

Article

Computing Analysis of Connection-Based Indices and Coindices for Product of Molecular Networks

Usman Ali ¹, Muhammad Javaid ^{1,*} and Abdulaziz Mohammed Alanazi ²

¹ Department of Mathematics, School of Science, University of Management and Technology, Lahore 54770, Pakistan; f2017265016@umt.edu.pk

² Department of Mathematics, University of Tabuk, Tabuk 71491, Saudi Arabia; am.alenezi@ut.edu.sa

* Correspondence: javaidmath@gmail.com or javaid@ustc.edu.cn

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Abstract: Gutman and Trinajstić (1972) defined the connection-number based Zagreb indices, where connection number is degree of a vertex at distance two, in order to find the electron energy of alternant hydrocarbons. These indices remain symmetric for the isomorphic (molecular) networks. For the prediction of physicochemical and symmetrical properties of octane isomers, these indices are restudied in 2018. In this paper, first and second Zagreb connection coindices are defined and obtained in the form of upper bounds for the resultant networks in the terms of different indices of their factor networks, where resultant networks are obtained from two networks by the product-related operations, such as cartesian, corona, and lexicographic. For the molecular networks linear polynomial chain, carbon nanotube, alkane, cycloalkane, fence, and closed fence, first and second Zagreb connection coindices are computed in the consequence of the obtained results. An analysis of Zagreb connection indices and coindices on the aforesaid molecular networks is also included with the help of their numerical values and graphical presentations that shows the symmetric behaviour of these indices and coindices with in certain intervals of order and size of the under study (molecular) networks.

Keywords: connection number; Zagreb indices; coindices; product of networks

MSC: 05C12; 05C90; 05C15; 05C62

1. Introduction

Topological indices (TIs) are functions that associate a numeric value with a finite, simple, and undirected network. The various types of TIs are widely used for the studies of the structural and chemical properties of the networks. These are also used in chemo-informatics modelings consisting of quantitative structures activity and property relationships that create a symmetrical link between a biological property and a molecular network. This symmetric relation can be shown mathematically as $\mathbb{P} = \chi(\mathbb{N})$, where \mathbb{P} is an activity or property, \mathbb{N} is a molecular network, and χ is a function that depends upon the molecular network \mathbb{N} , see [1,2]. Moreover, a number of drugs particles and the medical behaviors of the different compounds have established with the help of various TI's in the pharmaceutical industries, see [3]. In particular, the TIs called by connection based Zagreb indices are used to compute the correlation values among various octane isomers, such as acentric factor, connectivity, heat of evaporation, molecular weight, density, critical temperature, and stability, see [4,5].

Operations on networks play an important role to develop the new molecular networks from the old ones that are known as the resultant networks. Graovac et al. [6] was the first who used some operations on networks and computed exact formulae of Wiener index for the resultant networks.

In particular, Cartesian products of P_m & P_2 and C_m & P_2 present the polynomial chain and nanotube ($TUC_4(m, n)$), respectively, alkane (C_3H_8) is the corona product of P_3 and N_3 , cyclobutane (C_4H_8) is the corona product of C_4 and N_2 , and lexicographic products of P_m & P_2 and C_m & P_2 are fence and closed fence, respectively, where P_m , C_m and N_m are path, cycle and null networks of order m respectively. For further study, see [7–13]. Now, we define these operations, as follows:

Definition 1. Cartesian product of two networks G_1 and G_2 is a network $G_1 \times G_2$ with vertex-set: $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and edge-set: $E(G_1 \times G_2) = \{(a_1, b_1)(a_2, b_2); \text{ where } (a_1, b_1), (a_2, b_2) \in V(G_1) \times V(G_2)\}$ and

- Either $[a_1 = a_2 \in V(G_1) \wedge b_1b_2 \in E(G_2)]$ or $[b_1 = b_2 \in V(G_2) \wedge a_1a_2 \in E(G_1)]$. For more detail, see Figure 1.

Definition 2. Corona product ($G_1 \odot G_2$) of two networks G_1 and G_2 is obtained by taking one copy of G_1 and n_1 copies of G_2 (i.e., $\{G_2^i : 1 \leq i \leq n_1\}$) then by joining each vertex of the i th copy of G_2 to the i th vertex of one copy of G_1 , where $1 \leq i \leq n_1$, $|V(G_1 \odot G_2)| = n_1n_2 + n_1$ and $|E(G_1 \odot G_2)| = e_1 + n_1e_2 + n_1n_2$. For more detail, see Figure 2.

Definition 3. Lexicographic product of two networks G_1 and G_2 is a graph $G_1 \cdot G_2$ with vertex-set : $V(G_1 \cdot G_2) = V(G_1) \cdot V(G_2)$ and edge-set : $E(G_1 \cdot G_2) = \{(a_1, b_1)(a_2, b_2); \text{ where } (a_1, b_1), (a_2, b_2) \in V(G_1) \cdot V(G_2)\}$ and

- Either $[a_1 = a_2 \in V(G_1) \wedge b_1b_2 \in E(G_2)]$ or $[b_1, b_2 \in V(G_2) \wedge a_1a_2 \in E(G_1)]$. For more detail, see Figure 3.

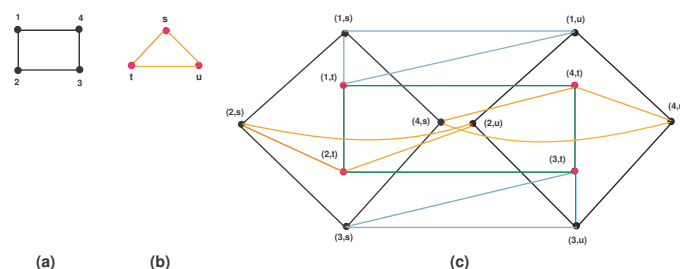


Figure 1. (a) $G_1 \cong C_4$, (b) $G_2 \cong C_3$ and (c) Cartesian Product ($C_4 \times C_3$).

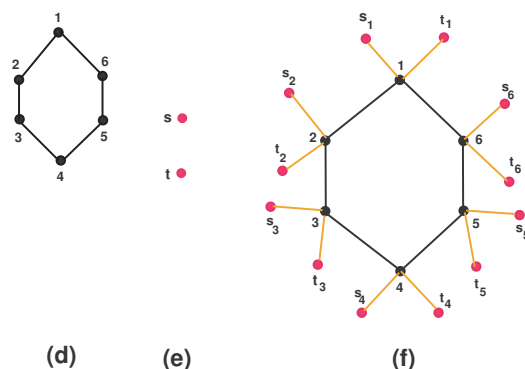


Figure 2. (d) $G_1 \cong C_6$, (e) $G_2 \cong N_2$ and (f) Cyclohexane ($C_6H_{12} = C_6 \odot N_2$).

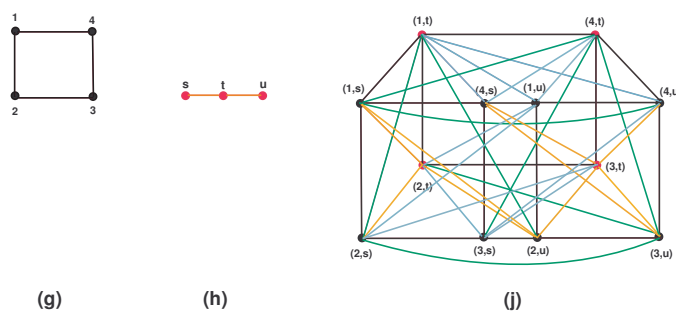


Figure 3. (g) $G_1 \cong C_4$, (h) $G_2 \cong P_3$ and (j) Lexicographic Product ($C_4 \cdot P_3$).

Thus, the theory of networks gives the significant techniques in the field of modern chemistry that is exploited to develop the several types of molecular networks and also predicts their chemical properties. Gutman and Trinajstić [14] defined the first degree-based (number of vertices at distance one) TI called by the first Zagreb index to compute the total π -electron energy of the molecules in molecular networks. There are several TIs in literature but degree-based are studied more than others, see [15]. Recently, Ashrafi et al. [16] defined the concept of coindices associated with the classical Zagreb indices for the resultant networks of different operations. Relations between Zagreb coindices and some distance-based TIs are established in [17]. The multiplicative, first, second, third, and hyper Zagreb coindices with certain properties are defined in [18–23]. Munir et al. [24] found closed relations for M-polynomial of polyhex networks and also computed closed relation for degree-based TIs of networks. Moreover, the various degree-based TIs of different networks, such as icosahedral honey comb, carbon nanotubes, oxide, rhombus type silicate, hexagonal, octahedral, neural, and metal-organic, are computed in [25–29].

In 2018, the concept of connection-based (number of vertices at distance two) TIs is restudied [30]. The origin of these indices can be found in the work of Gutman and Trinajstić [14]. It is found that the correlation values for the various physicochemical and symmetrical properties of the octane isomers measured by Zagreb connection indices are better than the classical Zagreb indices. Ali and Javaid [31] computed the formulae for Zagreb connection indices of disjunction and symmetric difference operations on networks. For further studies of these indices on acyclic (alkane), unicycle, product, subdivided, and semi-total point networks, we refer to [32–37].

In this paper, we compute the coindices associated with the first and second Zagreb connection indices of the resultant networks as upper bounds in the terms of their factor networks, where resultant networks are obtained by Cartesian, corona and lexicographic products of two networks. As the consequences of these results, first and second Zagreb connection coindices of the linear polynomial chain, carbon nanotube, alkane, cyclobutane, fence, and closed fence networks are also obtained. Moreover, at the end, an analysis of connection-based Zagreb indices and coindices on the aforesaid molecular networks is included with the help of their numerical values and graphical presentations.

Moreover, in this note, Section 2 represents the preliminaries and some important lemmas, Section 3 covers the few molecular networks, Section 4 contains the main results of product based networks, and Section 5 includes the applications, comparisons, and conclusions.

2. Preliminaries

For the vertex set $V(G)$ and edge set $E(G) \subseteq V(G) \times V(G)$, we present a simple and undirected (molecular) network by $G = (V(G), E(G))$, such that $|V(G)|$ and $|E(G)|$ are order and size of G , respectively. A network denoted by N is called null if it has at least exactly one vertex and there exists no edge. A null network becomes trivial if it has one vertex. The complement of a network G is denoted by \bar{G} . It is also simple with same vertex set as of G , but edge set is defined as $E(\bar{G}) = \{ab : a, b \in V(G) \wedge ab \notin E(G)\}$, thus $E(G) \cup E(\bar{G}) = E(K_n)$, where K_n is a complete network of order n and size $|E(K_n)| = \binom{n}{2}$. Moreover, if $|E(G)| = e$, then $|E(\bar{G})| = \binom{n}{2} - e = \mu$ and $d_{\bar{G}}(b) = n - 1 - d_G(b)$, where $d_G(b)$ and $d_{\bar{G}}(b)$ are the degrees of the vertex b in G and \bar{G} , respectively. In addition, we assume that

$\tau_G(b)$ denotes the connection number (number of vertices at distance 2) of the vertex b in G (distance between two vertices is number of edges of the shortest path between them).

Now, throughout the paper, for two networks G_1 and G_2 , we assume that $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, $|E(G_1)| = e_1$ and $|E(G_2)| = e_2$. Finally, it is important to note that Zagreb connection coindices of G are not Zagreb connection indices of \bar{G} , because the connection number works according to G . For further basic terminologies, see [38].

Definition 4. For a (molecular) network G , the first Zagreb index ($M_1(G)$) and second Zagreb index ($M_2(G)$) are defined as

$$M_1(G) = \sum_{ab \in E(G)} [d_G(a) + d_G(b)] \quad \text{and} \quad M_2(G) = \sum_{ab \in E(G)} [d_G(a) \times d_G(b)].$$

Gutman, Trinajstić, and Ruscic [14,39] defined these indices to predict better outcomes of the various parameters related to the molecular networks, such as chirality, complexity, entropy, heat energy, ZE-isomerism, heat capacity, absolute value of correlation coefficient, chromatographic, retention times in chromatographic, pH, and molar ratio, see [4,14,29,40]. The connection-based TIs are discussed, as follows:

Definition 5. For a (molecular) network G , the modified first Zagreb connection index ($ZC_1^*(G)$) and second Zagreb connection index ($ZC_2(G)$) are defined as

$$ZC_1^*(G) = \sum_{ab \in E(G)} [\tau_G(a) + \tau_G(b)] \quad \text{and} \quad ZC_2(G) = \sum_{ab \in E(G)} [\tau_G(a) \times \tau_G(b)].$$

Definition 6. For a (molecular) network G , the first Zagreb coindex ($\bar{M}_1(G)$) and second Zagreb coindex ($\bar{M}_2(G)$) are defined as

$$\bar{M}_1(G) = \sum_{ab \notin E(G)} [d_G(a) + d_G(b)] \quad \text{and} \quad \bar{M}_2(G) = \sum_{ab \notin E(G)} [d_G(a) \times d_G(b)].$$

These coindices that are associated with the degree-based classical Zagreb indices are defined by Ashrafi et al. see [16]. The coindices associated with the Zagreb connection indices are defined in Definition 7.

Definition 7. For a (molecular) network G , the first Zagreb connection coindex ($\bar{Z}C_1(G)$) and second Zagreb connection coindex ($\bar{Z}C_2(G)$) are defined as

$$\bar{Z}C_1(G) = \sum_{ab \notin E(G)} [\tau_G(a) + \tau_G(b)] \quad \text{and} \quad \bar{Z}C_2(G) = \sum_{ab \notin E(G)} [\tau_G(a) \times \tau_G(b)].$$

The degree/connection based coindices defined in Definitions 6 and 7 study the various physicochemical and isomer properties of molecules on the bases of the adjacency and non-adjacency pairs of vertices in the molecular networks. For more detail, see [16,30,36,41].

Now, we present some important results that are used in the main results.

Lemma 1 (see [42]). Let G be a connected network with n vertices and e edges. Subsequently, $\tau_G(a) + d_G(a) \leq \sum_{b \in N_G(a)} d_G(b)$, where equality holds if and only if G is a $\{C_3, C_4\}$ -free network.

Lemma 2 (see [38]). Let G be a connected network with n vertices and e edges. Afterwards, $\sum_{b \in V(G)} d_G(b) = 2e$.

Lemma 3 (see [36]). Let G be a connected network with n vertices and e edges. Subsequently, $\sum_{b \in V(G)} \tau_G(b) \leq M_1(G) - 2e$, where equality holds iff G is a $\{C_3, C_4\}$ -free network.

3. A Few Molecular Networks

In this section, we define a few molecular networks, as follows:

- Alkanes (hydrocarbon compounds) are organic compounds consisting of carbon atoms joined by single bounds. The simple and Lewis networks of alkanes are given in Figure 4. Moreover, methane (CH_4), ethane ($H_3C - CH_3$), and propane ($H_3C - CH_2 - CH_3$) are examples of alkanes that are given in Figure 5. This alkane series continues and follows general formula as C_nH_{2n+2} .
- Cyclic compounds are molecules consisting of closed chain (ring) of at least three carbon atoms. If the closed chain has only carbon atoms, then it is an organic cyclic molecule that is called by homocyclic compound. If the closed chain has both carbon and non-carbon atoms, then it is an inorganic cyclic molecule that is called the heterocyclic compound. Moreover, Cycloalkanes (C_nH_{2n}) are the isomers of alkenes consisting of exactly one cyclic compound joined by a single bond. Figure 6a,b presents the cyclic compounds (homocyclic and heterocyclic, respectively).

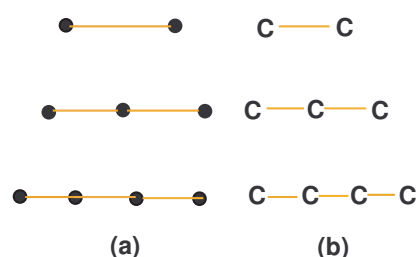


Figure 4. (a) P_2, P_3, P_4 are simple networks of alkanes and (b) P_2, P_3, P_4 are Lewis networks of alkanes.

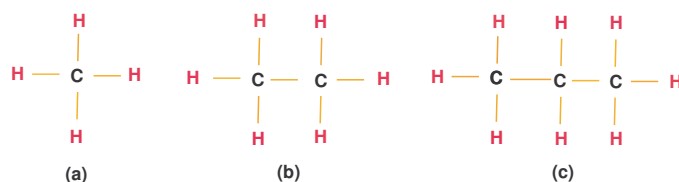


Figure 5. Lewis network of (a) Methane, (b) Ethane and (c) Propane.

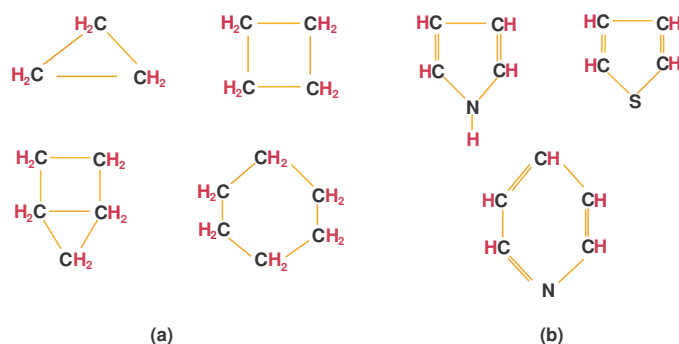


Figure 6. (a) The Lewis network of cyclopropane, cyclobutane, cyclopentane, and cyclohexane, (b) The Lewis network of pyrrole, thiophene, and pyridine.

4. Main Results

The first Zagreb connection coindex ($\bar{Z}C_1$) and second Zagreb connection coindex ($\bar{Z}C_2$) of the product based networks obtained under the operations of Cartesian product, corona product and lexicographic product are studied in third section.

Theorem 1. Let G_1 and G_2 be two networks. Then, $\bar{Z}C_1$ and $\bar{Z}C_2$ of the Cartesian product $G_1 \times G_2$ are

$$(a) \bar{Z}C_1(G_1 \times G_2) \leq n_2 \bar{Z}C_1(G_1) + n_1 \bar{Z}C_1(G_2) + 2e_2 \bar{M}_1(G_1) + 2e_1 \bar{M}_1(G_2) + 2\mu_2[M_1(G_1) - 2e_1] + 2\mu_1[M_1(G_2) - 2e_2],$$

$$(b) \bar{Z}C_2(G_1 \times G_2) \leq \bar{Z}C_1(G_1)[M_1(G_2) - 2e_2] + \bar{Z}C_1(G_2)[M_1(G_1) - 2e_1] + ZC_1(G_1)\bar{M}_1(G_2) + ZC_1(G_2)\bar{M}_1(G_1) + n_2 \bar{Z}C_2(G_1) + n_1 \bar{Z}C_2(G_2) + \mu_2 ZC_1(G_1) + \mu_1 ZC_1(G_2) + M_1(G_1)\bar{M}_1(G_2) + 2e_2 \bar{M}_1(G_1) + 2e_1 \sum_{a_1 a_2 \notin E(G_1)} [d_{G_1}(a_1)\tau_{G_1}(a_2) + d_{G_1}(a_2)\tau_{G_1}(a_1)] + 2e_1 \sum_{b_1 b_2 \notin E(G_2)} [d_{G_2}(b_1)\tau_{G_2}(b_2) + d_{G_2}(b_2)\tau_{G_2}(b_1)].$$

where equality holds iff $G_1 \times G_2$ is a $\{C_3, C_4\}$ -free network.

Proof. (a). For $a \in V(G_1)$, $b \in V(G_2)$ and $(a, b) \in V(G_1 \times G_2)$, we have, $\tau_{G_1 \times G_2}(a, b) = \tau_{G_1}(a) + d_{G_1}(a)d_{G_2}(b) + \tau_{G_2}(b)$.

$$\begin{aligned} \bar{Z}C_1(G_1 \times G_2) &= \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \times G_2)} [\tau_{G_1 \times G_2}(a_1, b_1) + \tau_{G_1 \times G_2}(a_2, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \times G_2}(a, b_1) + \tau_{G_1 \times G_2}(a, b_2)] + \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \times G_2}(a_1, b) + \tau_{G_1 \times G_2}(a_2, b)] \end{aligned}$$

Taking

$$\begin{aligned} &\sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \times G_2}(a, b_1) + \tau_{G_1 \times G_2}(a, b_2)] \\ &\leq \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\{\tau_{G_1}(a) + d_{G_1}(a)d_{G_2}(b_1) + \tau_{G_2}(b_1)\} + \{\tau_{G_1}(a) + d_{G_1}(a)d_{G_2}(b_2) + \tau_{G_2}(b_2)\}] \\ &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [2\tau_{G_1}(a) + d_{G_1}(a)\{d_{G_2}(b_1) + d_{G_2}(b_2)\} + \{\tau_{G_2}(b_1) + \tau_{G_2}(b_2)\}] \\ &= 2\mu_2[M_1(G_1) - 2e_1] + 2e_1 \bar{M}_1(G_2) + n_1 \bar{Z}C_1(G_2). \end{aligned}$$

Also taking

$$\begin{aligned} &\sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \times G_2}(a_1, b) + \tau_{G_1 \times G_2}(a_2, b)] \\ &\leq \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\{\tau_{G_1}(a_1) + d_{G_1}(a_1)d_{G_2}(b) + \tau_{G_2}(b)\} + \{\tau_{G_1}(a_2) + d_{G_1}(a_2)d_{G_2}(b) + \tau_{G_2}(b)\}] \\ &= n_2 \bar{Z}C_1(G_1) + 2e_2 \bar{M}_1(G_1) + 2\mu_1[M_1(G_2) - 2e_2]. \end{aligned}$$

Consequently,

$$\bar{Z}C_1(G_1 \times G_2) \leq n_2 \bar{Z}C_1(G_1) + n_1 \bar{Z}C_1(G_2) + 2e_2 \bar{M}_1(G_1) + 2e_1 \bar{M}_1(G_2) + 2\mu_2[M_1(G_1) - 2e_1] + 2\mu_1[M_1(G_2) - 2e_2].$$

(b).

$$\begin{aligned} \bar{Z}C_2(G_1 \times G_2) &= \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \times G_2)} [\tau_{G_1 \times G_2}(a_1, b_1) \times \tau_{G_1 \times G_2}(a_2, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \times G_2}(a, b_1) \times \tau_{G_1 \times G_2}(a, b_2)] + \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \times G_2}(a_1, b) \times \tau_{G_1 \times G_2}(a_2, b)] \end{aligned}$$

Taking

$$\begin{aligned} & \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \times G_2}(a, b_1) \times \tau_{G_1 \times G_2}(a, b_2)] \\ & \leq \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\{\tau_{G_1}(a) + d_{G_1}(a)d_{G_2}(b_1) + \tau_{G_2}(b_1)\} \times \{\tau_{G_1}(a) + d_{G_1}(a)d_{G_2}(b_2) + \tau_{G_2}(b_2)\}] \\ & = \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1}^2(a) + \tau_{G_1}(a)d_{G_1}(a)d_{G_2}(b_2) + \tau_{G_1}(a)\tau_{G_2}(b_2) + d_{G_1}(a)d_{G_2}(b_1)\tau_{G_1}(a) + d_{G_1}(a)d_{G_2}(b_1) \end{aligned}$$

$$d_{G_1}(a)d_{G_2}(b_2) + d_{G_1}(a)d_{G_2}(b_1)\tau_{G_2}(b_2) + \tau_{G_2}(b_1)\tau_{G_1}(a) + \tau_{G_2}(b_1)d_{G_1}(a)d_{G_2}(b_2) + \tau_{G_1}(b_1)\tau_{G_2}(b_2)]$$

We know that, $\sum_{b_1 b_2 \notin E(G_2)} = \binom{n_2}{2} - e_2 = \mu_2$

$$= \mu_2 ZC_1(G_1) + ZC_1(G_1)\bar{M}_1(G_2) + \bar{Z}C_1(G_2)[M_1(G_1) - 2e_1] + M_1(G_1)\bar{M}_1(G_2) + 2e_1 \sum_{b_1 b_2 \notin E(G_2)}$$

$$[d_{G_2}(b_1)\tau_{G_2}(b_2) + d_{G_2}(b_2)\tau_{G_2}(b_1)] + n_1 \bar{Z}C_2(G_2).$$

Also taking

$$\begin{aligned} & \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \times G_2}(a_1, b) \times \tau_{G_1 \times G_2}(a_2, b)] \\ & \leq \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\{\tau_{G_1}(a_1) + d_{G_1}(a_1)d_{G_2}(b) + \tau_{G_2}(b)\} \times \{\tau_{G_1}(a_2) + d_{G_1}(a_2)d_{G_2}(b) + \tau_{G_2}(b)\}] \end{aligned}$$

We know that, $\sum_{a_1 a_2 \notin E(G_1)} = \binom{n_1}{2} - e_1 = \mu_1$

$$= n_2 \bar{Z}C_2(G_1) + 2e_2 \sum_{a_1 a_2 \notin E(G_1)} [d_{G_1}(a_1)\tau_{G_1}(a_2) + d_{G_1}(a_2)\tau_{G_1}(a_1)] + \bar{Z}C_1(G_1)[M_1(G_2) - 2e_2]$$

$$+ 2e_2 \bar{M}_1(G_1) + \bar{M}_1(G_1)ZC_1^*(G_2) + \mu_1 ZC_1(G_2).$$

Consequently,

$$\bar{Z}C_2(G_1 \times G_2) \leq \bar{Z}C_1(G_1)[M_1(G_2) - 2e_2] + \bar{Z}C_1(G_2)[M_1(G_1) - 2e_1] + ZC_1(G_1)\bar{M}_1(G_2) + ZC_1(G_2)$$

$$\bar{M}_1(G_1) + n_2 \bar{Z}C_2(G_1) + n_1 \bar{Z}C_2(G_2) + \mu_2 ZC_1(G_1) + \mu_1 ZC_1(G_2) + M_1(G_1)\bar{M}_1(G_2) + 2e_2 \bar{M}_1(G_1)$$

$$+ 2e_2 \sum_{a_1 a_2 \notin E(G_1)} [d_{G_1}(a_1)\tau_{G_1}(a_2) + d_{G_1}(a_2)\tau_{G_1}(a_1)] + 2e_1 \sum_{b_1 b_2 \notin E(G_2)} [d_{G_2}(b_1)\tau_{G_2}(b_2) + d_{G_2}(b_2)\tau_{G_2}(b_1)].$$

□

Theorem 2. Let G_1 and G_2 be two networks. Subsequently, $\bar{Z}C_1$ and $\bar{Z}C_2$ of the corona product $G_1 \odot G_2$ are

(a) $\bar{Z}C_1(G_1 \odot G_2) \leq \bar{Z}C_1(G_1) + n_2 \bar{M}_1(G_1) - n_1 \bar{M}_1(G_2) + 2\mu_2[n_1(n_2 - 1) + 2e_1],$

(b) $\bar{Z}C_2(G_1 \odot G_2) \leq \bar{Z}C_2(G_1) + n_2^2 \bar{M}_2(G_1) + n_1 \bar{M}_2(G_2) - n_1(n_2 - 1)\bar{M}_1(G_2) - 2e_1 \bar{M}_1(G_2) + \mu_2 M_1(G_1) + (n_2 - 1)\mu_2[n_1(n_2 - 1) + 4e_1] + n_2 \sum_{ab \notin E(G_1)} [d_{G_1}(a)\tau_{G_1}(b) + d_{G_1}(b)\tau_{G_1}(a)].$

where equality holds iff $G_1 \odot G_2$ is a $\{C_3, C_4\}$ -free network.

Proof. (a). For $b \in V(G_1 \odot G_2)$ either $b \in V(G_1)$ or $b \in V(G_2^i)$, where $1 \leq i \leq n_1$.

Case (I): If $b \in V(G_1)$, then $\tau_{G_1 \odot G_2}(b) = \tau_{G_1}(b) + n_2 d_{G_1}(b)$.

Case (II): If $b \in V(G_2^i)$, then $\tau_{G_1 \odot G_2}(b) = (n_2 - 1) - d_{G_2^i}(b) + d_{G_1}(b_i)$.

$$\begin{aligned} \bar{Z}C_1(G_1 \odot G_2) &= \sum_{ab \notin E(G_1 \odot G_2)} [\tau_{(G_1 \odot G_2)}(a) + \tau_{(G_1 \odot G_2)}(b)] \\ &= \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_1)}} [\tau_{G_1}(a) + \tau_{G_1}(b)] + \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_2)}} [\tau_{G_2}(a) + \tau_{G_2}(b)] + \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a \in V(G_1) \wedge b \in V(G_2)}} [\tau_{G_1}(a) + \tau_{G_2}(b)]. \end{aligned}$$

Taking

$$\begin{aligned} &\sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_1)}} [\tau_{G_1}(a) + \tau_{G_1}(b)] \\ &\leq \sum_{ab \notin E(G_1)} [\{\tau_{G_1}(a) + n_2 d_{G_1}(a)\} + \{\tau_{G_1}(b) + n_2 d_{G_1}(b)\}] \\ &= \sum_{ab \notin E(G_1)} [\{\tau_{G_1}(a) + \tau_{G_1}(b)\} + n_2 \{d_{G_1}(a) + d_{G_1}(b)\}] = \bar{Z}C_1(G_1) + n_2 \bar{M}_1(G_1). \end{aligned}$$

Also taking

$$\begin{aligned} &\sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_2)}} [\tau_{G_2}(a) + \tau_{G_2}(b)] \\ &= \sum_{i=1}^{n_1} \sum_{ab \notin E(G_2^i)} [\{(n_2 - 1) - d_{G_2^i}(a) + d_{G_1}(b_i)\} + \{(n_2 - 1) - d_{G_2^i}(b) + d_{G_1}(b_i)\}] \\ &= 2n_1(n_2 - 1)\mu_2 - n_1 \bar{M}_1(G_2) + 4e_1 \mu_2. \end{aligned}$$

Consequently,

$$\bar{Z}C_1(G_1 \odot G_2) \leq \bar{Z}C_1(G_1) + n_2 \bar{M}_1(G_1) - n_1 \bar{M}_1(G_2) + 2\mu_2[n_1(n_2 - 1) + 2e_1].$$

(b).

$$\begin{aligned} \bar{Z}C_2(G_1 \odot G_2) &\leq \sum_{ab \notin E(G_1 \odot G_2)} [\tau_{(G_1 \odot G_2)}(a) \times \tau_{(G_1 \odot G_2)}(b)] \\ &= \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_1)}} [\tau_{G_1}(a) \times \tau_{G_1}(b)] + \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_2)}} [\tau_{G_2}(a) \times \tau_{G_2}(b)] + \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a \in V(G_1) \wedge b \in V(G_2)}} [\tau_{G_1}(a) \times \tau_{G_2}(b)]. \end{aligned}$$

Taking

$$\begin{aligned} &\sum_{\substack{uv \notin E(G_1 \odot G_2) \\ a, b \in V(G_1)}} [\tau_{G_1}(a) \times \tau_{G_1}(b)] \\ &\leq \sum_{ab \notin E(G_1)} [\{\tau_{G_1}(a) + n_2 d_{G_1}(a)\} \times \{\tau_{G_1}(b) + n_2 d_{G_1}(b)\}] \\ &= \bar{Z}C_2(G_1) + n_2^2 \bar{M}_2(G_1) + n_2 \sum_{ab \notin E(G_1)} [d_{G_1}(a) \tau_{G_1}(b) + d_{G_1}(b) \tau_{G_1}(a)]. \end{aligned}$$

Also taking

$$\sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a, b \in V(G_2)}} [\tau_{G_2}(a) \times \tau_{G_2}(b)]$$

$$\leq \sum_{i=1}^{n_1} \sum_{ab \notin E(G_2^i)} [\{(n_2 - 1) - d_{G_2^i}(a) + d_{G_1}(b_i)\} \times \{(n_2 - 1) - d_{G_2^i}(b) + d_{G_1}(b_i)\}]$$

We know that, $\sum_{ab \notin E(G_2^i)} = \binom{n_2}{2} - e_2 = \mu_2$ (Say)

$$= n_1(n_2 - 1)^2\mu_2 - n_1(n_2 - 1)\bar{M}_1(G_2) + 4(n_2 - 1)e_1\mu_2 + n_1\bar{M}_2(G_2) - 2e_1\bar{M}_1(G_2) + \mu_2 M_1(G_1).$$

Again taking (Null case)

$$N = \sum_{\substack{ab \notin E(G_1 \odot G_2) \\ a \in V(G_1) \wedge b \in V(G_2)}} [\tau_{G_1}(a) \times \tau_{G_2}(b)] = 0.$$

Consequently,

$$\bar{Z}C_2(G_1 \odot G_2) \leq \bar{Z}C_2(G_1) + n_2^2\bar{M}_2(G_1) + n_1\bar{M}_2(G_2) - n_1(n_2 - 1)\bar{M}_1(G_2) - 2e_1\bar{M}_1(G_2) + \mu_2 M_1(G_1)$$

$$+ (n_2 - 1)\mu_2[n_1(n_2 - 1) + 4e_1] + n_2 \sum_{ab \notin E(G_1)} [d_{G_1}(a)\tau_{G_1}(b) + d_{G_1}(b)\tau_{G_1}(a)].$$

□

Theorem 3. Let G_1 and G_2 be networks. Subsequently, $\bar{Z}C_1$ and $\bar{Z}C_2$ of the lexicographic product $G_1 \cdot G_2$ are

$$(a) \bar{Z}C_1(G_1 \cdot G_2) \leq n_2(n_2 + 2\mu_2)\bar{Z}C_1(G_1) - 2\mu_1\bar{M}_2(G_2) - n_1\bar{M}_1(G_2) + 2n_2\mu_2[M_1(G_1) - 2e_1] + 2(n_2 - 1)$$

$$\mu_2(n_1 + 2\mu_1) + 2\mu_1[n_2(n_2 - 1) - 2e_2],$$

$$(b) \bar{Z}C_2(G_1 \cdot G_2) \leq n_2[n_2(n_2 - 1) - 2e_2 + 2(n_2 - 1)\mu_2]\bar{Z}C_1(G_1) + n_2^2(n_2 + 2\mu_2)\bar{Z}C_2(G_1) + n_2^2\mu_2 ZC_1(G_1)$$

$$+ (n_1 + 2\mu_1)\bar{M}_2(G_2) - [n_2(M_1(G_1) - 2e_1) + n_1(n_2 - 1) + 2(n_2 - 1)\mu_1]\bar{M}_1(G_2) + \mu_1 M_1(G_2) + 2n_2(n_2 - 1)$$

$$\mu_2[M_1(G_1) - 2e_1] + (n_2 - 1)^2\mu_2(n_1 + 2\mu_1) + (n_2 - 1)\mu_1[n_2(n_2 - 1) - 4e_2] - 2n_2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}}$$

$$[d_{G_2}(b_1)\tau_{G_1}(a_2) + d_{G_2}(b_2)\tau_{G_1}(a_1)].$$

where equality holds iff $G_1[G_2]$ is a $\{C_3, C_4\}$ -free network.

Proof. (a). For $a \in V(G_1)$, $b \in V(G_2)$ and $(a, b) \in V(G_1 \cdot G_2)$, we have $\tau_{G_1[G_2]}(a, b) = n_2\tau_{G_1}(a) + d_{G_2}(b) = n_2\tau_{G_1}(a) + (n_2 - 1) - d_{G_2}(b)$.

$$\bar{Z}C_1(G_1 \cdot G_2) = \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \cdot G_2)} [\tau_{G_1 \cdot G_2}(a_1, b_1) + \tau_{G_1 \cdot G_2}(a_2, b_2)]$$

$$= \sum_{a \in V(G_1)} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ a_1 = a_2}} [\tau_{G_1 \cdot G_2}(a, b_1) + \tau_{G_1 \cdot G_2}(a, b_2)] + \sum_{b \in V(G_2)} \sum_{\substack{a_1 a_2 \notin E(G_1) \\ b_1 = b_2}} [\tau_{G_1 \cdot G_2}(a_1, b) + \tau_{G_1 \cdot G_2}(a_2, b)]$$

$$+ \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) + \tau_{G_1 \cdot G_2}(a_2, b_2)] + \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \text{ not parallel } b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) + \tau_{G_1 \cdot G_2}(a_2, b_2)]$$

Taking

$$\begin{aligned} & \sum_{a \in V(G_1)} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ a_1 = a_2}} [\tau_{G_1 \cdot G_2}(a, b_1) + \tau_{G_1 \cdot G_2}(a, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ a_1 = a_2}} [\{n_2 \tau_{G_1}(a) + (n_2 - 1) - d_{G_2}(b_1)\} + \{n_2 \tau_{G_1}(a) + (n_2 - 1) - d_{G_2}(b_2)\}] \\ &= 2n_2 \mu_2 [M_1(G_1) - 2e_1] + 2n_1(n_2 - 1)\mu_2 - n_1 \bar{M}_1(G_2). \end{aligned}$$

Also taking

$$\begin{aligned} & \sum_{b \in V(G_2)} \sum_{\substack{a_1 a_2 \notin E(G_1) \\ b_1 = b_2}} [\tau_{G_1 \cdot G_2}(a_1, b) + \tau_{G_1 \cdot G_2}(a_2, b)] \\ &= \sum_{b \in V(G_2)} \sum_{\substack{a_1 a_2 \notin E(G_1) \\ b_1 = b_2}} [\{n_2 \tau_{G_1}(a_1) + (n_2 - 1) - d_{G_2}(b)\} + \{n_2 \tau_{G_1}(a_2) + (n_2 - 1) - d_{G_2}(b)\}] \\ &= n_2^2 \bar{Z}C_1(G_1) + 2n_2(n_2 - 1)\mu_1 - 4e_2 \mu_1. \end{aligned}$$

Again taking

$$\begin{aligned} & \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) + \tau_{G_1 \cdot G_2}(a_2, b_2)] \\ &\leq 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\{n_2 \tau_{G_1}(a_1) + (n_2 - 1) - d_{G_2}(b_1)\} + \{n_2 \tau_{G_1}(a_2) + (n_2 - 1) - d_{G_2}(b_2)\}] \\ &= 2n_2 \mu_2 \bar{Z}C_1(G_1) + 4(n_2 - 1)\mu_1 \mu_2 - 2\mu_1 \bar{M}_2(G_2). \end{aligned}$$

Further taking (Null case)

$$N = \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \text{ not parallel } b_2}} [\tau_{G_1[G_2]}(a_1, b_1) + \tau_{G_1[G_2]}(a_2, b_2)] = 0.$$

Consequently,

$$\begin{aligned} \bar{Z}C_1(G_1 \cdot G_2) &\leq n_2(n_2 + 2\mu_2) \bar{Z}C_1(G_1) - 2\mu_1 \bar{M}_2(G_2) - n_1 \bar{M}_1(G_2) + 2n_2 \mu_2 [M_1(G_1) - 2e_1] + 2(n_2 - 1) \\ &\mu_2(n_1 + 2\mu_1) + 2\mu_1 [n_2(n_2 - 1) - 2e_2]. \end{aligned}$$

(b).

$$\begin{aligned} \bar{Z}C_2(G_1 \cdot G_2) &= \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \cdot G_2)} [\tau_{G_1 \cdot G_2}(a_1, b_1) \times \tau_{G_1 \cdot G_2}(a_2, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ a_1 = a_2}} [\tau_{G_1 \cdot G_2}(a, b_1) \times \tau_{G_1 \cdot G_2}(a, b_2)] + \sum_{b \in V(G_2)} \sum_{\substack{a_1 a_2 \notin E(G_1) \\ b_1 = b_2}} [\tau_{G_1 \cdot G_2}(a_1, b) \times \tau_{G_1 \cdot G_2}(a_2, b)] \end{aligned}$$

$$+ \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) \times \tau_{G_1 \cdot G_2}(a_2, b_2)] + \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \text{ not parallel } b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) \times \tau_{G_1 \cdot G_2}(a_2, b_2)]$$

Taking

$$\begin{aligned} & \sum_{a \in V(G_1)} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ a_1 = a_2}} [\tau_{G_1 \cdot G_2}(a, b_1) \times \tau_{G_1 \cdot G_2}(a, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ a_1 = a_2}} [\{n_2 \tau_{G_1}(a) + (n_2 - 1) - d_{G_2}(b_1)\} \times \{n_2 \tau_{G_1}(a) + (n_2 - 1) - d_{G_2}(b_2)\}] \\ &= n_2^2 \mu_2 ZC_1(G_1) + 2n_2(n_2 - 1)\mu_2 [M_1(G_1) - 2e_1] - n_2 \bar{M}_1(G_2) [M_1(G_1) - 2e_1] + n_1(n_2 - 1)^2 \mu_2 \\ & \quad - n_1(n_2 - 1) \bar{M}_1(G_2) + n_1 \bar{M}_2(G_2). \end{aligned}$$

Also taking

$$\begin{aligned} & \sum_{b \in V(G_2)} \sum_{\substack{a_1 a_2 \notin E(G_1) \\ b_1 = b_2}} [\tau_{G_1 \cdot G_2}(a_1, b) \times \tau_{G_1 \cdot G_2}(a_2, b)] \\ & \leq \sum_{b \in V(G_2)} \sum_{\substack{a_1 a_2 \notin E(G_1) \\ b_1 = b_2}} [\{n_2 \tau_{G_1}(a_1) + (n_2 - 1) - d_{G_2}(b)\} \times \{n_2 \tau_{G_1}(a_2) + (n_2 - 1) - d_{G_2}(b)\}] \\ &= n_2^3 \bar{Z}C_2(G_1) + n_2^2(n_2 - 1) \bar{Z}C_1(G_1) - 2n_2 e_2 \bar{Z}C_1(G_1) + n_2(n_2 - 1)^2 \mu_1 - 4(n_2 - 1)e_2 \mu_1 + \mu_1 M_1(G_2). \end{aligned}$$

Again taking

$$\begin{aligned} & \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) \times \tau_{G_1 \cdot G_2}(a_2, b_2)] \\ &= 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\{n_2 \tau_{G_1}(a_1) + (n_2 - 1) - d_{G_2}(b_1)\} \times \{n_2 \tau_{G_1}(a_2) + (n_2 - 1) - d_{G_2}(b_2)\}] \\ &= 2n_2^2 \mu_2 \bar{Z}C_2(G_1) + 2n_2(n_2 - 1)\mu_2 \bar{Z}C_1^*(G_1) - 2n_2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [d_{G_2}(b_1) \tau_{G_1}(a_2) \\ & \quad + d_{G_2}(b_2) \tau_{G_1}(a_1)] + 2(n_2 - 1)^2 \mu_1 \mu_2 - 2(n_2 - 1)\mu_1 \bar{M}_1(G_2) + 2\mu_1 \bar{M}_2(G_2). \end{aligned}$$

Further taking (Null case)

$$N = \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \text{ not parallel } b_2}} [\tau_{G_1 \cdot G_2}(a_1, b_1) \times \tau_{G_1 \cdot G_2}(a_2, b_2)] = 0.$$

Consequently,

$$\begin{aligned} \bar{Z}C_2(G_1 \cdot G_2) & \leq n_2[n_2(n_2 - 1) - 2e_2 + 2(n_2 - 1)\mu_2] \bar{Z}C_1(G_1) + n_2^2(n_2 + 2\mu_2) \bar{Z}C_2(G_1) + n_2^2 \mu_2 ZC_1(G_1) \\ & \quad + (n_1 + 2\mu_1) \bar{M}_2(G_2) - [n_2(M_1(G_1) - 2e_1) + n_1(n_2 - 1) + 2(n_2 - 1)\mu_1] \bar{M}_1(G_2) + \mu_1 M_1(G_2) + 2n_2(n_2 - 1) \\ & \quad \mu_2 [M_1(G_1) - 2e_1] + (n_2 - 1)^2 \mu_2 (n_1 + 2\mu_1) + (n_2 - 1)\mu_1 [n_2(n_2 - 1) - 4e_2] - 2n_2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} \end{aligned}$$

$$[d_{G_2}(b_1)\tau_{G_1}(a_2) + d_{G_2}(b_2)\tau_{G_1}(a_1)].$$

□

5. Applications, Comparisons and Conclusions

In this section, we compute Zagreb connection coindices ($\bar{Z}C_1, \bar{Z}C_2$) for the particular molecular networks, such as carbon nanotube, linear polynomial chain, alkane, cyclobutane, fence, and closed fence (see Figures 7–9, 11, 13, 15, and 17) as the consequence of the main results obtained in Section 4. We also construct the Tables 1–6 with the help of the numerical values of Zagreb connection coindices ($\bar{Z}C_1, \bar{Z}C_2$) and Zagreb connection indices (ZC_1^*, ZC_2) for the aforesaid molecular networks. The graphical presentations of the Zagreb connection coindices ($\bar{Z}C_1, \bar{Z}C_2$) and Zagreb connection indices (ZC_1^*, ZC_2) for these molecular networks are also presented in Figures 8, 10, 12, 14, 16, and 18. Assume that N_2 & N_3 be two null networks (with order 2 & 3), P_2, P_3, P_4 & P_6 be four particular alkanes called by paths (with order 2, 3, 4, & 6) and C_4, C_5 & C_6 be cycles (with order 4, 5, & 6).

5.1. Cartesian Product

(1) Polynomial chains: Let P_m and P_n be two particular path- alkanes, then the polynomial chains ($P_m \times P_n$) are obtained by the Cartesian product of P_m and P_n . For $m = 6$ and $n = 2$, see Figure 7.

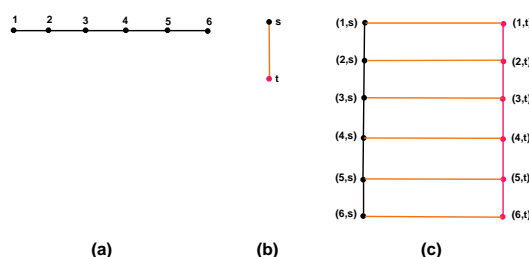


Figure 7. (a) $H_1 \cong P_6$ (b) $H_2 \cong P_2$ & (c) Polynomial chain ($P_6 \times P_2$).

Using Theorem 1, Zagreb connection coindices ($\bar{Z}C_1$ and $\bar{Z}C_2$) of polynomial chains are obtained, as follows:

- (a) $\bar{Z}C_1(P_m \times P_n) \leq 2m^2n + 2mn^2 - 4m^2 - 4n^2 + 8m + 34n - 32,$
 (b) $\bar{Z}C_2(P_m \times P_n) \leq 2mn^2 - 6n^2 + 22mn - 28m + 60n - 66.$

The Zagreb connection indices (ZC_1^* and ZC_2) of polynomial chains are as follows [43]:

ZC_1^* of polynomial chains: **(1)** If $m \geq 3$ & $n = 2$, $ZC_1^*(P_m \times P_n) \leq 32mn - 40m - 42n + 40$; **(2)** If $m \geq 3$ & $n \geq 3$, $ZC_1^*(P_m \times P_n) \leq 32mn - 42m - 42n + 40$

ZC_2 of polynomial chains: **(1)** If $m \geq 3$ & $n = 2$, $ZC_2(P_m \times P_n) \leq 120mn - 192m - 238n + 350$; **(2)** If $m \geq 3$ & $n = 3$, $ZC_2(P_m \times P_n) \leq 128mn - 238m - 246n + 402$; **(3)** If $m \geq 3$ & $n = 4$, $ZC_2(P_m \times P_n) \leq 128mn - 239m - 246n + 402$; **(4)** If $m \geq 5$ & $n \geq 5$, $ZC_2(P_m \times P_n) \leq 128mn - 240m - 246n + 402.$

Table 1 and Figure 8 present the numerical and graphical behaviours of the upper bound values of Zagreb connection indices and Zagreb connection coindices for polynomial chains with respect to different values of m and n .

Table 1. Polynomial chains of $\theta_1 = P_m \times P_n$.

(m,n)	$ZC_1^*(\theta_1)$	$ZC_2(\theta_1)$	$\bar{Z}C_1(\theta_1)$	$\bar{Z}C_2(\theta_1)$
(3,2)	28	18	68	102
(3,3)	76	102	130	228
(3,4)	130	237	196	354
(3,5)	184	372	266	480
(4,2)	52	66	84	126
(4,3)	130	248	170	284
(4,4)	216	510	264	446
(4,5)	302	772	366	612
(5,2)	76	114	100	150
(5,3)	184	394	214	340
(5,4)	302	783	340	538
(5,5)	420	1172	478	744
(6,2)	100	162	116	174
(6,3)	238	540	262	396
(6,4)	388	1056	424	630
(6,5)	538	1572	602	876

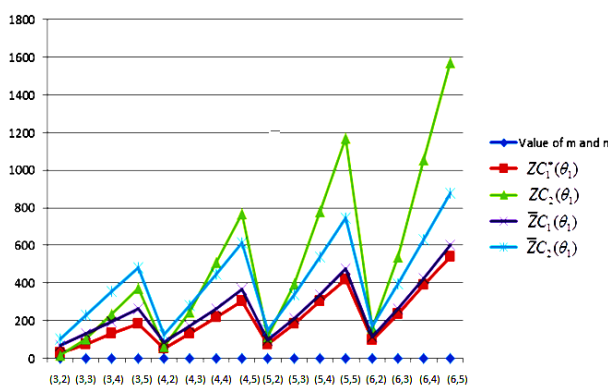


Figure 8. Polynomial chains of $\theta_1 = P_m \times P_n$ based on Table 1 with respect to indices and coincides .

(2) Carbon Nanotubes ($TUC_4(m, n)$): Let P_m and C_n be a particular alkane and cycloalkane called by path and cycle, then carbon nanotubes ($P_m \times C_n$) are obtained by the cartesian product of P_m and C_n . For $m = 4$ and $n = 5$, see Figure 9.

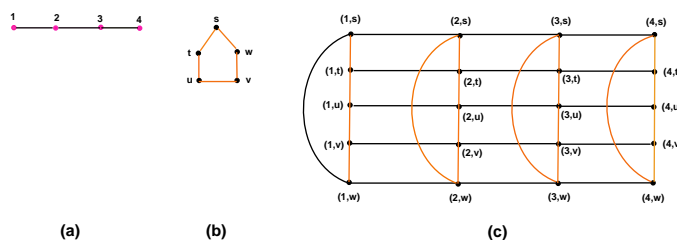


Figure 9. (a) $H_1 \cong P_4$ (b) $H_2 \cong C_5$ & (c) Carbon nanotube ($TUC_4(m, n) \cong P_4 \times C_5$).

Using Theorem 1, Zagreb connection coincides ($\bar{Z}C_1$ and $\bar{Z}C_2$) of carbon nanotubes are obtained as follows:

- (a) $\bar{Z}C_1(P_m \times C_n) \leq 2m^2n + 2mn^2 - 4n^2 + 10mn - 10n,$
- (b) $\bar{Z}C_2(P_m \times C_n) \leq 2m^2n + 2mn^2 - 6n^2 + 82mn - 131n.$

The Zagreb connection indices (ZC_1^* and ZC_2) of carbon nanotubes are as follows [43]:

- (1) $ZC_1^*(P_m \times C_n) \leq 32mn - 42n,$

(2) $ZC_2(P_m \times C_n) \leq 128mn - 238n$.

Table 2 and Figure 10 present the numerical and graphical behaviours of the Zagreb connection indices coincides for carbon nanotubes with respect to different values of m and n .

Table 2. Carbon nanotubes ($TUC_4(m, n)$) of $\theta_2 = P_m \times C_n$.

(m,n)	$ZC_1^*(\theta_2)$	$ZC_2(\theta_2)$	$\bar{Z}C_1(\theta_2)$	$\bar{Z}C_2(\theta_2)$
(3,2)	108	292	84	266
(3,3)	162	438	132	399
(3,4)	216	584	184	532
(3,5)	270	730	240	665
(4,2)	172	548	140	466
(4,3)	258	822	222	705
(4,4)	344	1096	312	948
(4,5)	430	1370	410	1195
(5,2)	236	804	204	674
(5,3)	354	1206	324	1023
(5,4)	472	1608	456	1380
(5,5)	590	2010	600	1745
(6,2)	300	1060	276	890
(6,3)	450	1590	438	1353
(6,4)	600	2120	616	1828
(6,5)	750	2650	810	2315

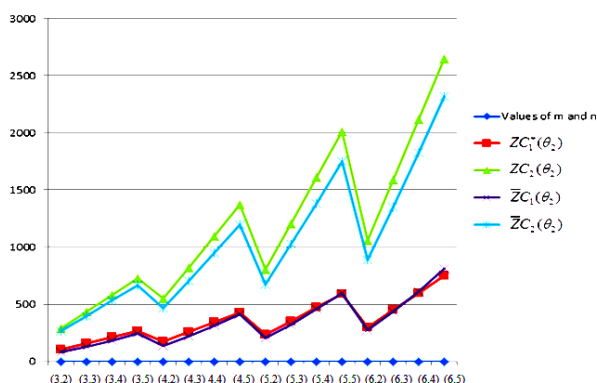


Figure 10. Carbon nanotubes ($TUC_4(m, n)$) of $\theta_2 = P_m \times C_n$ based on Table 2 with respect to indices and coincides.

5.2. Corona Product

(3) **Alkane** (C_3H_8) : Let P_m and N_n be a particular alkane called by paths and a null graph, then the alkanes ($P_m \odot N_n$) are obtained by the corona product of P_m and N_n . The corona product only has a chemical sense when for arbitrary $m > 0, n = 2$, and $n = 3$ provide equivalence chemical networks of alkenes and alkanes, respectively. Besides this sense, for $n > 3$, see no chemical context of corona product. For $m = 3$ and $n = 3$, see Figure 11.

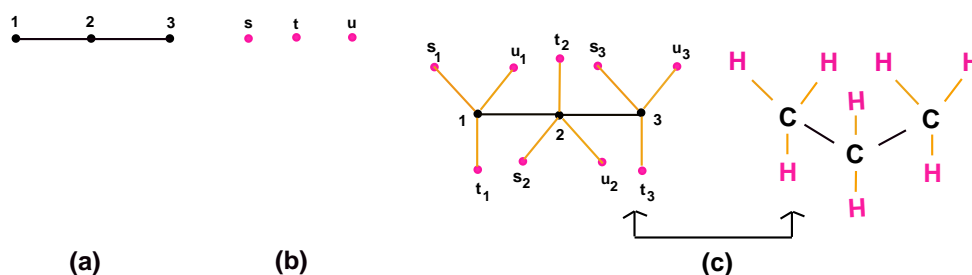


Figure 11. (a) $H_1 \cong P_3$ (b) $H_2 \cong N_3$ & (c) Alkane ($P_3 \odot N_3 \sim C_3H_8$).

Using Theorem 2, Zagreb connection coincides ($\bar{Z}C_1$ and $\bar{Z}C_2$) of alkanes are obtained as follows:

- (a) $\bar{Z}C_1(P_m \odot N_n) = mn + m - n - 1,$
 (b) $\bar{Z}C_2(P_m \odot N_n) = mn^2 - 2n^2 + mn + m - n - 2.$

The Zagreb connection indices (ZC_1^* and ZC_2) of alkanes are as follows [43]:

- (1) $ZC_1^*(P_m \odot N_n) = 3mn^2 - 2n^2 + 7mn + 4m - 12n - 10,$
 (2) $ZC_2(P_m \odot N_n) = 2mn^3 - 2n^3 + 8mn^2 - 16n^2 + 10mn - 26n.$

Table 3 and Figure 12 present the numerical and graphical behaviours of the Zagreb connection indices and coincides for alkanes with respect to different values of m and n .

Table 3. Alkanes of $\theta_3 = P_m \odot N_n$.

(m,n)	$ZC_1^*(\theta_3)$	$ZC_2(\theta_3)$	$\bar{Z}C_1(\theta_3)$	$\bar{Z}C_2(\theta_3)$
(3,2)	48	72	6	9
(3,3)	92	192	8	16
(3,4)	150	400	10	25
(3,5)	222	720	12	36
(4,2)	78	140	9	16
(4,3)	144	348	12	29
(4,4)	230	696	15	46
(4,5)	336	1220	18	67
(5,2)	108	208	12	23
(5,3)	196	504	16	42
(5,4)	310	992	20	67
(5,5)	450	1720	24	98
(6,2)	138	276	15	30
(6,3)	248	660	20	55
(6,4)	390	1288	25	88
(6,5)	564	2220	30	129

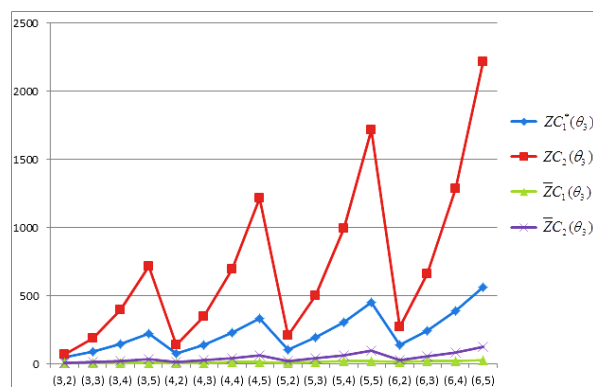


Figure 12. Alkanes of $\theta_3 = P_m \odot N_n$ based on Table 3 with respect to indices and coincides.

(4) Cyclobutane (C_4H_8): Let C_m and N_n be a cycle and a null graph, then Cyclobutanes ($C_m \odot N_n$) are obtained by the corona product of C_m and N_n . The corona product has a chemical sense only when for arbitrary $m > 0$, $n = 1$ and $n = 2$ provide equivalence chemical networks of cycloalkenes and cycloalkanes, respectively. Besides this sense, for $n > 2$ see no chemical context (cyclic compounds) of corona product. For $m = 4$ and $n = 2$, see Figure 13.

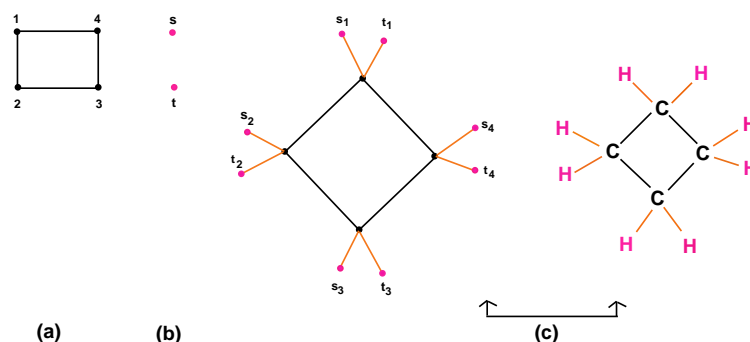


Figure 13. (a) $H_1 \cong C_4$ (b) $H_2 \cong N_2$ & (c) Cyclobutane ($C_4 \odot N_2 \cong C_4H_8$).

Using Theorem 2, Zagreb connection coindices ($\bar{Z}C_1$ and $\bar{Z}C_2$) of cyclobutanes are obtained, as follows:

- (a) $\bar{Z}C_1(C_m \odot N_n) \leq 2mn + 2m,$
 (b) $\bar{Z}C_2(C_m \odot N_n) \leq 2mn^2 + 4mn + 2m.$

The Zagreb connection indices (ZC_1^* and ZC_2) of cyclobutanes are as follows [43]:

- (1) $ZC_1^*(C_m \odot N_n) \leq 3mn^2 + 7mn + 4m,$
 (2) $ZC_2(C_m \odot N_n) \leq 2mn^3 + 8mn^2 + 10mn + 4m.$

Table 4 and Figure 14 present the numerical and graphical behaviours of the upper bound values of Zagreb connection indices and coindices for cyclobutanes with respect to different values of m and n .

Table 4. Cyclobutanes of $\theta_4 = C_m \odot N_n$.

(m,n)	$ZC_1^*(\theta_4)$	$ZC_2(\theta_4)$	$\bar{Z}C_1(\theta_4)$	$\bar{Z}C_2(\theta_4)$
(3,2)	90	216	18	54
(3,3)	156	480	24	96
(3,4)	240	900	30	150
(3,5)	342	1512	36	216
(4,2)	120	288	24	72
(4,3)	208	640	32	128
(4,4)	320	1200	40	200
(4,5)	456	2016	48	288
(5,2)	150	360	30	90
(5,3)	260	800	40	160
(5,4)	400	1500	50	250
(5,5)	570	2520	60	360
(6,2)	180	432	36	100
(6,3)	312	960	48	174
(6,4)	480	1800	60	268
(6,5)	684	3024	72	382

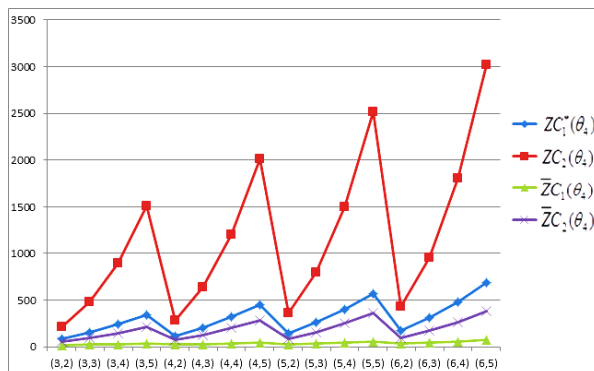


Figure 14. Cyclobutanes of $\theta_4 = C_m \odot N_n$ based on Table 4 with respect to indices and coindices.

5.3. Lexicographic Product

(5) Fence: Let P_m and P_n be two particular path-alkanes, then the fence $(P_m \cdot P_n)$ are obtained by the lexicographic product of P_m and P_n . For $m = 6$ and $n = 2$, see Figure 15.

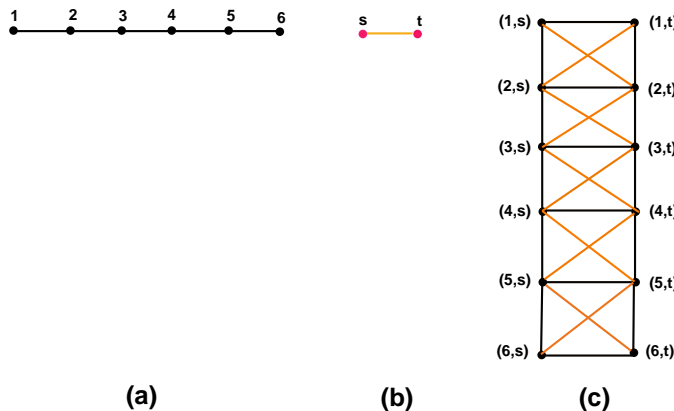


Figure 15. (a) $H_1 \cong P_6$ (b) $H_2 \cong P_2$ & (c) Fence $(P_6 \cdot P_2)$.

Using Theorem 3, Zagreb connection coindices ($\bar{Z}C_1$ and $\bar{Z}C_2$) of fence are obtained, as follows:

- (a) $\bar{Z}C_1(P_m \cdot P_n) \leq m^2n^2 - 3m^2n + mn^2 + 2m^2 + 4n^2 + 9mn - 6m - 6n + 4,$
- (b) $\bar{Z}C_2(P_m \cdot P_n) \leq \frac{m^2n^3}{2} - 3m^2n^2 + \frac{13}{2}m^2n - 5m^2 + \frac{13}{2}mn^3 - 3mn^2 - \frac{23}{2}mn + 15m - 5n^3 - 12n^2 + 17n - 10.$

The Zagreb connection indices (ZC_1^* and ZC_2) of fence are as follows [43]:

- (1) $ZC_1^*(P_m \cdot P_n) = 6mn^3 - 12n^3 + 4mn^2 - 6n^2 - 24mn + 24m + 20n - 16,$
- (2) $ZC_2(P_m \cdot P_n) = n^5 + 8mn^4 - 28n^4 + 5mn^3 - 6n^3 - 43mn^2 + 70n^2 + 71mn - 46m - 91n + 34.$

Table 5 and Figure 16 present the numerical and graphical behaviours of the upper bound values of Zagreb connection indices and coindices for fence with respect to different values of m and n .

Table 5. Fence of $\theta_5 = P_m \cdot P_n$.

(m,n)	$ZC_1^*(\theta_5)$	$ZC_2(\theta_5)$	$\bar{Z}C_1(\theta_5)$	$\bar{Z}C_2(\theta_5)$
(3,2)	24	-56	56	32
(3,3)	116	-107	130	194
(3,4)	328	16	236	602
(3,5)	696	781	374	1370
(4,2)	64	36	72	64
(4,3)	266	456	174	330
(4,4)	704	1934	324	974
(4,5)	1450	5640	522	2170
(5,2)	104	128	88	96
(5,3)	416	1019	222	468
(5,4)	1080	3852	424	1356
(5,5)	2204	10499	694	3000
(6,2)	144	220	104	128
(6,3)	566	1582	274	608
(6,4)	1456	5770	536	1748
(6,5)	2958	15358	890	3860

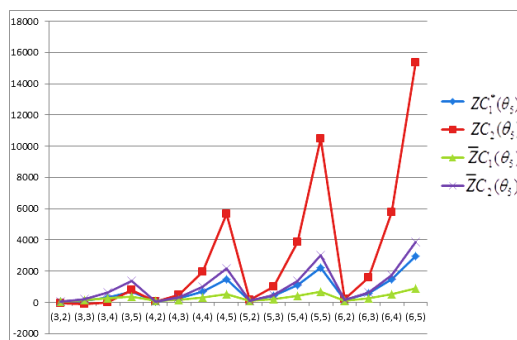


Figure 16. Fence of $\theta_5 = P_m \cdot P_n$ based on Table 5 with respect to indices and coincides.

(6) Closed fence: Let C_m and P_n be a cycle and a particular path-alkane, then closed fence ($C_m \cdot P_n$) is obtained by the lexicographic product of C_m and P_n . For $m = 6$ and $n = 2$, see Figure 17.

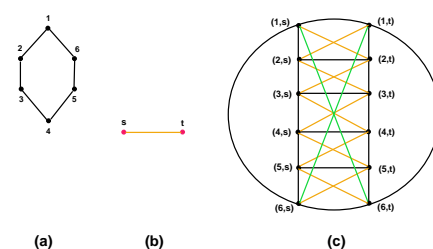


Figure 17. (a) $H_1 \cong C_6$ (b) $H_2 \cong P_2$ & (c) Closed fence $S(C_6 \cdot P_2)$.

Using Theorem 3, Zagreb connection coincides ($\bar{Z}C_1$ and $\bar{Z}C_2$) of closed fence are obtained, as follows:

- (a) $\bar{Z}C_1(C_m \cdot P_n) \leq m^2n^2 - 3m^2n + 2m^2 + 3mn^2 + 9mn - 6m,$
- (b) $\bar{Z}C_2(C_m \cdot P_n) \leq \frac{m^2n^3}{2} - 3m^2n^2 + \frac{13}{2}m^2n - 5m^2 + \frac{21}{2}mn^3 - 9mn^2 - \frac{15}{2}mn + 15m.$

The Zagreb connection indices (ZC_1^* and ZC_2) of the closed fence are as follows [43]:

- (1) $ZC_1^*(C_m \cdot P_n) \leq 4mn^3 + 4mn^2 - 24mn + 24m,$
- (2) $ZC_2(C_m \cdot P_n) \leq n^5 + 6mn^4 - 16n^4 + 7mn^3 - 8n^3 - 39mn^2 + 10n^2 + 67mn - 46m - 5n + 2.$

Table 6 and Figure 18 present the numerical and graphical behaviours of the upper bound values of Zagreb connection indices and coindices for closed fence with respect to different values of m and n .

Table 6. Closed fences of $\theta_6 = C_m \cdot P_n$.

(m,n)	$ZC_1^*(\theta_6)$	$ZC_2(\theta_6)$	$\bar{Z}C_1(\theta_6)$	$\bar{Z}C_2(\theta_6)$
(3,2)	72	-4	72	144
(3,3)	288	245	162	594
(3,4)	744	1304	288	1584
(3,5)	1512	4169	450	3330
(4,2)	96	80	96	192
(4,3)	384	724	224	796
(4,4)	992	2886	408	2132
(4,5)	2016	8108	648	4500
(5,2)	120	164	120	240
(5,3)	480	1203	290	1000
(5,4)	1240	4468	540	2690
(5,5)	2520	12047	870	5700
(6,2)	144	248	144	288
(6,3)	576	1682	360	1206
(6,4)	1488	6050	684	3258
(6,5)	3024	15986	1116	6930

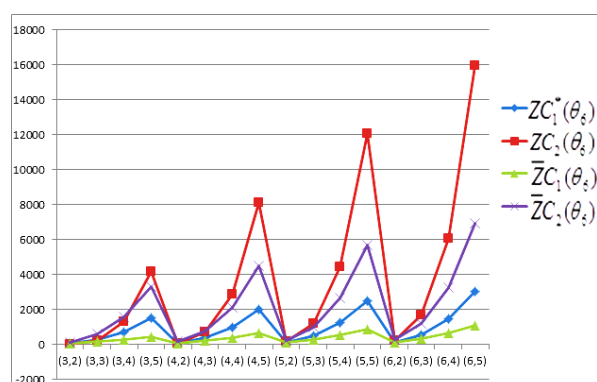


Figure 18. Closed fence of $\theta_6 = C_m \cdot P_n$ based on Table 6 with respect to indices and coindices.

Now, from Tables 1–6 and Figures 8, 10, 12, 14, 16, and 18–22, we close our discussion with the following conclusions:

- The behaviours of all the connection-based Zagreb indices and coindices for the molecular networks (polynomial chain, carbon nanotube, alkane, cycloalkane, fence, and closed fence) are symmetrise with some less or more values and the following orderings: (i) $ZC_2 \geq \bar{Z}C_2 \geq \bar{Z}C_1 \geq ZC_1^*$ (for polynomial chain), (ii) $ZC_2 \geq \bar{Z}C_2 \geq ZC_1^* \geq \bar{Z}C_1$ (for carbon nanotubes, fence and closed fence) and (iii) $ZC_2 \geq ZC_1^* \geq \bar{Z}C_2 \geq \bar{Z}C_1$ (for alkane and cycloalkane).
- For increasing values of m and n in all of the molecular networks (polynomial chain, carbon nanotube, alkane, cycloalkane, fence, and closed fence), the second Zagreb connection index, and the first Zagreb connection coindex are responding rapidly, and steadily, respectively.
- In the certain intervals of the values of m and n , all the connection-based indices and coindices attain the maximum and minimum values. These values are also lifting up in the intervals on increasing values of m and n in such a way that the response of maximum values is more rapid than the minimum values. In addition, we analyse that second the Zagreb connection index has attained more upper layer than other TIs in all pf the molecular networks.

- In particular, Figures 19–22 present that first Zagreb connection index, second Zagreb connection index, first Zagreb connection coindex, and second Zagreb connection coindex are dominant and auxiliary or incapable for the molecular networks from polynomial chain to closed fence, respectively. Moreover, we analyse that last molecular network i.e., closed fence has attain more upper layer than all other molecular networks for connection-based indices and coindices.

The investigation of these molecular descriptors for the resultant networks obtained from other operations of networks (switching, addition, rooted product, and Zig-zag product, etc.) is still open.

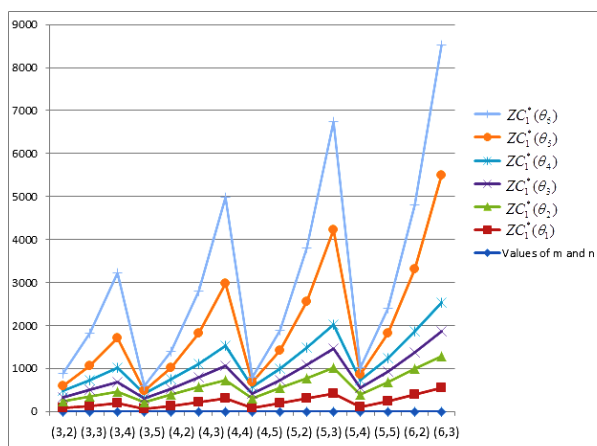


Figure 19. Comparison of first Zagreb connection indices.

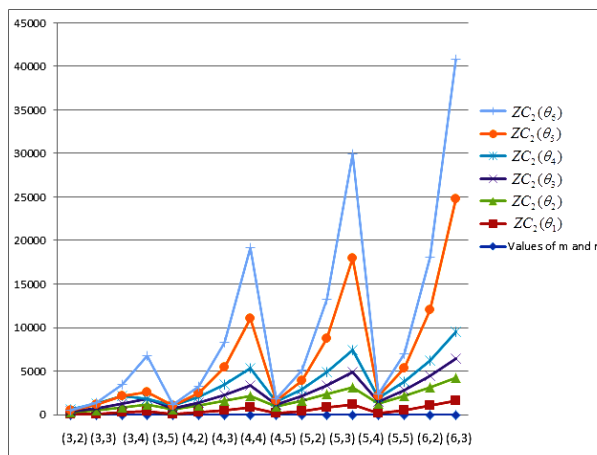


Figure 20. Comparison of second Zagreb connection indices.

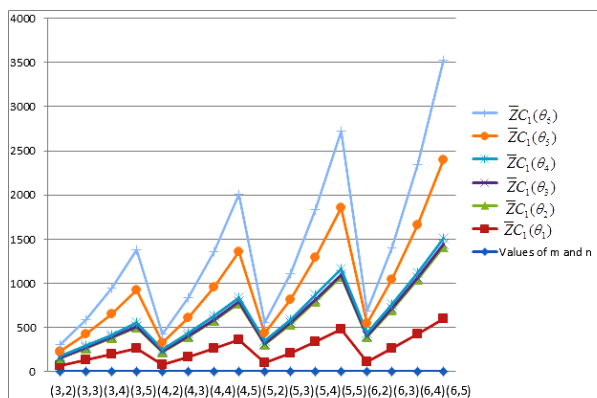


Figure 21. Comparison of first Zagreb connection coindices.

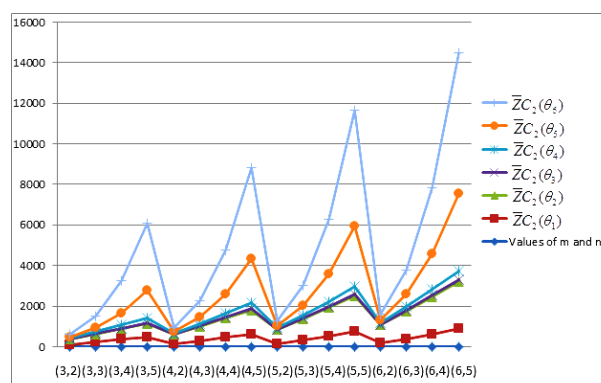


Figure 22. Comparison of second Zagreb connection coindices.

Author Contributions: Data curation, U.A.; Investigation, U.A.; Methodology, M.J. and A.M.A.; Supervision, M.J.; Validation, A.M.A.; Writing—original draft, U.A.; Writing—review and editing, M.J. and A.M.A. All authors have read and agreed to the published version of the manuscript.

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