properties and obtained explicit formula for the values under some graph operations. The results are also applied to find the first general Zagreb coindex of some special and chemically interesting graphs. However, there are still many other graph operations and special classes of graphs which are not covered here. Thus, for further research, the first general Zagreb coindex of other graph operations as well as determining extremal values of the first general Zagreb coindx over various classes of graphs shall be considered. In particular, if  $\alpha = 1$  (resp.  $\alpha = 2$ ) is substituted in all the results of this paper, it gives the first Zagreb coindex (resp. the F-coindex) of those studied graph operations.

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