Research Article

Computing Analysis for First Zagreb Connection Index and Coindex of Resultant Graphs

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A numeric parameter which studies the behaviour, structural, toxicological, experimental, and physicochemical properties of chemical compounds under several graphs' isomorphism is known as topological index. In 2018, Ali and Trinajstić studied the first Zagreb connection index (ZC_1) to evaluate the value of a molecule. This concept was first studied by Gutman and Trinajstić in 1972 to find the solution of π -electron energy of alternant hydrocarbons. In this paper, the first Zagreb connection index and coindex are obtained in the form of exact formulae and upper bounds for the resultant graphs in terms of different indices of their factor graphs, where the resultant graphs are obtained by the product-related operations on graphs such as tensor product, strong product, symmetric difference, and disjunction. At the end, an analysis of the obtained results for the first Zagreb connection index and coindex on the aforesaid resultant graphs is interpreted with the help of numerical values and graphical depictions.

1. Introduction

Topological indices (TIs) are used in the study of cheminformatics which has key role in the formational structure of quantitative structures' activity and property relationships to examine the chemical reactivity and experimental activity of a chemical compound in a molecular graph [1]. So, TIs predict both physical and chemical features that are defined in the molecular graphs such as surface tension, solubility, connectivity, freezing point, boiling point, melting point, critical temperature, polarizability, heat of evaporation, and formation [2]. In addition, the medical behaviours and a number of drug particles of different compounds have formed with the help of various TIs in the pharmaceutical networks (see [3]). In particular, the TIs called by connection number-based Zagreb indices are used to compute the correlation values among various octane isomers such as heat of evaporation, acentric factor, molecular weight, connectivity, critical temperature, stability, and density (see [4, 5]).

Product graphs play an essential part to develop new molecular graphs from simple graphs. For this purpose,

Ashrafi et al. [6] defined the concept of coindices for several products on graphs. Das et al. [7] computed upper bounds for multiplicative Zagreb indices of operations such as join, corona, Cartesian, disjunction, and composition. The reformulated, multiplicative, hyper, first, second, and third Zagreb coindices with certain properties are defined in [8–13]. Relations between Zagreb coindices and some distance-based indices are computed in [14]. For more details, see [15–18]. For this purpose, we can define some operations such as tensor product, strong product, symmetric difference, and disjunction in the following definitions.

Definition 1. Tensor (or Kronecker or conjunctive or direct) product of two graphs G_1 and G_2 is a graph $G_1 \otimes G_2$ with vertex set $V(G_1 \otimes G_2) = V(G_1) \otimes V(G_2)$ and edge set $E(G_1 \otimes G_2) = \{(a_1, b_1)(a_2, b_2), \text{ where } (a_1, b_1), (a_2, b_2) \in V(G_1) \otimes V(G_2)\}$ and

$$[a_1 a_2 \in E(G_1)] \wedge [b_1 b_2 \in E(G_2)]. \quad (1)$$

The connection number of a vertex (a, b) of $G_1 \otimes G_2$ is defined by $\tau_{Q_1 \otimes Q_2}(a, b) = \tau_{G_1}(a) + \tau_{G_2}(b) + \tau_{G_1}(a)\tau_{G_2}(b)$. For more details, see Figure 1.

Definition 2. Strong product or normal product $(G_1 \otimes G_2)$ of two graphs G_1 and G_2 is obtained by taking the vertex set and edge set as $V(Q_1 \otimes Q_2) = V(Q_1) \otimes V(Q_2)$ and $E(Q_1 \otimes Q_2) = \{(a_1, b_1)(a_2, b_2), \text{ where } (a_1, b_1), (a_2, b_2) \in V(Q_1) \otimes V(Q_2)\}$ with condition

$$\begin{aligned} &\text{either } [a_1 = a_2 \in V(G_1) \wedge b_1 b_2 \in E(Q_2)] \\ &\text{or } [b_1 = b_2 \in V(Q_2) \wedge a_1 a_2 \in E(Q_1)] \\ &\text{or } [a_1 a_2 \in E(Q_1)] \wedge [b_1 b_2 \in E(Q_2)]. \end{aligned} \quad (2)$$

The connection number of a vertex (a, b) of $Q_1 \otimes Q_2$ is defined by

$$\begin{aligned} \tau_{G_1 \otimes G_2}(a, b) &= \tau_{G_1}(a) + \tau_{G_2}(b) + d_{G_1}(a)\tau_{G_1}(a) \\ &\quad + d_{G_2}(b)\tau_{G_2}(b) + \tau_{G_1}(a)\tau_{G_2}(b) \\ &= \tau_{G_1}(a)[1 + d_{G_1}(a)] \\ &\quad + \tau_{G_2}(b)[1 + d_{G_2}(b) + \tau_{G_1}(a)], \end{aligned} \quad (3)$$

if $n_1, n_2 \geq 4$. For more details, see Figure 2.

Definition 3. Symmetric difference of two graphs Q_1 and Q_2 is a graph $G_1 \ominus G_2$ with vertex set $V(Q_1 \ominus Q_2) = V(Q_1) \ominus V(Q_2)$ and edge set $E(Q_1 \ominus Q_2) = \{(a_1, b_1)(a_2, b_2), \text{ where } (a_1, b_1), (a_2, b_2) \in V(Q_1) \ominus V(Q_2)\}$ and

$$\begin{aligned} &[a_1 a_2 \in E(Q_1)] \\ &\text{or } [b_1 b_2 \in E(Q_2)], \end{aligned} \quad (4)$$

but not both hold at the same time, respectively.

The connection number of a vertex (a, b) of $G_1 \ominus G_2$ is defined by

$$\begin{aligned} \tau_{G_1 \ominus G_2}(a, b) &= n_1 n_2 - 1 - n_2 d_{G_1}(a) - n_1 d_{G_2}(b) \\ &\quad + 2d_{G_1}(a)d_{G_2}(b) \\ &= n_2[n_1 - d_{G_1}(a)] + d_{G_2}(b)[2d_{G_1}(a) - n_1] - 1. \end{aligned} \quad (5)$$

For more details, see Figure 3.

Definition 4. Disjunction of two graphs G_1 and G_2 is a graph $G_1 \oplus G_2$ with vertex set $V(Q_1 \oplus Q_2) = V(Q_1) \oplus V(Q_2)$ and edge set $E(Q_1 \oplus Q_2) = \{(a_1, b_1)(a_2, b_2), \text{ where } (a_1, b_1), (a_2, b_2) \in V(Q_1) \oplus V(Q_2)\}$ and

$$\begin{aligned} &[a_1 a_2 \in E(Q_1)] \\ &\text{or } [b_1 b_2 \in E(Q_2)]. \end{aligned} \quad (6)$$

The connection number of a vertex (a, b) of $G_1 \oplus G_2$ is defined by

$$\begin{aligned} \tau_{G_1 \oplus G_2}(a, b) &= n_1 n_2 - 1 - n_2 d_{G_1}(a) - n_1 d_{G_2}(b) \\ &\quad + d_{G_1}(a)d_{G_2}(b) \\ &= n_2[n_1 - d_{G_1}(a)] + d_{G_2}(b)[d_{G_1}(a) - n_1] - 1. \end{aligned} \quad (7)$$

For more details, see Figure 4.

The graph theory provides the significant tools in the field of modern chemistry that is exploited to develop several types of molecular graphs and also predicts their chemical properties. In 1972, Gutman and Trinajstić [19] defined the first degree-based (number of vertices at distance one) TI called the first Zagreb index to compute the total π -electron energy of the molecules in molecular graphs. There are several TIs in literature, but degree-based TIs are studied more than others (see [20–29]).

Ali and Trinajstić [30] restudied the concept of connection number-based (number of vertices at distance two) TIs that were also defined by Gutman and Trinajstić in the same paper in 1972 to compute the total electron energy of the alternant hydrocarbons. They recalled them as Zagreb connection indices and reported that the chemical capability of the Zagreb connection indices is better than the classical Zagreb indices for the thirteen physicochemical properties of octane isomers. After two years, a few works have delivered on these connection number-based descriptors. Ali et al. [31] computed the analysis of Zagreb connection indices and coindices for some chemical structures of operations on graphs. For further studies and properties of the Zagreb connection indices, we refer to [32–40]. Recently, Gong et al. [41, 42] developed blocking lot-streaming flow shop scheduling problems and dynamic interval multi-objective optimization problems. These problems have been considered in various studies which have a close relation with the topic considered in this paper. For more details, see [43, 44].

In this paper, we compute the analysis for the first Zagreb connection index and coindex of the resultant graphs in the shape of exact formulae and upper bounds in terms of their factor graphs, where resultant graphs are obtained by operations such as tensor product, strong product, symmetric difference, and disjunction. Moreover, at the end, an analysis of the first Zagreb connection index and coindex on the aforesaid operations is included with the help of their numerical values and graphical depictions.

The rest of the paper is as follows: Section 2 represents the preliminary definitions and key results which are used in the main results, Section 3 contains the main results of product on graphs, and Section 4 includes the analysis and conclusions.

2. Preliminaries

Let $G = (V(G), E(G))$ be a simple graph such that the order and size of G are $|V(G)| = n$ and $|E(G)| = e$. The distance $d(a, b)$ between any two vertices a and b of a graph G is equal to the length of a shortest path connecting them. For $b \in V(G)$ and a positive integer p , $N_p(b/G) =$

FIGURE 1: (a) $G_1 \cong P_4$, (b) $G_2 \cong P_4$, and (c) tensor product $(P_4 \otimes P_4)$. FIGURE 2: (a) $G_1 \cong C_4$, (b) $G_2 \cong P_3$, and (c) strong product $(C_4 \otimes P_3)$. FIGURE 3: (a) $G_1 \cong C_3$, (b) $G_2 \cong P_2$, and (c) symmetric difference $(C_3 \oplus P_2)$.

$\{u \in V(G) : d(a, u) = p\}$ denotes the open p -neighborhood of a in a graph G , where $d_p(a/G) = |N_p(a/G)|$ is called p -distance degree of a vertex a in any graph G . The degree of a vertex a in a graph G is the number of edges incident on it, and it is denoted by $d_G(a)$. In particular:

If $p = 1$, $d_1(a/G) = |N_1(a/G)| = d_G(a) = \text{degree of } a$
(number of vertices at distance one from a)

If $p = 2$, $d_2(a/G) = |N_2(a/G)| = \tau_G(a) = \text{connection number of } a$ (number of vertices at distance two from a)

The complement of a graph G is denoted by $\overline{G}$. It is also simple with the same vertex set as of G , but edge set is defined as $E(\overline{G}) = \{ab : a, b \in V(G) \wedge ab \notin E(G)\}$. Thus, $E(G) \cup E(\overline{G}) = E(K_n)$, where K_n is a complete graph of

FIGURE 4: (a) $G_1 \cong C_3$, (b) $G_2 \cong P_2$, and (c) disjunction $(C_3 \cdot P_2)$.

order n and size $|E(K_n)| = \binom{n}{2}$. Moreover, if $|E(G)| = e$, then $|E(\overline{G})| = \binom{n}{2} - e = \mu$ and $d_{\overline{G}}(b) = n - 1 - d_G(b)$, where $d_G(b)$ and $d_{\overline{G}}(b)$ are the degrees of the vertex b in G and $\overline{G}$, respectively. Now, throughout the paper, for two graphs 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 $\overline{G}$ because the connection number works according to G . For any terminology or notion which are not mentioned here, we refer to [45, 46].

Definition 5. For a graph G , the first Zagreb index ($M_1(G)$) and second Zagreb index ($M_2(G)$) are defined as

$$\begin{aligned} M_1(G) &= \sum_{ab \in E(G)} [d_G(a) + d_G(b)], \\ M_2(G) &= \sum_{ab \in E(G)} [d_G(a) \times d_G(b)]. \end{aligned} \quad (8)$$

These degree-based indices are defined by Gutman, Trinajstić, and Ruscic (see [19, 47]) which are frequently used 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 [19, 48]. Symmetrical to these degree-based TIs, the connection-based TIs are discussed in Definitions 6 and 7.

Definition 6. For a graph G , the first Zagreb connection index ($ZC_1(G)$) is defined as

$$ZC_1(G) = \sum_{b \in V(G)} [\tau_G(b)]^2. \quad (9)$$

Definition 7. For a graph G , the modified first Zagreb connection index ($ZC_1^*(G)$) and second Zagreb connection index ($ZC_2(G)$) are defined as

$$\begin{aligned} ZC_1^*(G) &= \sum_{ab \in E(G)} [\tau_G(a) + \tau_G(b)], \\ ZC_2(G) &= \sum_{ab \in E(G)} [\tau_G(a) \times \tau_G(b)]. \end{aligned} \quad (10)$$

Definition 8. For a graph G , the first Zagreb coindex ($\overline{M}_1(G)$) and second Zagreb coindex ($\overline{M}_2(G)$) are defined as

$$\begin{aligned} \overline{M}_1(G) &= \sum_{ab \notin E(G)} [d_G(a) + d_G(b)], \\ \overline{M}_2(G) &= \sum_{ab \notin E(G)} [d_G(a) \times d_G(b)]. \end{aligned} \quad (11)$$

These coindices associated with the degree-based classical Zagreb indices are defined by Ashrafi et al. (see [6]). The coindices associated with the connection-based Zagreb indices are defined in Definition 9.

Definition 9. For a graph G , the first Zagreb connection coindex ($\overline{ZC}_1(G)$) and second Zagreb connection coindex ($\overline{ZC}_2(G)$) are defined as

$$\begin{aligned} \overline{ZC}_1(G) &= \sum_{ab \notin E(G)} [\tau_G(a) + \tau_G(b)], \\ \overline{ZC}_2(G) &= \sum_{ab \notin E(G)} [\tau_G(a) \times \tau_G(b)]. \end{aligned} \quad (12)$$

The modified coindices associated with the connection number-based Zagreb indices are defined in Definition 10. These modified coindices associated with the connection number-based Zagreb indices are defined by Ali et al. (see [49]).

Definition 10. For a graph G , the modified first Zagreb connection coindex ($M\overline{ZC}_1(G)$) and the modified second Zagreb connection coindex ($M\overline{ZC}_2(G)$) are defined as

$$\begin{aligned} M\bar{Z}C_1(K) &= \sum_{uv \notin E(K)} [d_K(u)\tau_K(v) + d_K(v)\tau_K(u)], \\ M\bar{Z}C_2(K) &= \sum_{uv \notin E(K)} [d_K(u)\tau_K(u) + d_K(v)\tau_K(v)]. \end{aligned} \quad (13)$$

The degree/connection-based coindices defined in Definitions 8–10 study the various physicochemical and isomer properties of molecules on the basis of the adjacency and nonadjacency pairs of vertices in the molecular networks. For more details, see [6, 30, 31, 36].

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

Lemma 1 (see [50]). *Let G be a connected graph and $\bar{G}$ be its complement with n vertices and e edges. Then,*

- (a) $\sum_{b \in V(G)} d_G(b) = 2e$
- (b) $M_1(\bar{G}) \geq M_1(G) - 4$

Lemma 2 (see [36]). *Let G be a connected and $\{C_3, C_4\}$ -free graph with n vertices and e edges. Then,*

- (a) $\sum_{b \in V(G_1)} \tau_{G_1}(b) = M_1(G_1) - 2e_1 = A$
- (b) $\sum_{b \in V(G_2)} \tau_{G_2}(b) = M_1(G_2) - 2e_2 = B$

3. Main Results

This section contains the main results for the first Zagreb connection index (ZC_1) and first Zagreb connection coindex ($\bar{Z}C_1$) of the product on graphs obtained under the operations of tensor product, strong product, symmetric difference, and disjunction.

Theorem 1. *Let G_1 and G_2 be two connected and $\{C_3, C_4\}$ -free graphs. Then, ZC_1 and $\bar{Z}C_1$ of the tensor product $(G_1 \otimes G_2)$ are*

$$ZC_1(G_1 \otimes G_2) = n_2 ZC_1(G_1) + n_1 ZC_1(G_2) + ZC_1(G_1)ZC_1(G_2) + 2AB + 2AZC_1(G_2) + 2BZC_1(G_1), \quad (14)$$

$$\bar{Z}C_1(G_1 \otimes G_2) = 2\mu_2 \bar{Z}C_1(G_1) + 2\mu_1 \bar{Z}C_1(G_2) + 2 \sum_{a_1 a_2 \notin E(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1}(a_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)]. \quad (15)$$

Proof. Since $\tau_{G_1 \otimes G_2}(a, b) = \tau_{G_1}(a) + \tau_{G_2}(b) + \tau_{G_1}(a)\tau_{G_2}(b)$, where $a \in V(G_1)$, $b \in V(G_2)$, and $(a, b) \in G_1 \otimes G_2$,

$$\begin{aligned} ZC_1(G_1 \otimes G_2) &= \sum_{(a,b) \in V(G_1 \otimes G_2)} [\tau_{G_1 \otimes G_2}(a, b)]^2 \\ &= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [\tau_{G_1}(a) + \tau_{G_2}(b) + \tau_{G_1}(a)\tau_{G_2}(b)]^2 \\ &= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [\tau_{G_1}^2(a) + \tau_{G_2}^2(b) + \tau_{G_1}^2(a)\tau_{G_2}^2(b) + 2\tau_{G_1}(a) + \tau_{G_2}(b) + 2\tau_{G_1}(a)\tau_{G_2}^2(b) + 2\tau_{G_1}^2(a)\tau_{G_2}(b)] \\ &= \sum_{a \in V(G_1)} [n_2 \tau_{G_1}^2(a) + ZC_1(G_2) + \tau_{G_1}^2(a)ZC_1(G_2) + 2\tau_{G_1}(a)\{M_1(G_2) - 2e_2\} \\ &\quad + 2\tau_{G_1}(a)ZC_1(G_2) + 2\tau_{G_1}^2(a)\{M_1(G_2) - 2e_2\}]. \end{aligned} \quad (16)$$

Using Lemma 2 (a) and (b),

$$ZC_1(G_1 \otimes G_2) = n_2 ZC_1(G_1) + n_1 ZC_1(G_2) + ZC_1(G_1)ZC_1(G_2) + 2AB + 2AZC_1(G_2) + 2BZC_1(G_1), \quad (17)$$

$$\begin{aligned} \bar{Z}C_1(G_1 \otimes G_2) &= \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \otimes G_2)} [\tau_{G_1 \otimes G_2}(a_1, b_1) + \tau_{G_1 \otimes G_2}(a_2, b_2)] \\ &= 2 \sum_{a_1 a_2 \notin E(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\{\tau_{G_1}(a_1) + \tau_{G_2}(b_1) + \tau_{G_1}(a_1)\tau_{G_2}(b_1)\} + \{\tau_{G_1}(a_2) + \tau_{G_2}(b_2) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)\}] \\ &= 2 \sum_{a_1 a_2 \notin E(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\{\tau_{G_1}(a_1) + \tau_{G_1}(a_2)\} + \{\tau_{G_2}(b_1) + \tau_{G_2}(b_2)\} + \{\tau_{G_1}(a_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)\}] \\ \bar{Z}C_1(G_1 \otimes G_2) &= 2\mu_2 \bar{Z}C_1(G_1) + 2\mu_1 \bar{Z}C_1(G_2) + 2 \sum_{a_1 a_2 \notin E(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1}(a_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)]. \end{aligned} \quad (18)$$

□

Theorem 2. Let G_1 and G_2 be two connected and $\{C_3, C_4\}$ -free graphs. Then, ZC_1 and $\overline{ZC}_1$ of the strong product $(G_1 \otimes G_2)$ are

$$\begin{aligned} ZC_1(G_1 \otimes G_2) = & 2BZC_1^*(G_1) + 2AZC_1^*(G_2) + 2ZC_1^*(G_1)ZC_1^*(G_2) + (n_2 + 2B)ZC_1(G_1) \\ & + (n_1 + 2A)ZC_1(G_2) + ZC_1(G_1)ZC_1(G_2) + 2AB + 2(n_2 + B) \sum_{a \in V(G_1)} d_{G_1}(a)\tau_{G_1}^2(a) + 2(n_1 + A) \\ & \cdot \sum_{b \in V(G_2)} d_{G_2}(b)\tau_{G_2}^2(b) + n_2 \sum_{a \in V(G_1)} d_{G_1}^2(a)\tau_{G_1}^2(a) + n_1 \sum_{b \in V(G_2)} d_{G_2}^2(b)\tau_{G_2}^2(b), \end{aligned} \quad (19)$$

$$\begin{aligned} \overline{ZC}_1(G_1 \otimes G_2) \leq & (n_2 + 2\mu_2)M\overline{ZC}_2(G_1) + (n_1 + 2\mu_1)M\overline{ZC}_2(G_2) + (n_2 + 2\mu_2 + B)\overline{ZC}_1(G_1) \\ & + (n_1 + 2\mu_1 + A)\overline{ZC}_1(G_2) + 2[\mu_2 ZC_1^*(G_1) + \mu_1 ZC_1^*(G_2)] + 2[\mu_2 A + \mu_1 B] \\ & + 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1}(a_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)]. \end{aligned} \quad (20)$$

Proof. Since $\tau_{G_1 \otimes G_2}(a, b) = \tau_{G_1}(a)[1 + d_{G_1}(a)] + \tau_{G_2}(b)[1 + d_{G_2}(b) + \tau_{G_1}(a)]$, where $a \in V(G_1)$, $b \in V(G_2)$, and $(a, b) \in G_1 \otimes G_2$,

$$\begin{aligned} ZC_1(G_1 \otimes G_2) = & \sum_{(a,b) \in V(G_1 \otimes G_2)} [\tau_{G_1 \otimes G_2}(a, b)]^2 \\ = & \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [\tau_{G_1}(a)\{1 + d_{G_1}(a)\} + \tau_{G_2}(b)\{1 + d_{G_2}(b) + \tau_{G_1}(a)\}]^2 \\ = & \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} \left[\tau_{G_1}^2(a)\{1 + d_{G_1}(a)\}^2 + \tau_{G_2}^2(b)\{1 + d_{G_2}(b) + \tau_{G_1}(a)\}^2 + \right. \\ & \left. 2\tau_{G_1}(a)\tau_{G_2}(b)\{1 + d_{G_1}(a)\}\{1 + d_{G_2}(b) + \tau_{G_1}(a)\} \right] \\ = & \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} \left[\tau_{G_1}^2(a)\{1 + d_{G_1}^2(a) + 2d_{G_1}(a)\} + \tau_{G_2}^2(b)\{1 + d_{G_2}(b)\}^2 + \tau_{G_1}^2(a) + 2\{1 + d_{G_2}(b)\}\tau_{G_1}(a) \right] \\ & + 2\tau_{G_1}(a)\tau_{G_2}(b)\{1 + d_{G_2}(b) + \tau_{G_1}(a) + d_{G_1}(a) + d_{G_1}(a)d_{G_2}(b) + d_{G_1}(a)\tau_{G_1}(a)\} \\ = & \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} \left[\tau_{G_1}^2(a) + d_{G_1}^2(a)\tau_{G_1}^2(a) + 2d_{G_1}(a)\tau_{G_1}^2(a) + \tau_{G_2}^2(b) + d_{G_2}^2(b)\tau_{G_2}^2(b) + d_{G_2}(b)\tau_{G_2}^2(b) \right. \\ & + \tau_{G_1}^2(a)\tau_{G_2}^2(b) + 2\tau_{G_1}(a)\tau_{G_2}^2(b) + 2d_{G_2}(b)\tau_{G_1}(a)\tau_{G_2}^2(b) + 2\tau_{G_1}(a)\tau_{G_2}(b) + 2d_{G_2}(b)\tau_{G_1}(a)\tau_{G_2}(b) \\ & \left. + 2\tau_{G_1}^2(a)\tau_{G_2}(b) + 2d_{G_1}(a)\tau_{G_1}(a)\tau_{G_2}(b) + 2d_{G_1}(a)\tau_{G_1}(a)d_{G_2}(b)\tau_{G_2}(b) + 2d_{G_1}(a)\tau_{G_1}^2(a)\tau_{G_2}(b) \right]. \end{aligned} \quad (21)$$

Using Lemma 2 (a) and (b),

$$\begin{aligned}
 ZC_1(G_1 \otimes G_2) &= 2BZC_1^*(G_1) + 2AZC_1^*(G_2) \\
 &\quad + 2ZC_1^*(G_1)ZC_1^*(G_2) + (n_2 + 2B)ZC_1(G_1) \\
 &\quad + (n_1 + 2A)ZC_1(G_2) + ZC_1(G_1)ZC_1(G_2) \\
 &\quad + 2AB + 2(n_2 + B) \sum_{a \in V(G_1)} d_{G_1}(a)\tau_{G_1}^2(a) \\
 &\quad + 2(n_1 + A) \sum_{b \in V(G_2)} d_{G_2}(b)\tau_{G_2}^2(b) \\
 &\quad + n_2 \sum_{a \in V(G_1)} d_{G_1}^2(a)\tau_{G_1}^2(a) + n_1 \sum_{b \in V(G_2)} d_{G_2}^2(b)\tau_{G_2}^2(b),
 \end{aligned} \tag{22}$$

$$\begin{aligned}
 \bar{Z}C_1(G_1 \otimes G_2) &= \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \otimes G_2)} [\tau_{G_1 \otimes G_2}(a_1, b_1) + \tau_{G_1 \otimes G_2}(a_2, b_2)] \\
 &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \otimes G_2}(a, b_1) + \tau_{G_1 \otimes G_2}(a, b_2)] \\
 &\quad + \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \otimes G_2}(a_1, b) + \tau_{G_1 \otimes G_2}(a_2, b)] \\
 &\quad + \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \otimes G_2}(a_1, b_1) + \tau_{G_1 \otimes G_2}(a_2, b_2)].
 \end{aligned} \tag{23}$$

We take

$$\begin{aligned}
 &\sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \otimes G_2}(a, b_1) + \tau_{G_1 \otimes G_2}(a, b_2)] \\
 &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} \left[\{ \tau_{G_1}(a) + \tau_{G_2}(b_1) + d_{G_1}(a)\tau_{G_1}(a) + d_{G_2}(b_1)\tau_{G_2}(b_1) + \tau_{G_1}(a)\tau_{G_2}(b_1) \} \right. \\
 &\quad \left. + \{ \tau_{G_1}(a) + d_{\tau_{G_2}(b_2)G_1}(a)\tau_{G_1}(a) + d_{G_2}(b_2)\tau_{G_2}(b_2) + \tau_{G_1}(a)\tau_{G_2}(b_2) \} \right] \\
 &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [2\tau_{G_1}(a) + \{ \tau_{G_2}(b_1) + \tau_{G_2}(b_2) \} + 2d_{G_1}(a)\tau_{G_1}(a) + \{ d_{G_2}(b_1)\tau_{G_2}(b_1) \\
 &\quad + d_{G_2}(b_2)\tau_{G_2}(b_2) \} + \tau_{G_1}(a)\{ \tau_{G_2}(b_1) + \tau_{G_2}(b_2) \}].
 \end{aligned} \tag{24}$$

We know that

$$\begin{aligned}
 \sum_{b_1 b_2 \notin E(G_2)} &= \binom{n_2}{2} - e_2 = \mu_2 \\
 &= 2\mu_2 A + n_1 \bar{Z}C_1(G_2) + 2\mu_2 ZC_1^*(G_1) + n_1 M \bar{Z}C_2(G_2) + A \bar{Z}C_1(G_2).
 \end{aligned} \tag{25}$$

Also, we take

$$\begin{aligned}
 &\sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \otimes G_2}(a_1, b) + \tau_{G_1 \otimes G_2}(a_2, b)] \\
 &\sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} \left[\{ \tau_{G_1}(a_1) + \tau_{G_2}(b) + d_{G_1}(a_1)\tau_{G_1}(a_1) + d_{G_2}(b)\tau_{G_2}(b) + \tau_{G_1}(a_1)\tau_{G_2}(b) \} \right. \\
 &\quad \left. + \{ \tau_{G_1}(a_2) + \tau_{G_2}(b) + d_{G_1}(a_2)\tau_{G_1}(a_2) + d_{G_2}(b)\tau_{G_2}(b) + \tau_{G_1}(a_2)\tau_{G_2}(b) \} \right] \\
 &= n_2 \bar{Z}C_1(G_1) + 2\mu_1 B + n_2 M \bar{Z}C_2(G_1) + 2\mu_1 ZC_1^*(G_2) + B \bar{Z}C_1(G_1).
 \end{aligned} \tag{26}$$

Again, we take

$$\begin{aligned}
& \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \otimes G_2}(a_1, b_1) + \tau_{G_1 \otimes G_2}(a_2, b_2)] \\
& \leq 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\{\tau_{G_1}(a_1) + \tau_{G_2}(b_1) + d_{G_1}(a_1)\tau_{G_1}(a_1) + d_{G_2}(b_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_1)\tau_{G_2}(b_1) \\
& + \{\tau_{G_1}(a_2) + \tau_{G_2}(b_2) + d_{G_1}(a_2)\tau_{G_1}(a_2) + d_{G_2}(b_2)\tau_{G_2}(b_2) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)\}].
\end{aligned} \tag{27}$$

Similarly = $2\mu_2 \overline{ZC}_1(G_1) + 2\mu_1 \overline{ZC}_1(G_2) + 2\mu_2 M \overline{ZC}_2(G_1) + 2\mu_1 M \overline{ZC}_2(G_2)$

$$+ 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1}(a_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)].$$

Consequently,

$$\begin{aligned}
\overline{ZC}_1(G_1 \otimes G_2) & \leq (n_2 + 2\mu_2)M \overline{ZC}_2(G_1) + (n_1 + 2\mu_1)M \overline{ZC}_2(G_2) + (n_2 + 2\mu_2 + B)\overline{ZC}_1(G_1) \\
& + (n_1 + 2\mu_1 + A)\overline{ZC}_1(G_2) + 2[\mu_2 ZC_1^*(G_1) + \mu_1 ZC_1^*(G_2)] + 2[\mu_2 A + \mu_1 B] \\
& + 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1}(a_1)\tau_{G_2}(b_1) + \tau_{G_1}(a_2)\tau_{G_2}(b_2)].
\end{aligned} \tag{28}$$

□

Theorem 3. Let G_1 and G_2 be two connected and $\{C_3, C_4\}$ -free graphs. Then, ZC_1 and $\overline{ZC}_1$ of the symmetric difference $(G_1 \ominus G_2)$ are

$$\begin{aligned}
ZC_1(G_1 \ominus G_2) & = n_2(n_2^2 - 8e_2)M_1(G_1) + n_1(n_1^2 - 8e_1)M_1(G_2) + 4M_1(G_1)M_1(G_2) \\
& + n_1 n_2(n_1^2 n_2^2 - 4n_2^2 e_1 - 4n_1^2 e_2 - 2n_1 n_2 + 24e_1 e_2 + 1) + 4(n_1^2 e_2 + n_2^2 e_1 - 4e_1 e_2),
\end{aligned} \tag{29}$$

$$\begin{aligned}
\overline{ZC}_1(G_1 \ominus G_2) & = (4e_2 - n_2^2)\overline{M}_1(G_1) + (4e_1 - n_1^2)\overline{M}_1(G_2) + 2\mu_1(n_1 n_2^2 - n_2 - 2n_1 e_2) \\
& + 2\mu_2(n_1^2 n_2 - n_1 - 2n_2 e_1).
\end{aligned} \tag{30}$$

Proof. Since $\tau_{G_1 \ominus G_2}(a, b) = n_2[n_1 - d_{G_1}(a)] + d_{G_2}(b) [2d_{G_1}(a) - n_1] - 1$, where $a \in V(G_1)$, $b \in V(G_2)$, and $(a, b) \in G_1 \ominus G_2$,

$$\begin{aligned}
ZC_1(G_1 \ominus G_2) &= \sum_{(a,b) \in V(G_1 \ominus G_2)} [\tau_{G_1 \ominus G_2}(a, b)]^2 \\
&= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [n_2 \{n_1 - d_{G_1}(a)\} + d_{G_2}(b) \{2d_{G_1}(a) - n_1\} - 1]^2 \\
&= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [n_2^2 \{n_1 - d_{G_1}(a)\}^2 + d_{G_2}^2(b) \{2d_{G_1}(a) - n_1\}^2 + 1 + 2n_2 d_{G_2}(b) \{n_1 - d_{G_1}(a)\} \\
&\quad \{2d_{G_1}(a) - n_1\} - 2d_{G_2}(b) \{2d_{G_1}(a) - n_1\} - 2n_2 \{n_1 - d_{G_1}(a)\}] \\
&= n_1^3 n_2^3 + n_2^3 M_1(G_1) - 4n_1 n_2^3 e_1 + 4M_1(G_1) M_1(G_2) + n_1^3 M_1(G_2) - 8n_1 e_1 M_1(G_2) + n_1 n_2 \\
&\quad + 16n_1 n_2 e_1 e_2 - 4n_1^3 n_2 e_2 - 8n_2 e_2 M_1(G_1) + 8n_1 n_2 e_1 e_2 - 16e_1 e_2 + 4n_1^2 e_2 - 2n_1^2 n_2^2 + 4n_2^2 e_1, \\
ZC_1(G_1 \ominus G_2) &= n_2(n_2^2 - 8e_2) M_1(G_1) + n_1(n_1^2 - 8e_1) M_1(G_2) + 4M_1(G_1) M_1(G_2) + n_1 n_2 \\
&\quad (n_1^2 n_2^2 - 4n_2^2 e_1 - 4n_1^2 e_2 - 2n_1 n_2 + 24e_1 e_2 + 1) + 4(n_1^2 e_2 + n_2^2 e_1 - 4e_1 e_2).
\end{aligned} \tag{31}$$

$$\begin{aligned}
\bar{Z}C_1(G_1 \ominus G_2) &= \sum_{(a_1, b_1), (a_2, b_2) \notin E(G_1 \ominus G_2)} [\tau_{G_1 \ominus G_2}(a_1, b_1) + \tau_{G_1 \ominus G_2}(a_2, b_2)] \\
&= \sum_{a \in V(G_1)} \sum_{b_1, b_2 \notin E(G_2)} [\tau_{G_1 \ominus G_2}(a, b_1) + \tau_{G_1 \ominus G_2}(a, b_2)] + \sum_{b \in V(G_2)} \sum_{a_1, a_2 \notin E(G_1)} [\tau_{G_1 \ominus G_2}(a_1, b) + \tau_{G_1 \ominus G_2}(a_2, b)] \\
&\quad \cdot \sum_{a \in V(G_1)} \sum_{b_1, b_2 \notin E(G_2)} [\tau_{G_1 \ominus G_2}(a, b_1) + \tau_{G_1 \ominus G_2}(a, b_2)] \sum_{b \in V(G_2)} \sum_{a_1, a_2 \notin E(G_1)} [\tau_{G_1 \ominus G_2}(a_1, b) + \tau_{G_1 \ominus G_2}(a_2, b)] \\
&\quad \cdot [\tau_{G_1 \ominus G_2}(a_1, b_1) + \tau_{G_1 \ominus G_2}(a_2, b_2)].
\end{aligned} \tag{32}$$

We take

$$\begin{aligned}
&\sum_{a \in V(G_1)} \sum_{b_1, b_2 \notin E(G_2)} [\tau_{G_1 \ominus G_2}(a, b_1) + \tau_{G_1 \ominus G_2}(a, b_2)] \\
&= \sum_{a \in V(G_1)} \sum_{b_1, b_2 \notin E(G_2)} [\{n_1 n_2 - 1 - n_2 d_{G_1}(a) - n_1 d_{G_2}(b_1) + 2d_{G_1}(a) d_{G_2}(b_1)\} \\
&\quad + \{n_1 n_2 - 1 - n_2 d_{G_1}(a) - n_1 d_{G_2}(b_2) + 2d_{G_1}(a) d_{G_2}(b_2)\}].
\end{aligned} \tag{33}$$

$$\text{Similarly} = 2n_1^2 n_2 \mu_2 - 2n_1 \mu_2 - 4n_2 e_1 \mu_2 - n_1^2 \bar{M}_1(G_2) + 4e_1 \bar{M}_1(G_2).$$

Also, we take

$$\sum_{b \in V(G_2)} \sum_{a_1, a_2 \notin E(G_1)} [\tau_{G_1 \ominus G_2}(a_1, b) + \tau_{G_1 \ominus G_2}(a_2, b)]. \tag{34}$$

$$\text{Similarly} = 2n_1 n_2^2 \mu_1 - 2n_2 \mu_1 - n_2^2 \bar{M}_1(G_1) - 4n_1 e_2 \mu_1 + 4e_2 \bar{M}_1(G_1).$$

Again, we take (null case)

$$N = \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \uparrow b_2}} [\tau_{G_1 \ominus G_2}(a_1, b_1) + \tau_{G_1 \ominus G_2}(a_2, b_2)] = 0. \quad (35)$$

We further take (also null case)

$$N = \sum_{\substack{b_1 b_2 \notin E(G_1) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} \sum_{\substack{a_1 a_2 \notin E(G_2) \\ a_1 \neq a_2 \wedge a_1 \uparrow a_2}} [\tau_{G_1 \ominus G_2}(a_1, b_1) + \tau_{G_1 \ominus G_2}(a_2, b_2)] = 0. \quad (36)$$

Consequently,

$$\begin{aligned} \overline{ZC}_1(G_1 \oplus G_2) &= (4e_2 - n_2^2) \overline{M}_1(G_1) + (4e_1 - n_1^2) \overline{M}_1(G_2) \\ &\quad + 2\mu_1(n_1 n_2^2 - n_2 - 2n_1 e_2) \\ &\quad + 2\mu_2(n_1^2 n_2 - n_1 - 2n_2 e_1). \end{aligned} \quad (37)$$

□

Theorem 4. Let G_1 and G_2 be two connected and $\{C_3, C_4\}$ -free graphs. Then, ZC_1 and $\overline{ZC}_1$ of the disjunction $(G_1 \oplus G_2)$ are

$$\begin{aligned} ZC_1(G_1 \oplus G_2) &= n_2(n_2^2 - 4e_2)M_1(G_1) + n_1(n_1^2 - 4e_1)M_1(G_2) + M_1(G_1)M_1(G_2) + n_1 n_2 \\ &\quad (n_1^2 n_2^2 - 4n_2^2 e_1 - 4n_1^2 e_2 - 2n_1 n_2 + 16e_1 e_2 + 1) + 4(n_1^2 e_2 + n_2^2 e_1 - 2e_1 e_2), \end{aligned} \quad (38)$$

$$\begin{aligned} \overline{ZC}_1(G_1 \oplus G_2) &= (2e_2 - n_2^2 - 2n_2 \mu_2) \overline{M}_1(G_1) + (2e_1 - n_1^2 - 2n_1 \mu_1) \overline{M}_1(G_2) \\ &\quad + 2\mu_1(n_1 n_2^2 - n_2 - 2n_1 e_2) + 2\mu_2(n_1^2 n_2 - n_1 - 2n_2 e_1) + 4\mu_1 \mu_2 (n_1 n_2 - 1) \\ &\quad + 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [d_{G_1}(a_1) d_{G_2}(b_1) + d_{G_1}(a_2) d_{G_2}(b_2)]. \end{aligned} \quad (39)$$

Proof. Since $\tau_{G_1 \oplus G_2}(a, b) = n_2[n_1 - d_{G_1}(a)] + d_{G_2}(b)[d_{G_1}(a) - n_1] - 1$, where $a \in V(G_1)$, $b \in V(G_2)$, and $(a, b) \in G_1 \oplus G_2$,

$$\begin{aligned} ZC_1(G_1 \oplus G_2) &= \sum_{(a,b) \in V(G_1 \oplus G_2)} [\tau_{G_1 \oplus G_2}(a, b)]^2 \\ &= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [n_2\{n_1 - d_{G_1}(a)\} + d_{G_2}(b)\{d_{G_1}(a) - n_1\} - 1]^2. \end{aligned} \quad (40)$$

Similarly,

$$ZC_1(G_1 \oplus G_2) = n_2(n_2^2 - 4e_2)M_1(G_1) + n_1(n_1^2 - 4e_1)M_1(G_2) + M_1(G_1)M_1(G_2) + n_1n_2 \cdot (n_1^2n_2^2 - 4n_2^2e_1 - 4n_1^2e_2 - 2n_1n_2 + 16e_1e_2 + 1) + 4(n_1^2e_2 + n_2^2e_1 - 2e_1e_2). \quad (41)$$

$$\begin{aligned} \bar{Z}C_1(G_1 \oplus G_2) &= \sum_{(a_1, b_1)(a_2, b_2) \notin E(G_1 \oplus G_2)} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \oplus G_2}(a, b_1) + \tau_{G_1 \oplus G_2}(a, b_2)] + \sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \oplus G_2}(a_1, b) + \tau_{G_1 \oplus G_2}(a_2, b)] \\ &\quad \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)] \\ &\quad \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \uparrow b_2}} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)] \\ &+ \sum_{\substack{b_1 b_2 \notin E(G_1) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} \sum_{\substack{a_1 a_2 \notin E(G_2) \\ a_1 \neq a_2 \wedge a_1 \uparrow a_2}} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)]. \end{aligned} \quad (42)$$

We take

$$\begin{aligned} &\sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\tau_{G_1 \oplus G_2}(a, b_1) + \tau_{G_1 \oplus G_2}(a, b_2)] \\ &= \sum_{a \in V(G_1)} \sum_{b_1 b_2 \notin E(G_2)} [\{n_1n_2 - 1 - n_2d_{G_1}(a) - n_1d_{G_2}(b_1) + d_{G_1}(a)d_{G_2}(b_1)\} \\ &\quad + \{n_1n_2 - 1 - n_2d_{G_1}(a) - n_1d_{G_2}(b_2) + d_{G_1}(a)d_{G_2}(b_2)\}]. \end{aligned} \quad (43)$$

$$\text{Similarly} = 2n_1^2n_2\mu_2 - 2n_1\mu_2 - 4n_2e_1\mu_2 - n_1^2\bar{M}_1(G_2) + 2e_1\bar{M}_1(G_2).$$

Also, we take

$$\begin{aligned} &\sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)] \\ &= 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [\{n_1n_2 - 1 - n_2d_{G_1}(a_1) - n_1d_{G_2}(b_1) + d_{G_1}(a_1)d_{G_2}(b_1)\} \\ &\quad + \{n_1n_2 - 1 - n_2d_{G_1}(a_2) - n_1d_{G_2}(b_2) + d_{G_1}(a_2)d_{G_2}(b_2)\}]. \end{aligned} \quad (44)$$

$$\text{Similarly} = 4n_1n_2\mu_1\mu_2 - 4\mu_1\mu_2 - 2n_2\mu_2\bar{M}_1(G_1) - 2n_1\mu_1\bar{M}_1(G_2)$$

$$+ 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [d_{G_1}(a_1)d_{G_2}(b_1) + d_{G_1}(a_2)d_{G_2}(b_2)].$$

Again, we take

$$\sum_{b \in V(G_2)} \sum_{a_1 a_2 \notin E(G_1)} [\tau_{G_1 \oplus G_2}(a_1, b) + \tau_{G_1 \oplus G_2}(a_2, b)], \quad (45)$$

Similarly $= 2n_1 n_2^2 \mu_1 - 2n_2 \mu_1 - n_2^2 \overline{M}_1(G_1) - 4n_1 e_2 \mu_1 + 2e_2 \overline{M}_1(G_1).$

We further take (null case)

$$N = \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \uparrow b_2}} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)] = 0. \quad (46)$$

Furthermore, we take (also null case)

$$N = \sum_{\substack{b_1 b_2 \notin E(G_1) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} \sum_{\substack{a_1 a_2 \notin E(G_2) \\ a_1 \neq a_2 \wedge a_1 \uparrow a_2}} [\tau_{G_1 \oplus G_2}(a_1, b_1) + \tau_{G_1 \oplus G_2}(a_2, b_2)] = 0. \quad (47)$$

Consequently,

$$\begin{aligned} \overline{ZC}_1(G_1 \oplus G_2) &= (2e_2 - n_2^2 - 2n_2 \mu_2) \overline{M}_1(G_1) + (2e_1 - n_1^2 - 2n_1 \mu_1) \overline{M}_1(G_2) \\ &\quad + 2\mu_1(n_1 n_2^2 - n_2 - 2n_1 e_2) + 2\mu_2(n_1^2 n_2 - n_1 - 2n_2 e_1) + 4\mu_1 \mu_2(n_1 n_2 - 1) \\ &\quad + 2 \sum_{\substack{a_1 a_2 \notin E(G_1) \\ a_1 \neq a_2 \wedge a_1 \sim a_2}} \sum_{\substack{b_1 b_2 \notin E(G_2) \\ b_1 \neq b_2 \wedge b_1 \sim b_2}} [d_{G_1}(a_1) d_{G_2}(b_1) + d_{G_1}(a_2) d_{G_2}(b_2)]. \end{aligned} \quad (48)$$

□

4. Analysis and Conclusions

In this section, we compute the analysis for the first Zagreb connection index (ZC_1) and coindex ($\overline{ZC}_1$) of product on graphs such as tensor product, strong product, symmetric difference, and disjunction with the help of Tables 1–5 which are constructed by using numerical values of the aforesaid Zagreb index and coindex, respectively. The graphical depictions of the exact formulae and upper bounds for ZC_1 and $\overline{ZC}_1$ are also depicted in Figures 5–9. Moreover, in this section, for particular cases of main results, we compute all the results in the shape of upper bounds as $\{C_3, C_4\}$ are not free graphs and G_1 and G_2 are two undirected graphs.

4.1. Tensor Product. Let P_m and P_n be two particular alkanes called by paths, then the tensor product ($P_m \otimes P_n$) is obtained by the product of P_m and P_n . For $m = 3$ and $n = 3$, see Figure 10.

Using Theorem 1, the exact formulae for the first Zagreb connection index ($ZC_1(\theta_1)$) and first Zagreb connection coindex ($\overline{ZC}_1(\psi_1)$) of tensor product are obtained as follows:

- (a) $ZC_1(P_m \otimes P_n) \leq 64mn - 138m - 138n + 292$
- (b) $\overline{ZC}_1(P_m \otimes P_n) \leq 4mn - 4m - 6n + 6$

The upper bounds for the first Zagreb connection index ($ZC_1(\lambda_1)$) of tensor product are obtained as follows [39]:

$$ZC_1(P_m \otimes P_n) \leq 64mn - 56m - 124n + 100. \quad (49)$$

Table 1 and Figure 5 depict the numerical and graphical behaviours of the analysis between exact formulae and upper bounds for the first Zagreb connection index and coindex of tensor product by using values $m = n$.

4.2. Strong Product. Let P_m and P_n be two particular alkanes called by paths, then the strong product ($P_m \otimes P_n$) is

TABLE 1: Analysis for index and coindex of exact formulae and upper bounds of $\theta_1 = P_m \oslash P_n$, $\lambda_1 = P_m \oslash P_n$, and $\psi_1 = P_m \oslash P_n$, respectively.

$(m = n)$	$ZC_1(\theta_1)$	$ZC_1(\lambda_1)$	$\overline{ZC}_1(\psi_1)$
1	80	-16	0
2	-4	-4	2
3	40	136	12
4	212	404	30
5	512	800	56
6	940	1324	90
7	1496	1976	132
8	2180	2756	182
9	2992	3664	240
10	3932	4700	306
11	5000	5864	380
12	6196	7156	462
13	7520	8576	552
14	8972	10124	650
15	10552	11800	756

TABLE 2: Analysis for index and coindex of exact formulae and upper bounds of $\theta_2 = P_m \oslash P_n$, $\lambda_2 = P_m \oslash P_n$, and $\psi_2 = P_m \oslash P_n$, respectively.

$(m = n)$	$ZC_1(\theta_2)$	$ZC_1(\lambda_2)$	$\overline{ZC}_1(\psi_2)$
1	98	-13	22
2	56	-40	88
3	218	91	234
4	584	644	460
5	1154	1979	766
6	1928	4552	1152
7	2906	8915	1618
8	4088	15716	2164
9	5474	25699	2790
10	7064	39704	3496
11	8858	58667	4282
12	10856	83620	5148
13	13058	115691	6094
14	15464	156104	7120
15	18074	206179	8226

obtained by the product of P_m and P_n . For $m = 4$ and $n = 4$, see Figure 11.

Using Theorem 2, the exact formulae for the first Zagreb connection index ($ZC_1(\theta_2)$) and first Zagreb connection coindex ($\overline{ZC}_1(\psi_2)$) of strong product are obtained as follows:

- (a) $ZC_1(P_m \otimes P_n) \leq 102mn - 174m - 174n + 344$
- (b) $\overline{ZC}_1(P_m \otimes P_n) \leq 40mn - 26m - 28n + 36$

The upper bounds for first Zagreb connection index ($ZC_1(\lambda_2)$) of strong product are obtained as follows [39]:

$$ZC_1(P_m \otimes P_n) \leq 4mn^3 + 16mn^2 - 5mn - 4m - 12n^3 - 40n^2 + 24n + 4. \quad (50)$$

Table 2 and Figure 6 depict the numerical and graphical behaviours of the analysis between exact formulae and upper

TABLE 3: Analysis for index and coindex of exact formulae and upper bounds of $\theta_3 = P_m \oslash P_n$, $\lambda_3 = P_m \oslash P_n$, and $\psi_3 = P_m \oslash P_n$, respectively.

$(m = n)$	$ZC_1(\theta_3)$	$ZC_1(\lambda_3)$	$\overline{ZC}_1(\psi_3)$
1	12	33	0
2	4	34	0
3	116	153	44
4	912	390	264
5	4348	745	888
6	15332	1218	2240
7	44004	1809	4740
8	108736	2518	8904
9	239852	3345	15344
10	484068	4290	24768
11	909652	5353	37980
12	1612304	6534	55880
13	2721756	7833	79464
14	4409092	9250	109824
15	6894788	10785	148148

TABLE 4: Analysis for index and coindex of exact formulae and upper bounds of $\theta_4 = P_m \oslash P_n$, $\lambda_4 = P_m \oslash P_n$, and $\psi_4 = P_m \oslash P_n$, respectively.

$(m = n)$	$ZC_1(\theta_4)$	$ZC_1(\lambda_4)$	$\overline{ZC}_1(\psi_4)$
1	0	141	0
2	0	40	-2
3	40	189	40
4	492	588	378
5	2928	1237	1456
6	11680	2136	3910
7	36120	3285	8568
8	93660	4684	16450
9	213472	6333	28768
10	440928	8232	46926
11	842760	10381	72520
12	1512940	12780	107338
13	2579280	15429	153360
14	4210752	18328	212758
15	6676153	21477	287896

TABLE 5: Particular numeric values of obtained results for index and coindex.

Product graphs	$ZC_1(\theta)$	$ZC_1(\lambda)$	$\overline{ZC}_1(\psi)$
$(P_3 \oslash P_3)$	40	136	12
$(P_4 \otimes P_4)$	584	644	460
$(P_3 \oslash P_3)$	116	153	44
$(P_3 \oplus P_3)$	40	189	40

bounds for the first Zagreb connection index and coindex of strong product by using values $m = n$.

4.3. Symmetric Difference. Let P_m and P_n be two particular alkanes called by paths, then the symmetric difference ($P_m \ominus P_n$) is obtained by the product of P_m and P_n . For $m = 3$ and $n = 3$, see Figure 12.

FIGURE 5: Analysis for index and coindex of tensor product with respect to Table 1.

FIGURE 7: Analysis for index and coindex of symmetric difference with respect to Table 3.

FIGURE 6: Analysis for index and coindex of strong product with respect to Table 2.

FIGURE 8: Analysis for index and coindex of disjunction with respect to Table 4.

Using Theorem 3, the exact formulae for the first Zagreb connection index ($ZC_1(\theta_3)$) and first Zagreb connection

coindex ($\bar{Z}C_1(\psi_3)$) of symmetric difference are obtained as follows:

$$ZC_1(P_m \ominus P_n) \leq m^3 n^3 - 4m^3 n^2 + 8m^3 n - 6m^3 - 4m^2 n^3 + 22m^2 n^2 - 52m^2 n + 44m^2 + 8mn^3 - 52mn^2 + 137mn - 128m - 6n^3 + 44n^2 - 128n + 128, \quad (51)$$

$$\bar{Z}C_1(P_m \ominus P_n) \leq 4m^2 n^2 - 9m^2 n + 5m^2 - 9mn^2 + 20mn - 12m + 5n^2 - 12n + 8. \quad (52)$$

The upper bounds for first Zagreb connection index ($ZC_1(\lambda_3)$) of symmetric difference are obtained as follows [40]:

$$ZC_1(P_m \ominus P_n) \leq 59mn - 88m - 88n + 150. \quad (53)$$

Table 3 and Figure 7 depict the numerical and graphical behaviours of the analysis between exact formulae and upper bounds for first Zagreb connection index and coindex of symmetric difference by using values $m = n$.

4.4. Disjunction. Let P_m and P_n be two particular alkanes called by paths, then the disjunction ($P_m \oplus P_n$) is obtained by the product of P_m and P_n . For $m = 3$ and $n = 3$, see Figure 13.

Using Theorem 4, the exact formulae for the first Zagreb connection index ($ZC_1(\theta_4)$) and first Zagreb connection coindex ($\bar{Z}C_1(\psi_4)$) of disjunction are obtained as follows:

FIGURE 9: Analysis of obtained results for product on graphs with respect to Table 5.

 FIGURE 10: (a) $G_1 \cong P_3$ (b) $G_2 \cong P_3$, and (c) tensor product $(P_3 \otimes P_3)$.

 FIGURE 11: (a) $G_1 \cong P_4$ (b) $G_2 \cong P_4$, and (c) strong product $(P_4 \otimes P_4)$.

FIGURE 12: (a) $G_1 \cong P_3$ (b) $G_2 \cong P_3$, and (c) symmetric difference $(P_3 \ominus P_3)$. FIGURE 13: (a) $G_1 \cong P_3$ (b) $G_2 \cong P_3$, and (c) disjunction $(P_3 \oplus P_3)$. FIGURE 14: Analysis for $ZC_1(\theta)$ of exact formula.

FIGURE 15: Analysis for $ZC_1(\lambda)$ of upper bound. FIGURE 16: Analysis for $\bar{Z}C_1(\psi)$ of exact formula.

$$ZC_1(P_m \oplus P_n) \leq m^3 n^3 - 4m^3 n^2 + 8m^3 n - 6m^3 - 4m^2 n^3 + 14m^2 n^2 - 28m^2 n + 20m^2 + 8mn^3 - 28mn^2 + 41mn - 40m - 6n^3 + 36n^2 - 40n + 28, \quad (54)$$

$$\bar{Z}C_1(P_m \odot P_n) \leq 8m^2 n^2 - 19m^2 n + 7m^2 - 19mn^2 + 36mn - 2m + 7n^2 - 4n - 14. \quad (55)$$

The upper bounds for first Zagreb connection index ($ZC_1(\lambda_4)$) of disjunction are obtained as follows [39]:

$$ZC_1(P_m \oplus P_n) \leq 125mn - 238m - 238n + 492. \quad (56)$$

Table 4 and Figure 8 depict the numerical and graphical behaviours of the analysis between exact formulae and upper bounds for the first Zagreb connection index and coindex of disjunction by using values $m = n$.

Now, from Tables 1–5 and Figures 5–9 and 14–16, we close our discussion with the following conclusions:

The behaviours of all the connection number-based Zagreb index and coindex for operations on graphs

such as tensor product, strong product, symmetric difference, and disjunction are increased in the following order, respectively, as $\bar{Z}C_1(\psi) \geq ZC_1(\lambda) \geq ZC_1(\theta)$.

For increasing values of m and n , the upper bound for the first Zagreb connection index of products on graphs are working rapidly than all the exact formula for the first Zagreb connection index, respectively.

In certain intervals of the values of m and n , all the first Zagreb connection coindices attain the maximum values on increasing values of m and n . In Figures 5–8, we analyse that the first Zagreb connection coindex

attains more upper layer than other TIs in all the operations.

Table 5 and Figure 9 interpret the particular analysis of the obtained results for index and coindex on operations such as tensor product, strong product, symmetric difference, and disjunction. This particular analysis also concludes that the first Zagreb connection coindex attains more upper layer than other TIs in all the operations.

In particular, Figures 14–16 interpret the exact formula for the first Zagreb connection index, upper bound for the first Zagreb connection index, and exact formula for the first Zagreb connection coindex which are dominant on operations from tensor product to disjunction, respectively. In addition, we analyse that the first Zagreb connection coindex of operation disjunction has attained more upper layer than all the other operations for connection number-based index and coindex.

The investigation of these indices and coindices for the resultant graphs obtained from other operations of graphs (subtraction, switching, zig-zag product, addition, rooted product, modular product etc.) is still open.

Data Availability

All data used to support the findings of this study are included within the article. However, additional data will be made available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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