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RESEARCH ARTICLE

Comparison Between Connection Based Modified Indices and Coindices for Product of Networks

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ABSTRACT Topological indices (TIs) are functional tools which correlate with a computational value through a undirected, finite and simple networks. Many physicochemical properties and chemical reactions are studied with the help of these TIs. Recently, they are commonly used in the behavior of quantitative structures activity as well as property relationships. In 1972, connection number based TIs are studied by Gutman and Trinajstić to calculate the entire π-electron energy of the alternant hydrocarbons. Moreover, the data provided by the website http://www.moleculardescriptors.eu shows that the relations between Zagreb indices and connection based indices that provide the better absolute values of the correlation coefficients for the thirteen physicochemical properties of the octane isomers. In this paper, we discuss the two invariants which are modified indices and modified coindices based on connection number of the resultant networks obtained by the different operations of product such as lexicographic and corona. For the molecular networks such as fence, closed fence, alkene and cycloalkane are depicted in the consequences of the obtained results. The comparisons between two invariants of the aforemention molecular networks are also presented through tables and graphical depictions. In addition, the uses and significance related to product of networks are also included.

INDEX TERMS Indices and coindices, product of networks, connection number.

NOMENCLATURE

Abbreviation	Meaning
TI	Topological index.
ZI	Zagreb index.
ZC	Zagreb coindex.
ZCI	Zagreb connection index.
ZCCI	Zagreb connection coindex.
CGT	Chemical Graph Theory.

I. INTRODUCTION

A molecular-network is a graphical depiction of a chemical compounds that connects components of a compound via some tools. These tools in graph theory known as topological indices (TIs). The relation of TI is physically written as $\mathbb{Q} = \beta(\mathbb{M})$, here $\mathbb{Q}$ is any property or activity, β is any function and $\mathbb{M}$ is any molecular-network [2]. A molecular-network collects information of the relations between vertices (carbon atoms) and edges (covalent bonds) which comes up a huge variety of significance in various disciplines of science. This source of information is used to highlight the carbon-based (organic) molecules and networks protocol in mathematical chemistry [3] as well as computer science [4]. The purpose of a network is to enable the sharing of data with the help of some tools (TIs). So, the structural study of networks provides the useful tools in exploring new horizon in the modern chemistry.

Moreover, a number of drugs particles that are mostly used in nanotechnology and the medicinal contents have developed through these TIs, see [5]. Recently, the concept of connection number based Zagreb indices are proposed for the best chemical applicability of the molecule for testing the different apparatus of octane isomers, particular families of alkanes of the S-sum networks and also presented some molecular-networks, see [6], [7], and [8].

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There are several networks are working in chemical theory of networks. One of them is operations on networks. It depends on operations such as Cartesian, lexicographic, tensor, strong, zig-zag and disjunction. The networks based on operations play a significant position in constructing the new networks with the help of given conditions, such results are called resultant networks. A few decades ago, Graovac and Pisanski [9] initially computed different results for Wiener index based on Cartesian product. In particular, a rectangular grid, polyomino chain and carbon nanotube ($TUC_4(r, l)$) are the Cartesian product of P_r & P_l, P_r & P_2 and C_r & P_2 respectively, fence and closed fence are the lexicographic product of P_r & P_2 and C_r & P_2 respectively, alkene (C_3H_6) and cyclohexane (C_6H_{12}) are the corona product of P_3 & N_2 and C_6 & N_2 respectively, where N_l, P_l and C_l are null, path and cycle networks of specific order l. Up till now, a huge number of results related to product of molecular-networks for the TIs have been computed, see [10], [11], [12], [13], and [14].

Almost five decades ago, two famous mathematical chemist Gutman and Trinajstić [15] firstly studied the degree based TI known as first Zagreb index to compute the entire π-electron energy of the molecular-networks. A large variety of TIs is presented in literature but degree based TIs are extensively more discussed than others, see the survey report [16], [17]. The TIs based on degree of various networks such as metal-organic, oxide, hexagonal, icosahedral honey comb, octahedral, neural, rhombus type silicate and carbon nanotubes are computed in [18], [19], [20], and [21].

Recently, Ali and Trinajstić [6] reopened the concept of connection number (second degree) based TIs. Connection number means the cardinality of particular vertex from its neighbors vertices at distance two. They used this approach and defined modified first Zagreb connection index (ZCI) that was first time defined by Gutman and Trinajstić [15] to find the behavior of different molecular-networks. They also reported that the chemical possession of this connection based TI (ZC_1^*) is better than the degree based TI (M_1) for the thirteen physicochemical properties of octane isomers such as total surface area, acentric factor, entropy, molar volume, heat capacity at pressure, heat capacity at temperature, enthalpy of vaporization, boiling point, octanol water partition, enthalpy of formation, density, standard enthalpy of vaporization and standard enthalpy of formation. For further studies for the second degree-based TIs on unicycle, acyclic (alkane), operations, subdivision and semi-total point networks, we refer to [22], [23], [24], [25], [26], and [27].

Almost two decades ago, Nikolić et al. [28] defined the modified ZIs. Hao et al. [29] presented some formulae for the modified ZIs and also computed the comparative relations between ZIs and modified ZIs. Dhanalakshmi et al. [30], [31] showed different results for modified and multiplicative ZIs of operations on networks and also computed some properties of bethe trees, fascia network, polytree, dendrimer trees for modified ZIs. The concept of coindices was defined by Ashrafi et. al [32] to compute the several results for product on networks. The Results of some distance based TIs and Zagreb coindices (ZCIs) have established in [33]. The second, multiplicative and reformulated ZCs and ZIs with certain chemical networks are defined in [34], [35], [36], and [37]. Ali et al. [1] computed the analysis between connection number based indices and coindices on product of molecular-networks.

In this paper, we computed connection based modified indices and coindices of the resultant networks such as lexicographic and corona products in the shape of exact solutions and upper bounds. Several molecular networks liked fence, closed fence, alkene and cyclohexane are presented by these aforesaid results. Moreover, the comparative relation between modified indices and modified coindices based on connection number of several molecular networks are also presented through tables and graphical depictions. The rest of the paper is settle as: Section II gives the basic definitions and key findings which are used in the main results, Section III covers a few molecular-networks, Section IV gives the uses and significance for product of networks, Section V and VI contain the main results for product of networks and Section VII presents the comparisons, applications and conclusions. At the end, a list of abbreviation is also included.

II. PRELIMINARIES

Let $\Gamma = (V(\Gamma), E(\Gamma))$ be a simple and undirected molecular-network. The cardinality of vertex set $V(\Gamma)$ and edge set $E(\Gamma) \subseteq V(\Gamma) \times V(\Gamma)$ are called order and size of Γ respectively. The neighborhood set of a vertex $t \in V(\Gamma)$ is obtained all those pairs of vertices which are adjacent to t. It is symbolically ($N_\Gamma(t)$) and mathematically written as $N_\Gamma(t) = \{s \in V(\Gamma); \quad s \text{ is adjacent with } t\}$. If $d_\Gamma(t) = |N_\Gamma(t)|$ is called degree of vertex t. If $d_\Gamma(t)$ = exactly 1 and at least 2 without edge, then networks become trivial and null respectively. If a network is Γ then its complement represents as $\bar{\Gamma}$. The degree of the vertex t in $\bar{\Gamma}$ is $d_{\bar{\Gamma}}(b) = p - 1 - d_\Gamma(t)$. Connection number means number of those vertices whose distance from particular vertex t must be two. It is denoted by $\tau_\Gamma(t)$. The atoms depict vertices and the bonds depict edges in both chemical and graphical terminology of molecular descriptors. Since Γ_1 and Γ_2 are two molecular-networks in all over the study and suppose that $|V(\Gamma_1)| = p_1$, $|V(\Gamma_2)| = p_2$, $|E(\Gamma_1)| = q_1$, $|E(\Gamma_2)| = q_2$ and $|E(\bar{\Gamma})| = \binom{p}{2} - q = \mu$. Moreover, it is interested to explain that both indices ZCIs and ZCCs related to Γ and $\bar{\Gamma}$ respectively, are not same because the connection number operates through Γ. For more preliminary notions and terminologies, we refer to [38].

Let $V_0(\Gamma)$ be the set of isolated vertices of the graph Γ and $|V_0(\Gamma)| = n_0$. The following relation was computed [39]:

$$\sum_{a \in V(\Gamma) \setminus V_0(\Gamma)} d_\Gamma(s) g(d_\Gamma(s)) = \sum_{st \in E(\Gamma)} [g(d_\Gamma(s)) + g(d_\Gamma(t))],$$

where g denotes the set of degree of vertices which is also real valued function of network Γ. The truthness of this relation is defined by Ali and Trinajstić [6] on the equal pattern:

$\sum_{s\in V(\Gamma)\setminus V_0(\Gamma)} d_\Gamma(s)f(s) = \sum_{st\in E(\Gamma)}[f(s)+f(t)]$, where g and f have equal conditions. They have to use $f(s) = \tau_G(s)$ and $f(t) = \tau_\Gamma(t)$ in the above identity and find modified first ZCI ($ZC_1^*(\Gamma)$) as

$$ZC_1^*(\Gamma) = \sum_{st\in E(\Gamma)} [\tau_\Gamma(s) + \tau_\Gamma(t)].$$

Ali et al. [27] uses the above pattern on the similar way by putting $f(s) = d_\Gamma(s)\tau_\Gamma(t)$ and $f(t) = d_\Gamma(t)\tau_\Gamma(s)$ or $f(s) = d_\Gamma(s)\tau_\Gamma(s)$ and $f(t) = d_\Gamma(t)\tau_\Gamma(t)$. We get the modified second ZCI (ZC_2^*) and modified third ZCI (ZC_3^*), as follows:

(a)

$$ZC_2^*(\Gamma) = \sum_{st\in E(\Gamma)} [d_\Gamma(s)\tau_\Gamma(t) + d_\Gamma(t)\tau_\Gamma(s)],$$

(b)

$$ZC_3^*(\Gamma) = \sum_{st\in E(\Gamma)} [d_\Gamma(s)\tau_\Gamma(s) + d_\Gamma(t)\tau_\Gamma(t)].$$

The first and second ZIs (M_1, M_2) [15], [40] are classical degree-based TIs. If we replace degree of a vertex into connection number. We get first ZCI and second ZCI. These are called second degree (connection number) [6] based TIs. Mathematically, first ZI (M_1), second ZI (M_2), first ZCI (ZC_1) and second ZCI (ZC_1) can be inserted as

(a)

$$M_1(\Gamma) = \sum_{t\in V(\Gamma)} [d_\Gamma(t)]^2 = \sum_{st\in E(\Gamma)} [d_\Gamma(s) + d_\Gamma(t)],$$

(b)

$$M_2(\Gamma) = \sum_{st\in E(\Gamma)} [d_\Gamma(s) \times d_\Gamma(t)],$$

(c)

$$ZC_1(\Gamma) = \sum_{t\in V(\Gamma)} [\tau_\Gamma(t)]^2,$$

(d)

$$ZC_2(\Gamma) = \sum_{st\in E(\Gamma)} [\tau_\Gamma(s) \times \tau_\Gamma(t)].$$

For a (molecular) network Γ, modified first ZCCI ($M\bar{Z}C_1(\Gamma)$) and modified second ZCCI ($M\bar{Z}C_2(\Gamma)$) are written as

(a)

$$M\bar{Z}C_1(\Gamma) = \sum_{st\notin E(\Gamma)} [d_\Gamma(s)\tau_\Gamma(t) + d_\Gamma(t)\tau_\Gamma(s)],$$

(b)

$$M\bar{Z}C_2(\Gamma) = \sum_{st\notin E(\Gamma)} [d_\Gamma(s)\tau_\Gamma(s) + d_\Gamma(t)\tau_\Gamma(t)].$$

A few list of ZIs, ZCIs and ZCCIs in the form of Table 1 is listed below

Definition 2.2: Lexicographic product or composition ($\Gamma_1 \cdot \Gamma_2$) of two networks Γ_1 and Γ_2 are given with vertex set : $V(\Gamma_1 \cdot \Gamma_2) = V(\Gamma_1) \cdot V(\Gamma_2)$ and edge set : $E(\Gamma_1 \cdot \Gamma_2) = \{(s_1, t_1)(s_2, t_2)$; where $(s_1, t_1), (s_2, t_2) \in V(\Gamma_1) \cdot V(\Gamma_2)\}$ with conditions: either $[s_1 = s_2 \in V(\Gamma_1) \wedge t_1t_2 \in E(\Gamma_2)]$ or $[t_1, t_2 \in V(\Gamma_2) \wedge s_1s_2 \in E(\Gamma_1)]$. For further learning, see Figure 1.

TABLE 1. A few list of ZIs, ZCIs and ZCCIs.

Molecular Descriptors
Third Zagren index or Forgotten index
(In 2015, Furtula and Gutman [20]
$M_3(\Gamma) = \sum_{st\in E(\Gamma)}[d_\Gamma^2(s) + d_\Gamma^2(t)] = F(\Gamma)$
First and second Zagreb coindex
(In 2010, Ashrafi et al. [32])
$\bar{M}_1(\Gamma) = \sum_{st\notin E(\Gamma)}[d_\Gamma(s) + d_\Gamma(t)]$
$\bar{M}_2(\Gamma) = \sum_{st\notin E(\Gamma)}[d_\Gamma(s) \times d_\Gamma(t)]$
Third Zagreb coindex or F-coindex
(In 2016, De et al. [13])
$\bar{M}_3 = \sum_{st\notin E(\Gamma)}[d_\Gamma^2(s) + d_\Gamma^2(t)] = \bar{F}(\Gamma)$
First and second Zagreb connection coindex
(In 2020, Ali et al. [1])
$\bar{Z}C_1(\Gamma) = \sum_{st\notin E(\Gamma)}[\tau_\Gamma(s) + \tau_\Gamma(t)]$
$\bar{Z}C_2(\Gamma) = \sum_{st\notin E(\Gamma)}[\tau_\Gamma(s) \times \tau_\Gamma(t)]$

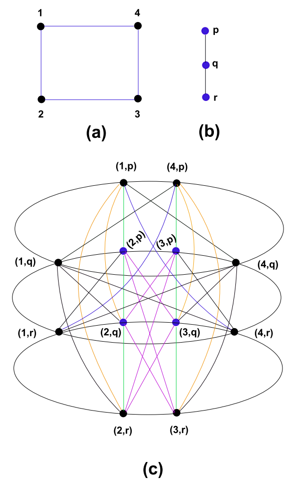

FIGURE 1. (a)$\Gamma_1 \cong C_4$, (b)$\Gamma_2 \cong P_3$ and (c)*Closed fence*($C_6H_{12} = C_4 \cdot P_3$).

Definition 2.3: Corona product ($\Gamma_1 \odot \Gamma_2$) of two graphs Γ_1 and Γ_2 is given with one copy of Γ_1 and p_1 copies of Γ_2 (i.e $\{\Gamma_2^i : 1 \le i \le p_1\}$) then by joining each vertex of the i^{th} copy of Γ_2 to the i^{th} vertex of one copy of Γ_1, where $1 \le i \le p_1$. In corona product, $|V(\Gamma_1 \odot \Gamma_2)| = p_1p_2 + p_1$ and $|E(\Gamma_1 \odot \Gamma_2)| = q_1 + p_1q_2 + p_1p_2$ are the cardinality of vertex set and edge set respectively. For more detail, see Figure 2.

Now, it is necessary to define some useful identities which will have surely needed to use in the main section.

Lemma 2.1 (see [38]): Suppose that a connected graph Γ and $|V(\Gamma)| = p$ and $|E(\Gamma)| = q$. Then,

$$\sum_{t\in V(\Gamma)} d_\Gamma(t) = 2q.$$

Lemma 2.2 (see [7]): Suppose that a connected graph Γ with $\{C_3, C_4\}-$ free network and $|V(\Gamma)| = p$ and $|E(\Gamma)| = q$. Then,

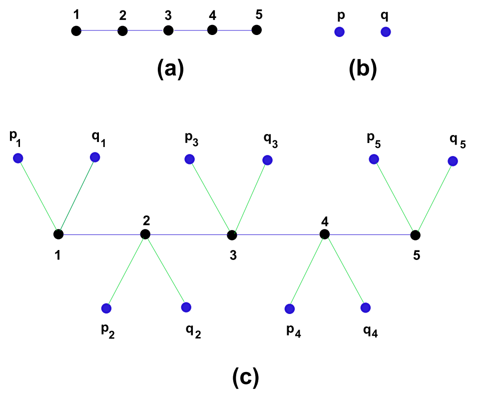

FIGURE 2. (a)$\Gamma_1 \cong P_5$, (b)$\Gamma_2 \cong N_2$ and (c)*Alkene*$(P_5 \odot N_2)$.

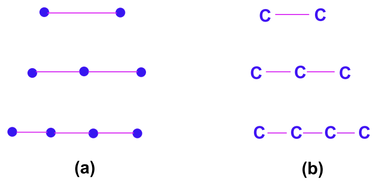

FIGURE 3. (a)P_2, P_3, P_4 are simple networks of alkanes and (b)P_2, P_3, P_4 are Lewis networks of alkanes.

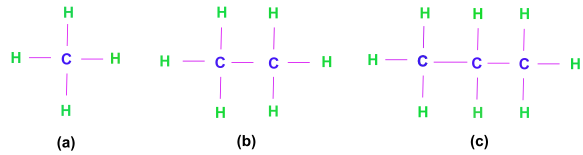

FIGURE 4. Lewis networks of (a) Methane, (b) Ethane and (c) Propane.

(a) $\tau_\Gamma(s) + d_\Gamma(s) = \sum_{t \in N_\Gamma(s)} d_\Gamma(t)$,

(b) $\sum_{t \in V(\Gamma)} \tau_\Gamma(t) = M_1(\Gamma) - 2q$.

Lemma 2.3: Let suppose

(a)

$$J_1(\Gamma_1, \Gamma_2) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \in E(\Gamma_2)} [d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_2) + d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_1)],$$

(b)

$$J_1'(\Gamma_1, \Gamma_2) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \notin E(\Gamma_2)} [d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_2) + d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_1)].$$

Lemma 2.4 Let suppose

(a)

$$J_2(\Gamma_2, \Gamma_1) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \in E(\Gamma_2)} [d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_2) + d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_1)],$$

(b)

$$J_2'(\Gamma_2, \Gamma_1) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \notin E(\Gamma_2)} [d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_2) + d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_1)].$$

Lemma 2.5: Let suppose

(a)

$$J_3(\Gamma_1, \Gamma_2) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \in E(\Gamma_2)} [d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_1) + d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_2)],$$

(b)

$$J_3'(\Gamma_1, \Gamma_2) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \notin E(\Gamma_2)} [d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_1) + d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_2)].$$

Lemma 2.6: Let suppose

(a)

$$J_4(\Gamma_2, \Gamma_1) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \in E(\Gamma_2)} [d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_1) + d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_2)],$$

(b)

$$J_4'(\Gamma_2, \Gamma_1) = \sum_{s_1s_2 \in E(\Gamma_1)} \sum_{t_1t_2 \notin E(\Gamma_2)} [d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_1) + d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_2)].$$

Lemma 2.7: Let suppose

(a)

$$JC_1(\Gamma_1, \Gamma_2) = \sum_{\substack{s_1s_2 \notin E(\Gamma_1) \\ s_1 \neq s_2 \wedge s_1 \backsim s_2}} \sum_{\substack{t_1t_2 \notin E(\Gamma_2) \\ t_1 \neq t_2 \wedge t_1 \backsim t_2}} \times [d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_2) + d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_1)],$$

(b)

$$JC_2(\Gamma_2, \Gamma_1) = \sum_{\substack{s_1s_2 \notin E(\Gamma_1) \\ s_1 \neq s_2 \wedge s_1 \backsim s_2}} \sum_{\substack{t_1t_2 \notin E(\Gamma_2) \\ t_1 \neq t_2 \wedge t_1 \backsim t_2}} \times [d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_2) + d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_1)].$$

Lemma 2.8: Let suppose

(a)

$$JC_3(\Gamma_1, \Gamma_2) = \sum_{\substack{s_1s_2 \notin E(\Gamma_1) \\ s_1 \neq s_2 \wedge s_1 \backsim s_2}} \sum_{\substack{t_1t_2 \notin E(\Gamma_2) \\ t_1 \neq t_2 \wedge t_1 \backsim t_2}} \times [d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_1) + d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_2)],$$

(b)

$$JC_4(\Gamma_2, \Gamma_1) = \sum_{\substack{s_1s_2 \notin E(\Gamma_1) \\ s_1 \neq s_2 \wedge s_1 \backsim s_2}} \sum_{\substack{t_1t_2 \notin E(\Gamma_2) \\ t_1 \neq t_2 \wedge t_1 \backsim t_2}} \times [d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_1) + d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_2)].$$

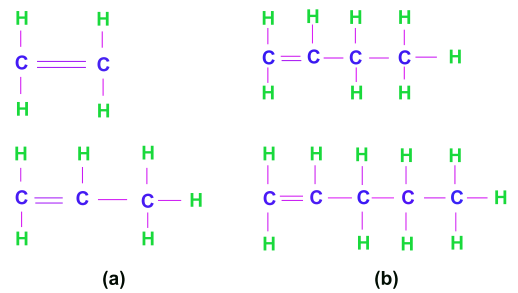

FIGURE 5. **(a) The Lewis networks of ethene and propene, (b) The Lewis networks of butene and pentene.**

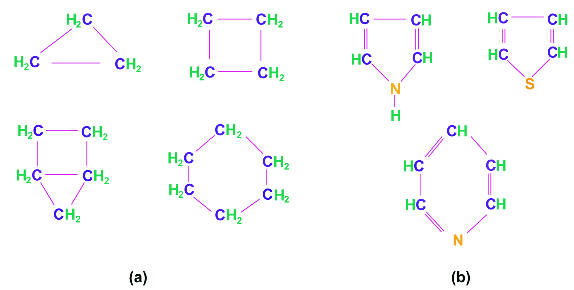

FIGURE 6. **(a) The Lewis network of 'cyclopropane, cyclobutane, cyclopentane and cyclohexane', (b) The Lewis network of 'pyrol, thiophene and pyridine'.**

III. UNDER STUDY MOLECULAR-NETWORKS

Under study molecular networks are defined as follows:

- The saturated hydrocarbon compounds are called alkanes which are also the simplest organic compounds obtained single bound between carbon atoms. It means single covalent bounds lies between carbon atoms which shares pair of electrons. Figure 3 shows its simple and Lewis networks. Methane (CH_4), ethane ($H_3C - CH_3$) and propane ($H_3C - CH_2 - CH_3$) are few examples of alkanes and their Lewis networks are shown in Figure 4. C_nH_{2n+2} is the general formula of this alkane series. A general formula gives us to encrypt a series of molecules that alter to each other by a constant unit. For example, let us look again propane (C_3H_8), where n represents 3 carbon atoms of propane. Then, $C_3H_{2(3)+2} = C_3H_8$. Using this, we can easily find the macular formula for other alkanes e.g. Decane ($H_3C(CH_2)_8CH_3$), an alkane has 10 carbon atoms. So, $C_{10}H_{22}$ is chemical formula of decane. Let us look now another molecular series that is alkenes which are unsaturated, so they contain double covalent bond between two carbon atoms. The some examples of alkenes are ethene, propene, butene & pentene and their Lewis networks are shown in Figure 5. C_nH_{2n} is the general formula of this alkene series. For example, the chemical formula of decene is $C_{10}H_{20}$ if $n = 10$ carbon atoms.
- In Chemistry, cyclic compounds are molecules obtained to each other by atom bond connection and form a ring network. Organic cyclic compounds are found when the ring consists of carbon atoms only. On the symmetric way, inorganic compounds are found when the ring consists of non-carbon atoms. They can be divided into two classes as homocyclic and heterocyclic compounds. The cyclo organic compounds are formed into small, medium and large according to their carbon atoms [1 to 5], [6 to 10] and [11 to on wards] respectively. C_nH_{2n} denotes the general formula of cyclic compounds. The examples of cyclic compounds which are homocyclic and heterocyclic compounds that are given in the form of sets {Cyclopropane, cyclobutane, cyclopentane etc.} and {pyrol, thiophene, pyridine etc.} respectively. Moreover, the Lewis networks of these cyclic compounds are depicted in the Figure 6.

IV. USES AND SIGNIFICANCE FOR PRODUCT OF NETWORKS

The graphs operations especially products of networks play an important role in the studies of complex structures related to chemistry and computer science [2], [4]. In particular, it is well known fact that many chemical graph structures can be molded from simple networks via product-related operations on networks. For detail study, see [41] and [42]. Moreover, molecular-networks such as fence and closed fence are formed by the lexicographic and strong product of paths and cycles. Khalifeh et al. [43] and Ashrafi et al. [32] studied different results of classical Zagreb indices and coindices via product of networks. So, the graphs operations have become a vast field of research in CGT because of its useful applications in various disciplines of science i.e. chemo-informatics (combination of three subjects mathematics, chemistry and informatics), pharmaceutical industries and drug discovery labs. The following are some important significance related to product of networks discussed below:

- Topological indices (TIs) are numeric values which correlate the chemical structures with its several chemical reactions, physical properties and biological experiments under various product of networks. So, they are used in nano-technology in isomer, chemistry, biochemistry, organic compounds, pharmaceutical industries, crystalline materials and mostly applied in QSAR/QSPR ([13], [44]).
- The product of networks are mostly used in CGT for chemical structures such as carbonnano tube, bottleneck graph, linear polyomino chain, fence, closed fence, alkane and cyclohexane ([1], [8], [13], [45]).
- The product of networks are also used in mathematics, chemistry as well as computer science. Model for linking computers are defined by Cartesian product. For the modeling of this model, we synchronize Hamiltonian paths and cycles in the network ([46]).

- Several drug structures have been determined by applying the product of networks i.e. Zig-Zag chain is used in the field of pharmacy engineering ([47]).
- Moreover, in the treatment of pandemic virus COVID-19, we can use two TIs sum-connectivity index and ZI to investigate the topological polar surface area and the molecular weight of phytochemical ([48]).
- Recently, corona product have been directly used in chemistry to make chemical structures such as alkanes, alkenes, cycloalkane and cycloalkenes ([1]).

V. RESULTS FOR MODIFIED INDICES

This section contains the general results for the modified second ZCI (ZC_2^*) and modified third ZCI (ZC_3^*) on product of molecular-networks i.e. lexicographic product and corona product.

Theorem 4.1: Let Γ_1 and Γ_2 be two connected graphs. Then, ZC_2^* and ZC_3^* of the composition or lexicographic product $(\Gamma_1 \cdot \Gamma_2)$ of Γ_1 and Γ_2 are as follows:

(a)

$$\begin{aligned}
&ZC_2^*(\Gamma_1 \cdot \Gamma_2)\\
&\leq p_2^2(p_2+2q_2+\delta_2)ZC_2^*(\Gamma_1)+2p_2(p_2+1)\\
&\quad\times q_2ZC_1^*(\Gamma_1)-2(p_1+2q_1)M_2(\Gamma_2)\\
&\quad+p_2[p_2(p_2-1)-2q_2+2\\
&\quad\times(p_2-1)q_2+(p_2-1)\delta_2]M_1(\Gamma_1)\\
&\quad+[2q_1(p_2-2)+p_1(p_2-1)\\
&\quad-4p_2q_1]M_1(\Gamma_2)+p_2M_1(\Gamma_1)M_1(\Gamma_2)+4(p_2^2-1)q_1q_2\\
&\quad-2q_1\bar{M}_2(\Gamma_2)+(p_2-1)q_1\bar{M}_1(\Gamma_2)\\
&\quad-2p_2J_1(\Gamma_1,\Gamma_2)+2p_2\\
&\quad\times J_2(\Gamma_2,\Gamma_1)-p_2J_1'(\Gamma_1,\Gamma_2)+p_2J_2'(\Gamma_2,\Gamma_1),
\end{aligned}$$

(b)

$$\begin{aligned}
&ZC_3^*(\Gamma_1 \cdot \Gamma_2)\\
&\leq p_2^2(p_2+2q_2+\delta_2)ZC_3^*(\Gamma_1)+2p_2(p_2+1)\\
&\quad\times q_2ZC_1^*(\Gamma_1)-(p_1+2q_1)M_3(\Gamma_2)\\
&\quad+[p_2(p_2-1)(p_2+2q_2+\delta_2)\\
&\quad-2p_2q_2]M_1(\Gamma_1)+[(p_2-1)(p_1+2q_1)\\
&\quad-2(2p_2+1)q_1]M_1(\Gamma_2)\\
&\quad+p_2M_1(\Gamma_1)M_1(\Gamma_2)+4(p_2^2-1)q_1q_2-q_1\bar{F}(\Gamma_2)\\
&\quad+(p_2-1)q_1\\
&\quad\times\bar{M}_1(\Gamma_2)-2p_2J_3(\Gamma_1,\Gamma_2)+2p_2J_4(\Gamma_2,\Gamma_1)\\
&\quad-p_2J_3'(\Gamma_1,\Gamma_2)+p_2J_4'(\Gamma_2,\Gamma_1).
\end{aligned}$$

Proof (a):

For $s \in V(\Gamma_1)$, $t \in V(\Gamma_2)$ and $(s,t) \in V(\Gamma_1 \cdot \Gamma_2)$, we have

- $d_{\Gamma_1\cdot\Gamma_2}(s,t) = p_2 d_{\Gamma_1}(s) + d_{\Gamma_2}(t)$,
- $\tau_{\Gamma_1\cdot\Gamma_2}(s,t) = p_2\tau_{\Gamma_1}(s) + d_{\bar{\Gamma}_2}(t) = p_2\tau_{\Gamma_1}(s) + (p_2-1) - d_{\Gamma_2}(t)$.

$$\begin{aligned}
&ZC_2^*(\Gamma_1 \cdot \Gamma_2)\\
&= \sum_{(s_1,t_1)(s_2,t_2)\in E(\Gamma_1\cdot\Gamma_2)} [d_{\Gamma_1\cdot\Gamma_2}(s_1,t_1)\\
&\quad\times\tau_{\Gamma_1\cdot\Gamma_2}(s_2,t_2)+d_{\Gamma_1\cdot\Gamma_2}(s_2,t_2)\tau_{\Gamma_1\cdot\Gamma_2}(s_1,t_1)]\\
&= \sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s,t_1)\tau(s,t_2)+d(s,t_2)\tau(s,t_1)]\\
&\quad+\sum_{t\in V(\Gamma_2)}\sum_{s_1s_2\in E(\Gamma_1)}[d(s_1,t)\tau(s_2,t)+d(s_2,t)\tau(s_1,t)]\\
&\quad+\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s_1,t_1)\tau(s_2,t_2)+d(s_2,t_2)\\
&\quad\times\tau(s_1,t_1)]+\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[d(s_1,t_1)\tau(s_2,t_2)\\
&\quad+d(s_2,t_2)\tau(s_1,t_1)]
\end{aligned}$$

Taking

$$\begin{aligned}
&\sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s,t_1)\tau(s,t_2)+d(s,t_2)\tau(s,t_1)]\\
&= \sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s)\\
&\quad+(p_2-1)-d_{\Gamma_2}(t_2)\}+\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s)\\
&\quad+(p_2-1)-d_{\Gamma_2}(t_1)\}]\\
&= \sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[p_2^2d_{\Gamma_1}(s)\tau_{\Gamma_1}(s)+p_2(p_2-1)d_{\Gamma_1}(s)\\
&\quad-p_2d_{\Gamma_1}(s)d_{\Gamma_2}(t_2)+p_2d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s)+(p_2-1)d_{\Gamma_2}(t_1)\\
&\quad-d_{\Gamma_2}(t_1)d_{\Gamma_2}(t_2)+p_2^2d_{\Gamma_1}(s)\tau_{\Gamma_1}(s)+p_2(p_2-1)d_{\Gamma_1}(s)\\
&\quad-p_2d_{\Gamma_1}(s)d_{\Gamma_2}(t_1)+p_2d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s)+(p_2-1)d_{\Gamma_2}(t_2)\\
&\quad-d_{\Gamma_2}(t_1)d_{\Gamma_2}(t_2)]\\
&= 2p_2^2q_2ZC_1^*(\Gamma_1)+4p_2(p_2-1)q_1q_2-2p_2q_1M_1(\Gamma_2)+p_2\\
&\quad\times M_1(\Gamma_2)[M_1(\Gamma_1)-2q_1]+p_1(p_2-1)M_1(\Gamma_2)\\
&\quad-2p_1M_2(\Gamma_2).
\end{aligned}$$

Also taking

$$\begin{aligned}
&\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[d(s_1,t_1)\tau(s_2,t_2)+d(s_2,t_2)\tau(s_1,t_1)]\\
&\leq \sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s_2)\\
&\quad+(p_2-1)-d_{\Gamma_2}(t_2)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s_1)\\
&\quad+(p_2-1)-d_{\Gamma_2}(t_1)\}]\\
&= \sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[p_2^2d_{\Gamma_1}(s_1)\tau_{\Gamma_1}(s_2)+p_2(p_2-1)\\
&\quad\times d_{\Gamma_1}(s_1)-p_2d_{\Gamma_1}(s_1)d_{\Gamma_2}(t_2)\\
&\quad+p_2d_{\Gamma_2}(t_1)\tau_{\Gamma_1}(s_2)+(p_2-1)\\
&\quad\times d_{\Gamma_2}(t_1)-d_{\Gamma_2}(t_1)d_{\Gamma_2}(t_2)\\
&\quad+p_2^2d_{\Gamma_1}(s_2)\tau_{\Gamma_1}(s_1)+p_2(p_2-1)\\
&\quad\times d_{\Gamma_1}(s_2)-p_2d_{\Gamma_1}(s_2)d_{\Gamma_2}(t_1)\\
&\quad+p_2d_{\Gamma_2}(t_2)\tau_{\Gamma_1}(s_1)+(p_2-1)\\
&\quad\times d_{\Gamma_2}(t_2)-d_{\Gamma_2}(t_1)d_{\Gamma_2}(t_2)]
\end{aligned}$$

Using Lemmas' 2.3 & 2.4 and suppose that

$$\sum_{t_1t_2\notin E(\Gamma_2)} = p_2(p_2-1)-2q_2=\delta_2$$
$$= p_2^2\delta_2 ZC_2^*(\Gamma_1)+p_2(p_2-1)\delta_2 M_1(\Gamma_1)-p_2J_1'(\Gamma_1,\Gamma_2)$$
$$+p_2J_2'(\Gamma_2,\Gamma_1)+(p_2-1)q_1\bar{M}_1(\Gamma_2)-2q_1\bar{M}_2(\Gamma_2).$$

Similarly,

$$\sum_{t\in V(\Gamma_2)}\sum_{s_1s_2\in E(\Gamma_1)}[d(s_1,t)\tau(s_2,t)+d(s_2,t)\tau(s_1,t)]$$
$$=\sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t)\}\{p_2\tau_{\Gamma_1}(s_2)$$
$$+(p_2-1)-d_{\Gamma_2}(t)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t)\}\{p_2\tau_{\Gamma_1}(s_1)$$
$$+(p_2-1)-d_{\Gamma_2}(t)\}]$$
$$=p_2^3ZC_2^*(\Gamma_1)+p_2^2(p_2-1)M_1(\Gamma_1)-2p_2q_2M_1(\Gamma_1)+2p_2q_2$$
$$\times ZC_1^*(\Gamma_1)+4(p_2-1)q_1q_2-2q_1M_1(\Gamma_2).$$

And

$$\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s_1,t_1)\tau(s_2,t_2)+d(s_2,t_2)\tau(s_1,t_1)]$$
$$\leq 2\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s_2)$$
$$+(p_2-1)-d_{\Gamma_2}(t_2)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s_1)$$
$$+(p_2-1)-d_{\Gamma_2}(t_1)\}]$$

Using Lemmas' 2.3 & 2.4, we have

$$=2p_2^2q_2ZC_2^*(\Gamma_1)+2p_2(p_2-1)q_2M_1(\Gamma_1)-2p_2J_1(\Gamma_1,\Gamma_2)$$
$$+2p_2J_2(\Gamma_2,\Gamma_1)+2(p_2-1)q_1M_1(\Gamma_2)-4q_1M_2(\Gamma_2).$$

Consequently,

$$ZC_2^*(\Gamma_1\cdot\Gamma_2)$$
$$\leq p_2^2(p_2+2q_2+\delta_2)ZC_2^*(\Gamma_1)+2p_2(p_2+1)$$
$$\times q_2ZC_1^*(\Gamma_1)-2(p_1+2q_1)M_2(\Gamma_2)$$
$$+p_2[p_2(p_2-1)-2q_2+2$$
$$\times(p_2-1)q_2+(p_2-1)\delta_2]M_1(\Gamma_1)$$
$$+[2q_1(p_2-2)+p_1(p_2-1)$$
$$-4p_2q_1]M_1(\Gamma_2)+p_2M_1(\Gamma_1)M_1(\Gamma_2)+4(p_2^2-1)q_1q_2$$
$$-2q_1\bar{M}_2(\Gamma_2)+(p_2-1)q_1\bar{M}_1(\Gamma_2)$$
$$-2p_2J_1(\Gamma_1,\Gamma_2)+2p_2$$
$$\times J_2(\Gamma_2,\Gamma_1)-p_2J_1'(\Gamma_1,\Gamma_2)+p_2J_2'(\Gamma_2,\Gamma_1).$$

Proof (b):

$$ZC_3^*(\Gamma_1\cdot\Gamma_2)$$
$$=\sum_{(s_1,t_1)(s_2,t_2)\in E(\Gamma_1\cdot\Gamma_2)}[d_{\Gamma_1\cdot\Gamma_2}(s_1,t_1)$$
$$\times\tau_{\Gamma_1\cdot\Gamma_2}(s_1,t_1)+d_{\Gamma_1\cdot\Gamma_2}(s_2,t_2)\tau_{\Gamma_1\cdot\Gamma_2}(s_2,t_2)]$$
$$=\sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s,t_1)\tau(s,t_1)+d(s,t_2)\tau(s,t_2)]$$
$$+\sum_{t\in V(\Gamma_2)}\sum_{s_1s_2\in E(\Gamma_1)}[d(s_1,t)\tau(s_1,t)+d(s_2,t)\tau(s_2,t)]$$
$$+\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s_1,t_1)\tau(s_1,t_1)+d(s_2,t_2)$$
$$\times\tau(s_2,t_2)]+\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[d(s_1,t_1)\tau(s_1,t_1)$$
$$+d(s_2,t_2)\tau(s_2,t_2)]$$

Taking

$$\sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s,t_1)\tau(s,t_1)+d(s,t_2)\tau(s,t_2)]$$
$$=\sum_{s\in V(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s)$$
$$+(p_2-1)-d_{\Gamma_2}(t_1)\}+\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s)$$
$$+(p_2-1)-d_{\Gamma_2}(t_2)\}]$$

Similarly,

$$=2p_2^2q_2ZC_1^*(\Gamma_1)+4p_2(p_2-1)q_1q_2-2p_2q_1M_1(\Gamma_2)+p_2$$
$$\times M_1(\Gamma_2)[M_1(\Gamma_1)-2q_1]$$
$$+p_1(p_2-1)M_1(\Gamma_2)-p_1M_3(\Gamma_2).$$

Also taking

$$\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[d(s_1,t_1)\tau(s_1,t_1)+d(s_2,t_2)\tau(s_2,t_2)]$$
$$\leq\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\notin E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s_1)$$
$$+(p_2-1)-d_{\Gamma_2}(t_1)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s_2)$$
$$+(p_2-1)-d_{\Gamma_2}(t_2)\}].$$

Using Lemmas' 2.5 & 2.6, we have

$$=p_2^2\delta_2ZC_3^*(\Gamma_1)+p_2(p_2-1)\delta_2M_1(\Gamma_1)-p_2J_3'(\Gamma_1,\Gamma_2)$$
$$+p_2J_4'(\Gamma_2,\Gamma_1)+(p_2-1)q_1\bar{M}_1(\Gamma_2)-q_1\bar{F}(\Gamma_2).$$

Similarly,

$$\sum_{t\in V(\Gamma_2)}\sum_{s_1s_2\in E(\Gamma_1)}[d(s_1,t)\tau(s_1,t)+d(s_2,t)\tau(s_2,t)]$$
$$=p_2^3ZC_3^*(\Gamma_1)+p_2^2(p_2-1)M_1(\Gamma_1)-2p_2q_2M_1(\Gamma_1)$$
$$+2p_2q_2ZC_1^*(\Gamma_1)+4(p_2-1)q_1q_2-2q_1M_1(\Gamma_2).$$

And

$$\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[d(s_1,t_1)\tau(s_1,t_1)+d(s_2,t_2)\tau(s_2,t_2)]$$
$$\leq 2\sum_{s_1s_2\in E(\Gamma_1)}\sum_{t_1t_2\in E(\Gamma_2)}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s_1)$$
$$+(p_2-1)-d_{\Gamma_2}(t_1)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s_2)$$
$$+(p_2-1)-d_{\Gamma_2}(t_2)\}]$$

Using Lemmas' 2.5 & 2.6, we have,

$$=2p_2^2q_2ZC_3^*(\Gamma_1)+2p_2(p_2-1)q_2M_1(\Gamma_1)-2p_2J_3(\Gamma_1,\Gamma_2)$$
$$+2p_2J_4(\Gamma_2,\Gamma_1)+2(p_2-1)q_1M_1(\Gamma_2)-2q_1M_3(\Gamma_2).$$

Consequently,

$$\begin{aligned} &ZC_3^*(\Gamma_1 \cdot \Gamma_2) \\ &\leq p_2^2(p_2+2q_2+\delta_2)ZC_3^*(\Gamma_1)+2p_2(p_2+1) \\ &\quad \times q_2 ZC_1^*(\Gamma_1)-(p_1 \\ &\quad +2q_1)M_3(\Gamma_2)+[p_2(p_2-1)(p_2+2q_2+\delta_2) \\ &\quad -2p_2q_2]M_1(\Gamma_1)+[(p_2-1)(p_1+2q_1) \\ &\quad -2(2p_2+1)q_1]M_1(\Gamma_2) \\ &\quad +p_2M_1(\Gamma_1)M_1(\Gamma_2)+4(p_2^2-1)q_1q_2 \\ &\quad -q_1\bar{F}(\Gamma_2)+(p_2-1)q_1 \\ &\quad \times \bar{M}_1(\Gamma_2)-2p_2J_3(\Gamma_1,\Gamma_2) \\ &\quad +2p_2J_4(\Gamma_2,\Gamma_1)-p_2J_3'(\Gamma_1,\Gamma_2) \\ &\quad +p_2J_4'(\Gamma_2,\Gamma_1). \end{aligned}$$

Theorem 4.2: Let Γ_1 and Γ_2 be two connected and $\{C_3, C_4\}-$ free graphs. Then, ZC_2^* and ZC_3^* of the corona product of G_1 and G_2 are as follows:

(a)

$$\begin{aligned} &ZC_2^*(\Gamma_1 \odot \Gamma_2) \\ &= ZC_2^*(\Gamma_1)+p_2ZC_1^*(\Gamma_1)+2p_2M_2(\Gamma_1) \\ &\quad -2p_1M_2(\Gamma_2)+(p_2^2+2p_2 \\ &\quad +2q_2)M_1(\Gamma_1)+[p_1(p_2-1)-p_1 \\ &\quad +2q_1]M_1(\Gamma_2)+p_1p_2^2(p_2-1)+2p_2(3p_2-2)q_1-2p_1q_2 \\ &\quad +4(p_2-1)q_1q_2, \end{aligned}$$

(b)

$$\begin{aligned} &ZC_3^*(\Gamma_1 \odot \Gamma_2) \\ &= ZC_3^*(\Gamma_1)+2p_2ZC_1^*(\Gamma_1)+p_2M_3(\Gamma_1) \\ &\quad -p_1M_3(\Gamma_2)+3p_2^2M_1(\Gamma_1)+(p_1p_2-3p_1+2q_1)M_1(\Gamma_2) \\ &\quad +p_1p_2(p_2-1)+2p_2(p_2^2-p_2+1)q_1 \\ &\quad +2p_1(2p_2-3)q_2+8q_1q_2. \end{aligned}$$

Proof (a):

If for any $t \in V(\Gamma_1 \odot \Gamma_2)$ either $t \in V(\Gamma_1)$ or $t \in V(\Gamma_2^i)$, where $1 \leqslant i \leqslant p_1$ and we have

- Case(I): If $t \in V(\Gamma_1)$, then $d_{\Gamma_1 \odot \Gamma_2}(t) = d_{\Gamma_1}(t) + p_2$, Case(II): If $t \in V(\Gamma_2^i)$,then $d_{\Gamma_1 \odot \Gamma_2}(t) = d_{\Gamma_2^i}(t) + 1$.
- Case(I): If $t \in V(\Gamma_1)$, then $\tau_{\Gamma_1 \odot \Gamma_2}(t) = \tau_{\Gamma_1}(t) + n_2 d_{\Gamma_1}(t)$, Case(II): If $t \in V(\Gamma_2^i)$,then $\tau_{\Gamma_1 \odot \Gamma_2}(t) = (p_2-1) - d_{\Gamma_2^i}(t) + d_{\Gamma_1}(t_i)$.

$$\begin{aligned} &ZC_2^*(\Gamma_1 \odot \Gamma_2) \\ &\quad = \sum_{st \in E(\Gamma_1 \odot \Gamma_2)} [d_{(\Gamma_1 \odot \Gamma_2)}(s)\tau_{(\Gamma_1 \odot \Gamma_2)}(t) \\ &\qquad + d_{(\Gamma_1 \odot \Gamma_2)}(t)\tau_{(\Gamma_1 \odot \Gamma_2)}(s)] \\ &\quad = \sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2) \\ s,t \in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(t) + d_{\Gamma_1}(t)\tau_{\Gamma_1}(s)] \\ &\qquad + \sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2) \\ s,t \in V(\Gamma_2)}} [d_{\Gamma_2}(s)\tau_{\Gamma_2}(t) + d_{\Gamma_2}(t)\tau_{\Gamma_2}(s)] \\ &\qquad + \sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2) \\ s \in V(\Gamma_1) \wedge t \in V(\Gamma_2)}} [d_{\Gamma_1}(s)\tau_{\Gamma_2}(t) + d_{\Gamma_2}(t)\tau_{\Gamma_1}(s)]. \end{aligned}$$

Taking

$$\begin{aligned} &\sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2) \\ s,t \in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(t) + d_{\Gamma_1}(t)\tau_{\Gamma_1}(s)] \\ &= \sum_{st \in E(\Gamma_1)} [\{d_{\Gamma_1}(s)+p_2\}\{\tau_{\Gamma_1}(t)+p_2d_{\Gamma_1}(t)\} + \{d_{\Gamma_1}(t)+p_2\} \\ &\quad \times \{\tau_{\Gamma_1}(s)+p_2d_{\Gamma_1}(s)\}] \\ &= \sum_{st \in E(\Gamma_1)} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(t)+p_2d_{\Gamma_1}(s)d_{\Gamma_1}(t)+p_2\tau_{\Gamma_1}(t)+p_2^2 \\ &\quad \times d_{\Gamma_1}(t)+d_{\Gamma_1}(t)\tau_{\Gamma_1}(s)+p_2d_{\Gamma_1}(s)d_{\Gamma_1}(t)+p_2\tau_{\Gamma_1}(s) \\ &\quad +p_2^2d_{\Gamma_1}(s)] \\ &= ZC_2^*(\Gamma_1)+2p_2M_2(\Gamma_1)+p_2ZC_1^*(\Gamma_1)+p_2^2M_1(\Gamma_1). \end{aligned}$$

Also taking

$$\begin{aligned} &\sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2) \\ s,t \in V(\Gamma_2)}} [d_{\Gamma_2}(s)\tau_{\Gamma_2}(t) + d_{\Gamma_2}(t)\tau_{\Gamma_2}(s)] \\ &= \sum_{i=1}^{n_1} \sum_{st \in E(\Gamma_2^i)} [\{(d_{\Gamma_2^i}(s)+1\}\{(p_2-1)-d_{\Gamma_2^i}(t)+d_{\Gamma_1}(s_i)\} \\ &\quad +\{(d_{\Gamma_2^i}(t)+1\}\{(p_2-1)]-d_{\Gamma_2^i}(s)+d_{\Gamma_1}(s_i)\} \\ &= \sum_{i=1}^{p_1} [(p_2-1)M_1(\Gamma_2)-2M_2(\Gamma_2)+d_{\Gamma_1}(t_i)M_1(\Gamma_2)+2q_2 \\ &\quad \times(p_2-1)-M_1(\Gamma_2)+2q_2d_{\Gamma_1}(t_i)] \\ &= p_1(p_2-1)M_1(\Gamma_2)-2p_1M_2(\Gamma_2)+2q_1M_1(\Gamma_2)+2p_1 \\ &\quad \times(p_2-1)q_2-p_1M_1(\Gamma_2)+4q_1q_2. \end{aligned}$$

Again taking

$$\begin{aligned} &\sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2) \\ s \in V(\Gamma_1) \wedge t \in V(\Gamma_2)}} [d_{\Gamma_1}(s)\tau_{\Gamma_2}(t) + d_{\Gamma_2}(t)\tau_{\Gamma_1}(s)] \\ &= \sum_{i=1}^{p_1} \sum_{t \in V(\Gamma_2^i)} [\{d_{\Gamma_1}(s_i)+p_2\}\{(p_2-1)-d_{\Gamma_2^i}(t)+d_{\Gamma_1}(s_i)\} \\ &\quad +\{d_{\Gamma_2^i}(t)+1\}\{\tau_{\Gamma_1}(s_i)+p_2d_{\Gamma_1}(s_i)\}] \\ &= 2p_2(p_2-1)q_1-4q_1q_2+p_2M_1(\Gamma_1) \\ &\quad +p_1p_2^2(p_2-1)-2p_1p_2q_2 \\ &\quad +4p_2^2q_1+2q_2[M_1(\Gamma_1)-2q_1] \\ &\quad +4p_2q_1q_2+p_2[M_1(\Gamma_1)-2q_1]. \end{aligned}$$

Consequently,

$$\begin{aligned} &ZC_2^*(\Gamma_1 \odot \Gamma_2) \\ &= ZC_2^*(\Gamma_1)+p_2ZC_1^*(\Gamma_1)+2p_2M_2(\Gamma_1) \\ &\quad -2p_1M_2(\Gamma_2)+(p_2^2+2p_2+2q_2)M_1(\Gamma_1) \\ &\quad +[p_1(p_2-1)-p_1 \\ &\quad +2q_1]M_1(\Gamma_2)+p_1p_2^2(p_2-1)+2p_2(3p_2-2)q_1-2p_1q_2 \\ &\quad +4(p_2-1)q_1q_2. \end{aligned}$$

Proof (b):

$$\begin{aligned}
&ZC_3^*(\Gamma_1 \odot \Gamma_2)\\
&= \sum_{st \in E(\Gamma_1 \odot \Gamma_2)} [d_{(\Gamma_1 \odot \Gamma_2)}(s)\tau_{(\Gamma_1 \odot \Gamma_2)}(s)\\
&\quad + d_{(\Gamma_1 \odot \Gamma_2)}(t)\tau_{(\Gamma_1 \odot \Gamma_2)}(t)]\\
&= \sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2)\\ s,t \in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(s) + d_{\Gamma_1}(t)\tau_{\Gamma_1}(t)]\\
&\quad + \sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2)\\ s,t \in V(\Gamma_2)}} [d_{\Gamma_2}(s)\tau_{\Gamma_2}(s) + d_{\Gamma_2}(t)\tau_{\Gamma_2}(t)]\\
&\quad + \sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2)\\ s \in V(\Gamma_1) \wedge t \in V(\Gamma_2)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(s) + d_{\Gamma_2}(t)\tau_{\Gamma_2}(t)].
\end{aligned}$$

Taking

$$\begin{aligned}
&\sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2)\\ s,t \in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(s) + d_{\Gamma_1}(t)\tau_{\Gamma_1}(t)]\\
&= \sum_{st \in E(\Gamma_1)} [\{d_{\Gamma_1}(s) + p_2\}\{\tau_{\Gamma_1}(s) + p_2 d_{\Gamma_1}(s)\}\\
&\quad + \{d_{\Gamma_1}(t) + p_2\}\{\tau_{\Gamma_1}(t) + p_2 d_{\Gamma_1}(t)\}]\\
&= ZC_3^*(\Gamma_1) + p_2 M_3(\Gamma_1) + p_2 ZC_1^*(\Gamma_1) + p_2^2 M_1(\Gamma_1).
\end{aligned}$$

Also taking

$$\begin{aligned}
&\sum_{\substack{st \in E(\Gamma_1 \odot \Gamma_2)\\ s,t \in V(\Gamma_2)}} [d_{\Gamma_2}(s)\tau_{\Gamma_2}(s) + d_{\Gamma_2}(t)\tau_{\Gamma_2}(t)]\\
&= \sum_{i=1}^{p_1} \sum_{st \in E(\Gamma_2^i)} [\{(d_{\Gamma_2^i}(s) + 1\}\{(p_2 - 1) - d_{\Gamma_2^i}(s) + d_{\Gamma_1}(s_i)\}\\
&\quad + \{(d_{\Gamma_2^i}(t) + 1\}\{(p_2 - 1)] - d_{\Gamma_2^i}(t) + d_{\Gamma_1}(s_i)\}\\
&= p_1(p_2 - 1)M_1(\Gamma_2) - p_1 M_3(\Gamma_2) + 2q_1 M_1(\Gamma_2) + 2p_1\\
&\quad \times (p_2 - 1)q_2 - p_1 M_1(\Gamma_2) + 4q_1 q_2.
\end{aligned}$$

Again taking

$$\begin{aligned}
&\sum_{\substack{st \in E(\Gamma_1 \circ \Gamma_2)\\ s \in V(\Gamma_1) \wedge t \in V(\Gamma_2)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(s) + d_{\Gamma_2}(t)\tau_{\Gamma_2}(t)]\\
&= \sum_{i=1}^{n_1} \sum_{t \in V(\Gamma_2^i)} [\{d_{\Gamma_1}(s_i) + p_2\}\{\tau_{\Gamma_1}(s_i) + p_2 d_{\Gamma_1}(s_i)\}\\
&\quad + \{d_{\Gamma_2^i}(t) + 1\}\{(p_2 - 1) - d_{\Gamma_2^i}(t) + d_{\Gamma_1}(s_i)\}]\\
&= p_2 ZC_1^*(\Gamma_1) + p_2^2 M_1(\Gamma_1) + p_2^2[M_1(\Gamma_1) - 2q_1] + 2p_2^3 q_1\\
&\quad + 2p_1(p_2 - 1)q_2 - p_1 M_1(\Gamma_2) + 4q_1 q_2 + p_1 p_2(p_2 - 1)\\
&\quad - 2p_1 q_2 + 2p_2 q_1.
\end{aligned}$$

Consequently,

$$\begin{aligned}
&ZC_3^*(\Gamma_1 \odot \Gamma_2)\\
&= ZC_3^*(\Gamma_1) + 2p_2 ZC_1^*(\Gamma_1) + p_2 M_3(\Gamma_1)\\
&\quad - p_1 M_3(\Gamma_2) + 3p_2^2 M_1(\Gamma_1) + (p_1 p_2 - 3p_1 + 2q_1)M_1(\Gamma_2)\\
&\quad + p_1 p_2(p_2 - 1) + 2p_2(p_2^2 - p_2 + 1)q_1\\
&\quad + 2p_1(2p_2 - 3)q_2 + 8q_1 q_2.
\end{aligned}$$

VI. RESULTS FOR MODIFIED COINDICES

This section contains the general results for the modified first ZCCI ($M\bar{Z}C_1$) and modified second ZCCI ($M\bar{Z}C_2$) on product of molecular-networks i.e. lexicographic product and corona product.

Theorem 5.1: Let Γ_1 and Γ_2 be two connected and $\{C_3, C_4\}-$ free graphs. Then, $M\bar{Z}C_1$ and $M\bar{Z}C_2$ of the composition or lexicographic product $(\Gamma_1 \cdot \Gamma_2)$ of Γ_1 and Γ_2 are as follows:

(a)

$$\begin{aligned}
&M\bar{Z}C_1(\Gamma_1 \cdot \Gamma_2)\\
&= 2p_2^2\mu_2 ZC_1^*(\Gamma_1) + p_2^2(p_2 + 2\mu_2)\\
&\quad \times M\bar{Z}C_1(\Gamma_1) + 2p_2 q_2 \bar{Z}C_1(\Gamma_1) - 2(p_1 + 2\mu_1)\bar{M}_2(\Gamma_2)\\
&\quad + [p_2(p_2 - 1)(p_2 + 2\mu_2) - 2p_2 q_2]\bar{M}_1(\Gamma_1)\\
&\quad + [p_2(M_1(\Gamma_1) - 4q_1)\\
&\quad + (p_2 - 1)(p_1 + 2\mu_1)]\bar{M}_1(\Gamma_2) - 2\mu_1 M_1(\Gamma_2) + 4(p_2 - 1)\\
&\quad \times (p_2 q_1 \mu_2 + q_2 \mu_1) - 2p_2 JC_1(\Gamma_1, \Gamma_2) + 2p_2 JC_2(\Gamma_2, \Gamma_1),
\end{aligned}$$

(b)

$$\begin{aligned}
&M\bar{Z}C_2(\Gamma_1 \cdot \Gamma_2)\\
&= 2p_2^2\mu_2 ZC_1^*(\Gamma_1) + p_2^2(p_2 + 2\mu_2)\\
&\quad \times M\bar{Z}C_2(\Gamma_1) + 2p_2 q_2 \bar{Z}C_1(\Gamma_1) - (p_1 + 2\mu_1)\bar{F}(\Gamma_2)\\
&\quad + [p_2(p_2 - 1)(p_2 + 2\mu_2) - 2p_2 q_2]\bar{M}_1(\Gamma_1)\\
&\quad + [p_2(M_1(\Gamma_1) - 4q_1)\\
&\quad + (p_2 - 1)(p_1 + 2\mu_1)]\bar{M}_1(\Gamma_2) - 2\mu_1 M_1(\Gamma_2) + 4(p_2 - 1)\\
&\quad \times (p_2 q_1 \mu_2 + q_2 \mu_1) - 2p_2 JC_3(\Gamma_1, \Gamma_2) + 2p_2 JC_4(\Gamma_2, \Gamma_1).
\end{aligned}$$

Proof (a):

$$\begin{aligned}
&M\bar{Z}C_1(\Gamma_1 \cdot \Gamma_2)\\
&= \sum_{(s_1,t_1)(s_2,t_2) \notin E(\Gamma_1 \cdot \Gamma_2)} [d_{\Gamma_1 \cdot \Gamma_2}(s_1, t_1)\\
&\quad \times \tau_{\Gamma_1 \cdot \Gamma_2}(s_2, t_2) + d_{\Gamma_1 \cdot \Gamma_2}(s_2, t_2)\tau_{\Gamma_1 \cdot \Gamma_2}(s_1, t_1)]\\
&= \sum_{s \in V(\Gamma_1)} \sum_{\substack{t_1 t_2 \notin E(\Gamma_2)\\ s_1 = s_2}} [d(s, t_1)\tau(s, t_2) + d(s, t_2)\tau(s, t_1)]\\
&\quad + \sum_{t \in V(\Gamma_2)} \sum_{\substack{s_1 s_2 \notin E(\Gamma_1)\\ t_1 = t_2}} [d(s_1, t)\tau(s_2, t) + d(s_2, t)\tau(s_1, t)]\\
&\quad + \sum_{\substack{s_1 s_2 \notin E(\Gamma_1)\\ s_1 \neq s_2 \wedge s_1 \backsim s_2}} \sum_{\substack{t_1 t_2 \notin E(\Gamma_2)\\ t_1 \neq t_2 \wedge t_1 \backsim t_2}} [d(s_1, t_1)\tau(s_2, t_2) + d(s_2, t_2)\\
&\quad \times \tau(s_1, t_1)] + \sum_{\substack{s_1 s_2 \notin E(\Gamma_1)\\ s_1 \neq s_2 \wedge s_1 \backsim s_2}} \sum_{\substack{t_1 t_2 \notin E(\Gamma_2)\\ t_1 \neq t_2 \wedge t_1 \nsim t_2}} [d(s_1, t_1)\tau(s_2, t_2)\\
&\quad + d(s_2, t_2)\tau(s_1, t_1)]
\end{aligned}$$

Taking

$$\begin{aligned}
&\sum_{s \in V(\Gamma_1)} \sum_{\substack{t_1 t_2 \notin E(\Gamma_2)\\ s_1 = s_2}} [d(s, t_1)\tau(s, t_2) + d(s, t_2)\tau(s, t_1)]\\
&= \sum_{s \in V(\Gamma_1)} \sum_{\substack{t_1 t_2 \notin E(\Gamma_2)\\ s_1 = s_2}} [\{p_2 d_{\Gamma_1}(s) + d_{\Gamma_2}(t_1)\}\{p_2 \tau_{\Gamma_1}(s)
\end{aligned}$$

$$+(p_2-1)-d_{\Gamma_2}(t_2)\}+\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s)+(p_2-1)-d_{\Gamma_2}(t_1)\}]$$

Similarly,

$$=2p_2^2\mu_2ZC_1^*(\Gamma_1)+4p_2(p_2-1)q_1\mu_2-2p_2q_1\bar{M}_1(\Gamma_2)+p_2\times[M_1(\Gamma_1)-2q_1]\bar{M}_1(\Gamma_2)+p_1(p_2-1)\bar{M}_1(\Gamma_2)-2p_1\bar{M}_2(\Gamma_2).$$

Also taking

$$\sum_{t\in V(\Gamma_2)}\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ t_1=t_2}}[d(s_1,t)\tau(s_2,t)+d(s_2,t)\tau(s_1,t)]$$
$$=\sum_{t\in V(\Gamma_2)}\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ t_1=t_2}}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t)\}\{p_2\tau_{\Gamma_1}(s_2)+(p_2-1)-d_{\Gamma_2}(t)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t)\}\{p_2\tau_{\Gamma_1}(s_1)+(p_2-1)-d_{\Gamma_2}(t)\}]$$

Similarly,

$$=p_2^3M\bar{Z}C_1(\Gamma_1)+p_2^2(p_2-1)\bar{M}_1(\Gamma_1)-2p_2q_2\bar{M}_1(\Gamma_1)+2p_2q_2\bar{Z}C_1(\Gamma_1)+4(p_2-1)q_2\mu_1-2\mu_1M_1(\Gamma_2).$$

Again taking

$$\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\backsim t_2}}[d(s_1,t_1)\tau(s_2,t_2)+d(s_2,t_2)\tau(s_1,t_1)]$$
$$=2\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\backsim t_2}}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t_1)\}\times\{p_2\tau_{\Gamma_1}(s_2)+(p_2-1)-d_{\Gamma_2}(t_2)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t_2)\}\times\{p_2\tau_{\Gamma_1}(s_1)+(p_2-1)-d_{\Gamma_2}(t_1)\}]$$

Using Lemma 2.7, we have

$$=2p_2^2\mu_2M\bar{Z}C_1(\Gamma_1)+2p_2(p_2-1)\mu_2\bar{M}_1(\Gamma_1)-2p_2JC_1(\Gamma_1,\Gamma_2)+2p_2JC_2(\Gamma_2,\Gamma_1)+2(p_2-1)\mu_1\bar{M}_1(\Gamma_2)-4\mu_1\bar{M}_2(\Gamma_2).$$

Further taking (Null case)

$$N=\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\nsim t_2}}[d(s_1,t_1)\tau(s_2,t_2)+d(s_2,t_2)\tau(s_1,t_1)]=0$$

Consequently,

$$M\bar{Z}C_1(\Gamma_1\cdot\Gamma_2)=2p_2^2\mu_2ZC_1^*(\Gamma_1)+p_2^2(p_2+2\mu_2)\times M\bar{Z}C_1(\Gamma_1)+2p_2q_2\bar{Z}C_1(\Gamma_1)-2(p_1+2\mu_1)\bar{M}_2(\Gamma_2)+[p_2(p_2-1)(p_2+2\mu_2)-2p_2q_2]\bar{M}_1(\Gamma_1)+[p_2(M_1(\Gamma_1)-4q_1)+(p_2-1)(p_1+2\mu_1)]\bar{M}_1(\Gamma_2)-2\mu_1M_1(\Gamma_2)+4(p_2-1)\times(p_2q_1\mu_2+q_2\mu_1)-2p_2JC_1(\Gamma_1,\Gamma_2)+2p_2JC_2(\Gamma_2,\Gamma_1).$$

Proof (b):

$$M\bar{Z}C_2(\Gamma_1\cdot\Gamma_2)=\sum_{(s_1,t_1)(s_2,t_2)\notin E(\Gamma_1\cdot\Gamma_2)}[d_{\Gamma_1\cdot\Gamma_2}(s_1,t_1)\times\tau_{\Gamma_1\cdot\Gamma_2}(s_1,t_1)+d_{\Gamma_1\cdot\Gamma_2}(s_2,t_2)\tau_{\Gamma_1\cdot\Gamma_2}(s_2,t_2)]$$
$$=\sum_{s\in V(\Gamma_1)}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ s_1=s_2}}[d(s,t_1)\tau(s,t_1)+d(s,t_2)\tau(s,t_2)]+\sum_{t\in V(\Gamma_2)}\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ t_1=t_2}}[d(s_1,t)\tau(s_1,t)+d(s_2,t)\tau(s_2,t)]$$
$$+\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\backsim t_2}}[d(s_1,t_1)\tau(s_1,t_1)+d(s_2,t_2)\times\tau(s_2,t_2)]+\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\nsim t_2}}[d(s_1,t_1)\tau(s_1,t_2)+d(s_2,t_2)\tau(s_2,t_2)]$$

Taking

$$\sum_{s\in V(\Gamma_1)}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ s_1=s_2}}[d(s,t_1)\tau(s,t_1)+d(s,t_2)\tau(s,t_2)]$$
$$=\sum_{s\in V(\Gamma_1)}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ s_1=s_2}}[\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_1)\}\{p_2\tau_{\Gamma_1}(s)+(p_2-1)-d_{\Gamma_2}(t_1)\}+\{p_2d_{\Gamma_1}(s)+d_{\Gamma_2}(t_2)\}\{p_2\tau_{\Gamma_1}(s)+(p_2-1)-d_{\Gamma_2}(t_2)\}]$$

Similarly,

$$=2p_2^2\mu_2ZC_1^*(\Gamma_1)+4p_2(p_2-1)q_1\mu_2-2p_2q_1\bar{M}_1(\Gamma_2)+p_2[M_1(\Gamma_1)-2q_1]\bar{M}_1(\Gamma_2)+p_1(p_2-1)\bar{M}_1(\Gamma_2)-p_1\bar{F}(\Gamma_2).$$

Also taking

$$\sum_{t\in V(\Gamma_2)}\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ t_1=t_2}}[d(s_1,t)\tau(s_1,t)+d(s_2,t)\tau(s_2,t)]$$
$$=\sum_{t\in V(\Gamma_2)}\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ t_1=t_2}}[\{p_2d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t)\}\{p_2\tau_{\Gamma_1}(s_1)+(p_2-1)-d_{\Gamma_2}(t)\}+\{p_2d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t)\}\{p_2\tau_{\Gamma_1}(s_2)+(p_2-1)-d_{\Gamma_2}(t)\}]$$

Similarly,

$$=p_2^3M\bar{Z}C_2(\Gamma_1)+p_2^2(p_2-1)\bar{M}_1(\Gamma_1)-2p_2q_2\bar{M}_1(\Gamma_1)+2p_2q_2\bar{Z}C_1(\Gamma_1)+4(p_2-1)q_2\mu_1-2\mu_1M_1(\Gamma_2).$$

Again taking

$$\sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}}\sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\backsim t_2}}[d(s_1,t_1)\tau(s_1,t_1)+d(s_2,t_2)\tau(s_2,t_2)]$$

$$
\begin{aligned}
&= 2 \sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}} \sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\backsim t_2}} [\{p_2 d_{\Gamma_1}(s_1)+d_{\Gamma_2}(t_1)\}\\
&\quad\times\{p_2\tau_{\Gamma_1}(s_1)+(p_2-1)-d_{\Gamma_2}(t_1)\}\\
&\quad+\{p_2 d_{\Gamma_1}(s_2)+d_{\Gamma_2}(t_2)\}\\
&\quad\times\{p_2\tau_{\Gamma_1}(s_2)+(p_2-1)-d_{\Gamma_2}(t_2)\}]
\end{aligned}
$$

Using Lemma 2.8, we have

$$
\begin{aligned}
&= 2p_2^2\mu_2 M\bar{Z}C_2(\Gamma_1)+2p_2(p_2-1)\mu_2\bar{M}_1(\Gamma_1)-2p_2\\
&\quad\times JC_3(\Gamma_1,\Gamma_2)+2p_2 JC_4(\Gamma_2,\Gamma_1)\\
&\quad+2(p_2-1)\mu_1\bar{M}_1(\Gamma_2)-2\mu_1\bar{F}(\Gamma_2).
\end{aligned}
$$

Further taking (Null case)

$$
\begin{aligned}
N &= \sum_{\substack{s_1s_2\notin E(\Gamma_1)\\ s_1\neq s_2\wedge s_1\backsim s_2}} \sum_{\substack{t_1t_2\notin E(\Gamma_2)\\ t_1\neq t_2\wedge t_1\nsim t_2}} [d(s_1,t_1)\tau(s_1,t_1)\\
&\quad+d(s_2,t_2)\tau(s_2,t_2)]=0
\end{aligned}
$$

Consequently,

$$
\begin{aligned}
&M\bar{Z}C_2(\Gamma_1\cdot\Gamma_2)\\
&= 2p_2^2\mu_2 ZC_1^*(\Gamma_1)+p_2^2(p_2+2\mu_2)\\
&\quad\times M\bar{Z}C_2(\Gamma_1)+2p_2q_2\bar{Z}C_1(\Gamma_1)-(p_1+2\mu_1)\bar{F}(\Gamma_2)\\
&\quad+[p_2(p_2-1)(p_2+2\mu_2)-2p_2q_2]\bar{M}_1(\Gamma_1)\\
&\quad+[p_2(M_1(\Gamma_1)-4q_1)\\
&\quad+(p_2-1)(p_1+2\mu_1)]\bar{M}_1(\Gamma_2)-2\mu_1 M_1(\Gamma_2)+4(p_2-1)\\
&\quad\times(p_2q_1\mu_2+q_2\mu_1)-2p_2 JC_3(\Gamma_1,\Gamma_2)+2p_2 JC_4(\Gamma_2,\Gamma_1).
\end{aligned}
$$

Theorem 5.2: Let Γ_1 and Γ_2 be two connected and $\{C_3, C_4\}-$ free graphs. Then, $M\bar{Z}C_1$ and $M\bar{Z}C_2$ of the corona product $(G_1\odot G_2)$ of Γ_1 and Γ_2 are as follows:

(a)

$$
\begin{aligned}
&M\bar{Z}C_1(\Gamma_1\odot\Gamma_2)\\
&= M\bar{Z}C_1(\Gamma_1)+p_2\bar{Z}C_1(\Gamma_1)+2\\
&\quad\times[p_2\bar{M}_2(\Gamma_1)-p_1\bar{M}_2(\Gamma_2)]+p_2^2\bar{M}_1(\Gamma_1)\\
&\quad+[p_1(p_2-2)+2q_1]\\
&\quad\times\bar{M}_1(\Gamma_2)+2\mu_2[p_1(p_2-1)+2q_1],
\end{aligned}
$$

(b)

$$
\begin{aligned}
&M\bar{Z}C_2(\Gamma_1\odot\Gamma_2)\\
&= M\bar{Z}C_2(\Gamma_1)+p_2\bar{Z}C_1(\Gamma_1)+p_2\\
&\quad\times\bar{F}(\Gamma_1)-p_1\bar{F}(\Gamma_2)+p_2^2\bar{M}_1(\Gamma_1)+[p_1(p_2-2)+2q_1]\\
&\quad\times\bar{M}_1(\Gamma_2)+2\mu_2[p_1(p_2-1)+2q_1].
\end{aligned}
$$

Proof (a):

$$
\begin{aligned}
&M\bar{Z}C_1(\Gamma_1\odot\Gamma_2)\\
&= \sum_{st\notin E(\Gamma_1\odot\Gamma_2)} [d_{\Gamma_1\odot\Gamma_2}(s)\tau_{\Gamma_1\odot\Gamma_2}(t)\\
&\quad+d_{\Gamma_1\odot\Gamma_2}(t)\tau_{\Gamma_1\odot\Gamma_2}(s)]\\
&= \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(t)+d_{\Gamma_1}(t)\tau_{\Gamma_1}(s)] + \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_2)}}\\
&\quad\times[d_{\Gamma_2}(s)\tau_{\Gamma_2}(t)+d_{\Gamma_2}(t)\tau_{\Gamma_2}(s)] + \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s\in V(\Gamma_1)\wedge t\in V(\Gamma_2)}}\\
&\quad\times[d_{\Gamma_1}(s)\tau_{\Gamma_2}(t)+d_{\Gamma_2}(t)\tau_{\Gamma_1}(s)]
\end{aligned}
$$

Taking

$$
\begin{aligned}
&\sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(t)+d_{\Gamma_1}(t)\tau_{\Gamma_1}(s)]\\
&\quad= \sum_{st\notin E(\Gamma_1)} [\{d_{\Gamma_1}(s)+p_2\}\{\tau_{\Gamma_1}(t)+p_2 d_{\Gamma_1}(t)\}\\
&\qquad+\{d_{\Gamma_1}(t)+p_2\}\{\tau_{\Gamma_1}(s)+p_2 d_{\Gamma_1}(s)\}]
\end{aligned}
$$

Similarly,

$$
= M\bar{Z}C_1(\Gamma_1)+2p_2\bar{M}_2(\Gamma_1)+p_2\bar{Z}C_1(\Gamma_1)+p_2^2\bar{M}_1(\Gamma_1).
$$

Also taking

$$
\begin{aligned}
&\sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_2)}} [d_{\Gamma_2}(s)\tau_{\Gamma_2}(t)+d_{\Gamma_2}(t)\tau_{\Gamma_2}(s)]\\
&= \sum_{i=1}^{n_1}\sum_{st\in E(\Gamma_2^i)} [\{d_{\Gamma_2^i}(s)+1\}\{(p_2-1)-d_{\Gamma_2^i}(t)+d_{\Gamma_1}(s_i)\}\\
&\quad+\{d_{\Gamma_2^i}(t)+1\}\{(p_2-1)-d_{\Gamma_2^i}(s)+d_{\Gamma_1}(s_i)\}]
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
&= p_1(p_2-1)\bar{M}_1(\Gamma_2)-2p_1\bar{M}_2(\Gamma_2)+2q_1\bar{M}_1(\Gamma_2)+2p_1\\
&\qquad\times(p_2-1)\mu_2-p_1\bar{M}_1(\Gamma_2)+4q_1\mu_2.
\end{aligned}
$$

Again taking (Null case)

$$
N = \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s\in V(\Gamma_1)\wedge t\in V(\Gamma_2)}} [d_{\Gamma_1}(s)\tau_{\Gamma_2}(t)+d_{\Gamma_2}(t)\tau_{\Gamma_1}(s)]=0.
$$

Consequently,

$$
\begin{aligned}
&M\bar{Z}C_1(\Gamma_1\odot\Gamma_2)\\
&= M\bar{Z}C_1(\Gamma_1)+n_2\bar{Z}C_1(\Gamma_1)+2[p_2\bar{M}_2(\Gamma_1)\\
&\quad-p_1\bar{M}_2(\Gamma_2)]+p_2^2\bar{M}_1(\Gamma_1)\\
&\quad+[p_1(p_2-2)+2q_1]\bar{M}_1(\Gamma_2)+2\mu_2\\
&\quad\times[p_1(p_2-1)+2q_1].
\end{aligned}
$$

Proof (b):

$$
\begin{aligned}
&M\bar{Z}C_2(\Gamma_1\odot\Gamma_2)\\
&= \sum_{st\notin E(\Gamma_1\odot\Gamma_2)} [d_{\Gamma_1\odot\Gamma_2}(s)\tau_{\Gamma_1\odot\Gamma_2}(s)\\
&\quad+d_{\Gamma_1\odot\Gamma_2}(t)\tau_{\Gamma_1\odot\Gamma_2}(t)]\\
&= \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_1)}} [d_{\Gamma_1}(s)\tau_{\Gamma_1}(s)+d_{\Gamma_1}(t)\tau_{\Gamma_1}(t)] + \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_2)}}\\
&\quad\times[d_{\Gamma_2}(s)\tau_{\Gamma_2}(s)+d_{\Gamma_2}(t)\tau_{\Gamma_2}(t)] + \sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s\in V(\Gamma_1)\wedge t\in V(\Gamma_2)}}\\
&\quad\times[d_{\Gamma_1}(s)\tau_{\Gamma_2}(s)+d_{\Gamma_2}(t)\tau_{\Gamma_1}(t)]
\end{aligned}
$$

Taking

$$\sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_1)}}[d_{\Gamma_1}(s)\tau_{\Gamma_1}(s)+d_{\Gamma_1}(t)\tau_{\Gamma_1}(t)]$$
$$=\sum_{st\notin E(\Gamma_1)}[\{d_{\Gamma_1}(s)+n_2\}\{\tau_{\Gamma_1}(s)+p_2d_{\Gamma_1}(s)\}+\{d_{\Gamma_1}(t)+p_2\}\times\{\tau_{\Gamma_1}(t)+p_2d_{\Gamma_1}(t)\}]$$

Similarly,

$$=M\bar{Z}C_2(\Gamma_1)+p_2\bar{F}(\Gamma_1)+p_2\bar{Z}C_1(\Gamma_1)+p_2^2\bar{M}_1(\Gamma_1).$$

Also taking

$$\sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s,t\in V(\Gamma_2)}}[d_{\Gamma_2}(s)\tau_{\Gamma_2}(s)+d_{\Gamma_2}(t)\tau_{\Gamma_2}(t)]$$
$$=\sum_{i=1}^{p_1}\sum_{st\in E(\Gamma_2^i)}[\{(d_{\Gamma_2^i}(s)+1\}\{(p_2-1)-d_{\Gamma_2^i}(s)+d_{\Gamma_1}(s_i)\}+\{(d_{\Gamma_2^i}(t)+1\}\{(p_2-1)]-d_{\Gamma_2^i}(t)+d_{\Gamma_1}(s_i)\}$$

Similarly,

$$=p_1(p_2-1)\bar{M}_1(\Gamma_2)-p_1\bar{F}_2(\Gamma_2)+2q_1\bar{M}_1(\Gamma_2)+2p_1\times(p_2-1)\mu_2-p_1\bar{M}_1(\Gamma_2)+4q_1\mu_2.$$

Again taking (Null case)

$$N=\sum_{\substack{st\notin E(\Gamma_1\odot\Gamma_2)\\ s\in V(\Gamma_1)\wedge t\in V(\Gamma_2)}}[d_{\Gamma_1}(s)\tau_{\Gamma_2}(s)+d_{\Gamma_2}(t)\tau_{\Gamma_1}(t)]=0.$$

Consequently,

$$\begin{aligned}&M\bar{Z}C_2(\Gamma_1\odot\Gamma_2)\\&=M\bar{Z}C_2(\Gamma_1)+p_2\bar{Z}C_1(\Gamma_1)+p_2\bar{F}(\Gamma_1)\\&\quad-p_1\bar{F}(\Gamma_2)+p_2^2\bar{M}_1(\Gamma_1)+[p_1(p_2-2)+2q_1]\bar{M}_1(\Gamma_2)\\&\quad+2\mu_2[p_1(p_2-1)+2q_1].\end{aligned}$$

VII. COMPARISONS, APPLICATIONS AND CONCLUSION

In that section, we compare modified indices and modified coindices based on connection number for the particular molecular networks such as fence, closed fence, alkene and cycloalkane, see Figures (7, 9, 11, and 13), related to the results given by Sections IV and V. We also develop the Tables $(2-6)$ with the help of numerical values for modified ZCIs (ZC_2^*, ZC_3^*) and modified ZCCs ($M\bar{Z}C_1, M\bar{Z}C_2$) of the aforesaid molecular-networks. The graphical depictions for connection based modified indices and coindices of above-said molecular networks are also depicted in Figures (8, 10, 12 and 14). Suppose that N_2 be a null network (of order 2), P_2, P_3, & P_5 be three particular alkanes known as paths (of orders 2, 3 & 5) and C_4 & C_6 be cycles (of orders 4 & 6). Moreover, for particular cases of main results in this section, we compare all results with respect to upper bounds due to $\{C_3, C_4\}$-not free networks and Γ_1 and Γ_2 are two undirected networks.

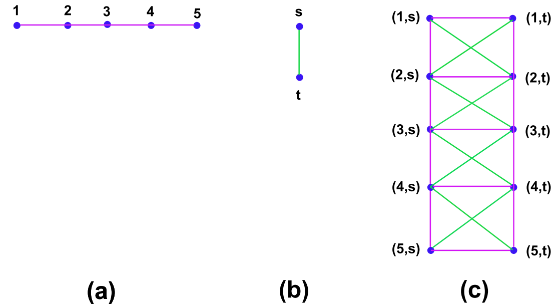

FIGURE 7. (a) $\Gamma_1 \cong P_5$ (b) $\Gamma_2 \cong P_2$ and (c) Fence $(P_5 \cdot P_2)$.

TABLE 2. Fence of $\theta_4 = P_m \cdot P_n$.

(m=n)	$ZC_2^*(\theta_4)$	$ZC_3^*(\theta_4)$	$M\bar{Z}C_4(\theta_4)$	$M\bar{Z}C_2(\theta_4)$
1	-18	-12	12	14
2	-128	-128	72	88
3	610	568	484	538
4	5568	5448	1728	1856
5	21958	21724	4476	4726
6	62272	61888	9592	10024
7	145722	145152	18132	18818
8	299680	298888	31344	32368
9	561118	560068	50668	52126
10	978048	976704	77736	79736
11	1610962	1609288	114372	117034
12	2534272	2532232	162592	166048
13	3837750	3835308	224604	228998
14	5627968	5625088	302808	308296
15	8029738	8026384	399796	406546

A. LEXICOGRAPHIC PRODUCT

(1) Fence: Let P_m and P_n be two particular alkanes called by paths, then the fence $(P_m \cdot P_n)$ are obtained by the lexicographic product of P_m and P_n. For $m = 5$ and $n = 2$, see Figure 7.

Using Theorem 5.1, modified ZCCs ($M\bar{Z}C_1$ and $M\bar{Z}C_2$) of fence are obtained as follows:

(i) $M\bar{Z}C_1(P_m \cdot P_n) \le 8mn^3 - 16mn - 8n^2 - 4n + 16m + 16$,

(ii) $M\bar{Z}C_2(P_m \cdot P_n) \le 8mn^3 - 16mn + 2n^3 - 8n^2 - 4n + 16m + 16$.

Using Theorem 4.1, modified ZCIs (ZC_2^* and ZC_3^*) of fence are as follows:

(i) $ZC_2^*(P_m \cdot P_n) \le 12mn^4 + 8mn^3 - 48mn - 28n^4 - 18n^3 + 48n + 40m - 32$,

(ii) $ZC_3^*(P_m \cdot P_n) \le 12mn^4 + 8mn^3 - 66mn - 28n^4 - 18n^3 + 60n + 76m - 56$.

Table 2 and Figure 8 depict the numerical and graphical behaviours for the modified ZCIs and modified ZCCs of fence using values $m = n$.

(2) Closed fence: Let C_m and P_n be a cycle and a particular alkane called by path, then the closed fence $(C_m \cdot P_n)$ are obtained by the lexicographic product of C_m and P_n. For $m = 4$ and $n = 2$, see Figure 9.

Using Theorem 5.1, modified ZCCs ($M\bar{Z}C_1$ and $M\bar{Z}C_2$) of closed fence are obtained as follows:

(i) $M\bar{Z}C_1(C_m \cdot P_n) \le 4mn^3 - 14mn - 8n^2 + 32n + 16m - 32$,

(ii) $M\bar{Z}C_2(C_m \cdot P_n) \le 4mn^3 - 14mn - 8n^2 + 32n + 16m - 32$.

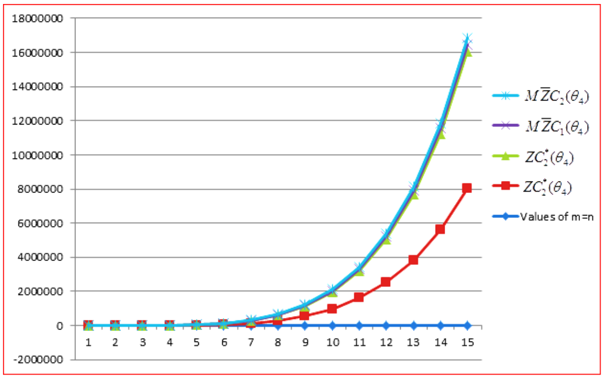

FIGURE 8. Fence of $\theta_4 = P_m \cdot P_n$ with respect to Table 2 for connection based modified indices and coindices.

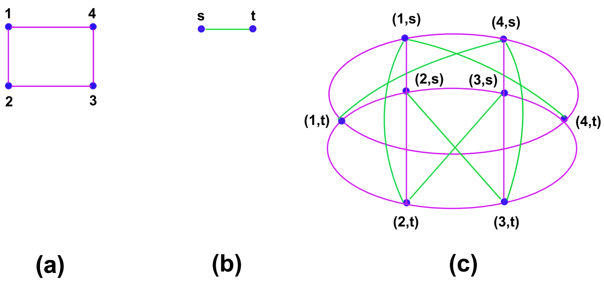

FIGURE 9. (a) $\Gamma_1 \cong C_4$ (b) $\Gamma_2 \cong P_2$ and (c) Closedfence ($C_4 \cdot P_2$).

TABLE 3. Closed fence of $\theta_5 = C_m \cdot P_n$.

(m=n)	$ZC_2^*(\theta_5)$	$ZC_3^*(\theta_5)$	$M\bar{Z}C_1(\theta_5)$	$M\bar{Z}C_2(\theta_5)$
1	4	22	-2	-2
2	208	208	40	40
3	1956	1902	238	238
4	8608	8464	832	832
5	26500	26230	2158	2158
6	65904	65472	4648	4648
7	141988	141358	8830	8830
8	275776	274912	15328	15328
9	495108	493974	24862	24862
10	835600	834160	38248	38248
11	1341604	1339822	56398	56398
12	2067168	2065008	80320	80320
13	3076996	3074422	111118	111118
14	4447408	4444384	149992	149992
15	6267300	6263790	198238	198238

Using Theorem 4.1, modified ZCIs (ZC_2^* and ZC_3^*) of closed fence are as follows:

(i) $ZC_2^*(C_m \cdot P_n) \leq 8mn^4 + 4mn^3 - 48mn + 40m$,

(ii) $ZC_3^*(C_m \cdot P_n) \leq 8mn^4 + 4mn^3 - 66mn + 76m$.

Table 3 and Figure 10 depict the numerical and graphical behaviours for the modified ZCIs and modified ZCCs of closed fence using values $m = n$.

B. CORONA PRODUCT

(3) Alkene (C_3H_6) : Let P_m and N_n be a particular alkene called by paths and a null graph, then the alkenes ($P_m \odot N_n$) are obtained by the corona product of P_m and N_n. For arbitrary $n = 2$, $n = 3$ and $m > 0$ yield equivalence

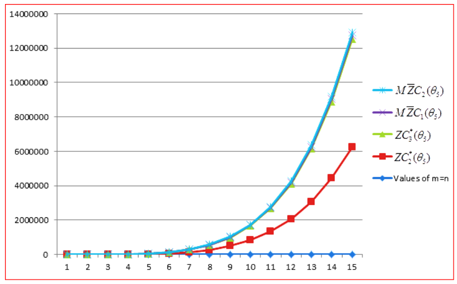

FIGURE 10. Closed fence of $\theta_5 = C_m \cdot P_n$ with respect to Table 3 for connection based modified indices and coindices.

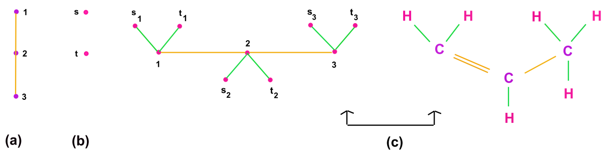

FIGURE 11. (a) $\Gamma_1 \cong P_3$ (b) $\Gamma_2 \cong N_2$ and (c) Alkene ($P_3 \odot N_2 \sim C_3H_6$).

TABLE 4. Alkanes of $\theta_6 = P_m \odot N_n$.

(m=n)	$ZC_2^*(\theta_6)$	$ZC_3^*(\theta_6)$	$M\bar{Z}C_1(\theta_6)$	$M\bar{Z}C_2(\theta_6)$
1	-18	-38	-2	0
2	39	30	7	9
3	262	308	32	32
4	765	970	79	75
5	1686	2238	154	144
6	3187	4382	263	245
7	5454	7720	412	384
8	8697	12618	607	567
9	13150	19490	854	800
10	19071	28798	1159	1089
11	26742	41052	1528	1440
12	36469	56810	1967	1859
13	48582	76678	2482	2352
14	63435	101310	3079	2925
15	81406	131408	3764	3584

alkenes and alkanes chemical networks, respectively. Any other sense liked as $n > 3$, we see their is no chemical shape of compounds with the help of corona product. So, we make alkene ($P_3 \odot N_2$) for $m = 3$ and $n = 2$, see Figure 11.

Using Theorem 5.2, modified ZCCs ($M\bar{Z}C_1$ and $M\bar{Z}C_2$) of alkanes are obtained as follows:

(i) $M\bar{Z}C_1(P_m \odot N_n) \leq mn^2 + 3mn - n^2 - 5n + m - 1$,

(ii) $M\bar{Z}C_2(P_m \odot N_n) \leq mn^2 + 2mn - n^2 - 2n + m - 1$.

Using Theorem 4.2, modified ZCIs (ZC_2^* and ZC_3^*) of alkanes are as follows:

(i) $ZC_2^*(P_m \odot N_n) \leq mn^3 + 9mn^2 + 16mn - 12n^2 - 34n + m + 1$,

(ii) $ZC_3^*(P_m \odot N_n) \leq 2mn^3 + 11mn^2 + 17mn - 2n^3 - 16n^2 - 36n + 8m - 22$.

Table 4 and Figure 12 depict the numerical and graphical behaviours for the modified ZCIs and modified ZCCs of alkanes using values $m = n$.

(7) Cyclohexane (C_6H_{12})**:** Let C_m and N_n be a cycle and a null graph, then Cycloalkanes ($C_m \odot N_n$) are obtained by the corona product of C_m and N_n. For arbitrary $n = 1$,

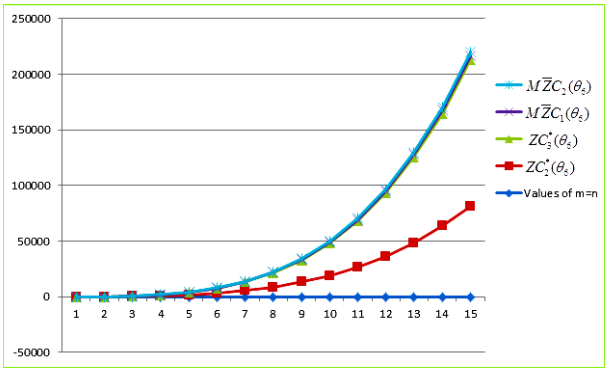

FIGURE 12. Alkanes of $\theta_6 = P_m \odot N_n$ with respect to Table 4 for connection based modified indices and coindices.

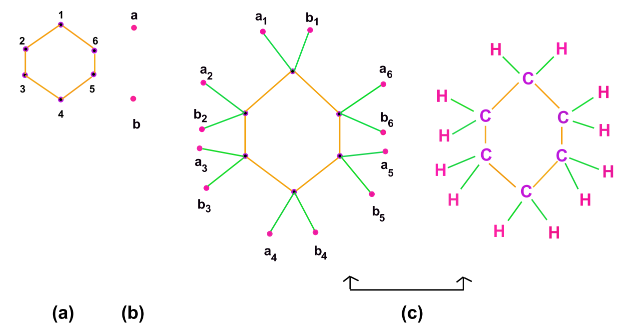

FIGURE 13. (a) $\Gamma_1 \cong C_6$ (b) $\Gamma_2 \cong N_2$ & (c) Cycloalkanes ($C_6 \odot N_2 \cong C_6H_{12}$).

TABLE 5. Cyclohenane of $\theta_7 = C_m \odot N_n$.

(m=n)	$ZC_2^*(\theta_7)$	$ZC_3^*(\theta_7)$	$M\bar{Z}C_1(\theta_7)$	$M\bar{Z}C_2(\theta_7)$
1	34	38	36	36
2	168	204	144	144
3	492	636	360	360
4	1120	1520	720	720
5	2190	3090	1260	1260
6	3864	5628	2016	2016
7	6328	9464	3024	3024
8	9792	14976	4320	4320
9	14490	22590	5940	5940
10	20680	32780	7920	7920
11	28644	46068	10296	10296
12	38688	63024	13104	13104
13	51142	84266	16380	16380
14	66360	110460	20160	20160
15	84720	142320	24480	24480

$n = 2$ and $m > 0$ yield equivalence cycloalkenes and cycloalkanes chemical networks, respectively. Any other sense liked as $n > 2$, we see their is no chemical shape of compounds with the help of corona product. So, we make Cycloalkanes ($C_6 \odot N_2$) for $m = 6$ and $n = 2$, see Figure 13.

Using Theorem 5.2, modified ZCCs ($M\bar{Z}C_1$ and $M\bar{Z}C_2$) of cycloalkanes are obtained as follows:

(i) $M\bar{Z}C_1(C_m \odot N_n) \leq 6mn^2 + 18mn + 12m$,

(ii) $M\bar{Z}C_2(C_m \odot N_n) \leq 6mn^2 + 18mn + 12m$.

Using Theorem 4.2, modified ZCIs (ZC_2^* and ZC_3^*) of cycloalkanes are as follows:

(i) $ZC_2^*(C_m \odot N_n) \leq mn^3 + 9mn^2 + 16mn + 8m$,

(ii) $ZC_3^*(C_m \odot N_n) \leq 2mn^3 + 11mn^2 + 17mn + 8m$.

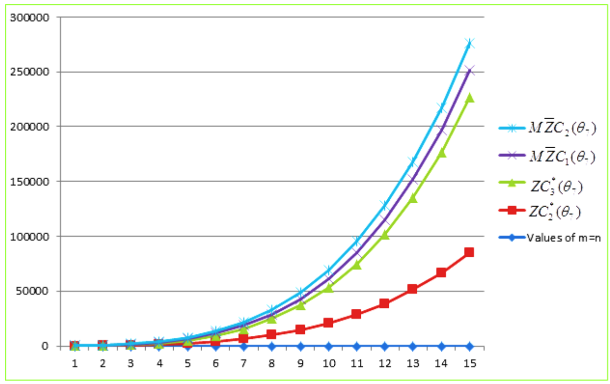

FIGURE 14. Cycloalkanes of $\theta_7 = C_m \circ N_n$ with respect to Table 7 for connection based modified indices and coindices.

TABLE 6. Particular numeric values for the obtained results of different molecular-networks.

Molecular-networks	ZC_2^*	ZC_3^*	$M\bar{Z}C_1$	$M\bar{Z}C_2$
$(P_4 \odot P_4)$	696	720	552	576
$(P_5 \odot P_2)$	208	212	156	168
$(P_3 \odot C_5)$	920	930	690	690
$(P_5[P_2])$	472	472	216	232
$(C_4[P_2])$	416	416	80	80
$(P_3 \circ N_2)$	116	132	18	18
$(C_6 \circ N_2)$	504	612	432	432

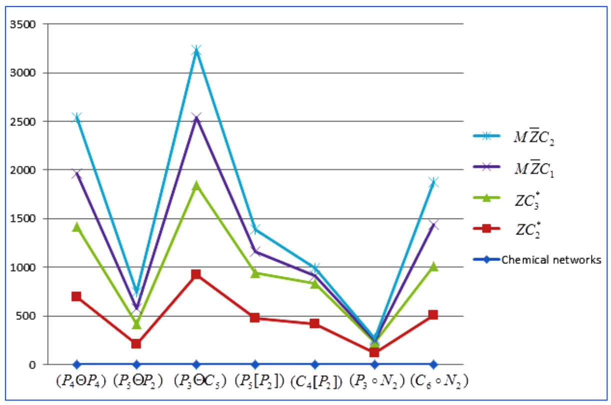

FIGURE 15. Comparisons of molecular-networks with respect to Table 6 for connection-based modified indices and coindices.

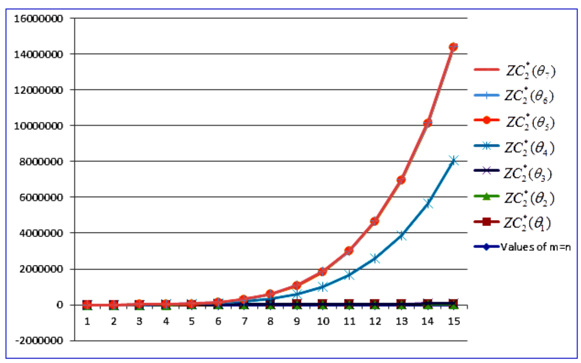

FIGURE 16. Comparisons of modified second ZCIs.

Table 5 and Figure 14 depict the numerical and graphical behaviours for the modified ZCIs and modified ZCCs of cycloalkanes using values $m = n$.

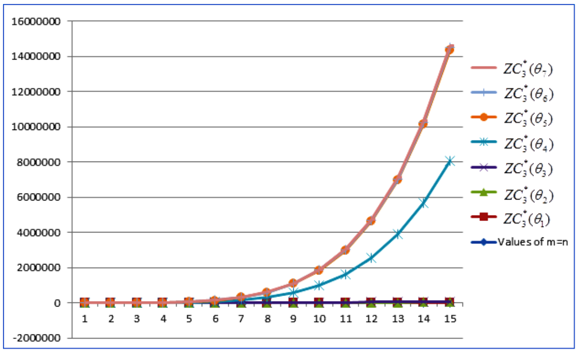

FIGURE 17. Comparisons of modified third ZCIs.

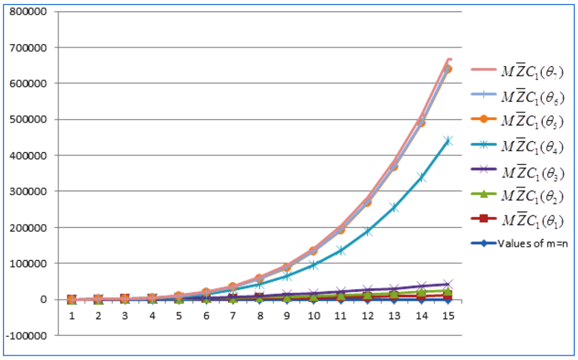

FIGURE 18. Comparisons of modified first ZCCIs.

VIII. CONCLUSION

Now, from Tables 2-6 and Figures 8, 10, 12, and 14-19, the discussion is closed with the following consequence's findings:

- All the modified indices and modified coindices based on connection number of the molecular-networks (fence, closed fence, alkene and cycloalkane) are similar with more values in ascending order respectively as: $M\bar{Z}C_2 \geq M\bar{Z}C_1 \geq ZC_3^* \geq ZC_2^*$.
- The modified third ZCI and the modified second ZCCI are responding steadily and quickly for increasing values of m and n in all the molecular networks (fence, closed fence, alkene and cycloalkane).
- In ascending order, all the modified indices and modified coindices based on connection number receive the upward values for different values of m and n. These general relations conclude that modified second ZCCI attains more upper layer than other TIs in all the molecular-networks.
- Table 6 and Figure 15 are depicted the particular comparisons for the obtained results of molecular-networks such as fence, closed fence, alkene and cycloalkane. This particular relation also concludes that modified second ZCCI attains more upper layer as similar to all the general relations.
- Moreover, Figures 16-19 provide the obtained results such as modified second ZCI, modified third ZCI, modified first ZCCI and modified second ZCC which are also depicted the molecular-networks fence to

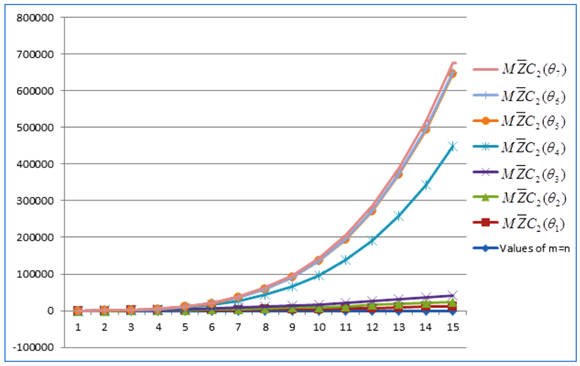

FIGURE 19. Comparisons of modified second ZCCIs.

cycloalkane in ascending order respectively. In addition, we also conclude that the last molecular network which is cycloalkane attains more upward layer than other molecular networks for modified indices and modified coindices based on connection number.

The resultant networks are obtained to the study of connection based modified indices and coindices via some other product of networks such as modular product, rooted product and zig zag product.

The investigation of these molecular descriptors for obtained from other operations of networks (subtration, addition, modular product and rooted product etc) is still open.

Conflicts of Interest: Authors declare that there is no conflict of interest.

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