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Modified Zagreb connection indices of the T-sum graphs

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Abstract: The quantitative structures activity relationships (QSAR) and quantitative structures property relationships (QSPR) between the chemical compounds are studied with the help of topological indices (TI's) which are the fixed real numbers directly linked with the molecular graphs. Gutman and Trinajstic (1972) defined the first degree based TI to measure the total π-electrone energy of a molecular graph. Recently, Ali and Trinajstic (2018) restudied the connection based TI's such as first Zagreb connection index, second Zagreb connection index and modified first Zagreb connection index to find entropy and accentric factor of the octane isomers. In this paper, we study the modified second Zagreb connection index and modified third Zagreb connection index on the T-sum (molecular) graphs obtained by the operations of subdivision and product on two graphs. At the end, as the applications of the obtained results for the modified Zagreb connection indices of the T-sum graphs of the particular classes of alkanes are also included. Mainly, a comparision among the Zagreb indices, Zagreb connection indices and modified Zagreb connection indices of the T-sum graphs of the particular classes of alkanes is performed with the help of numerical tables, 3D plots and line graphs using the statistical tools.

Keywords: modified Zagreb indices; connection number; T-sum graphs

1 Introduction

A topological index (TI) is represented as a graphical invariant in chemical graph theory with graphical terms vertex and edge are equal to chemical terms atom and bond respectively. Briefly, a TI is a numerical value for correlation between chemical structure and various physical properties of biological activity or chemical reactivity. So, these TI's predict the chemical and physical aspects that encoded or shown in the molecular graphs such as heat of formation, heat of evaporation, polarizability, solubility, surface tension, connectivity, critical temperature, boiling, melting and freezing point. The medical behaviors of the different drugs and their compounds, crystalline materials and their nano materials which are very important for the pharmaceutical fields, chemical industries and its widely extended networks have studied with the help of various TI's (Gonzalez-Diaz et al., 2007; Hall and Kier, 1976; Matamala and Estrada, 2005).

In addition, the quantitative structures activity relationships (QSAR) and quantitative structures property relationships (QSPR) are useful in the study of molecules with the help of these TI's. For more details, we refer to Todeschini and Consonni (2009, 2010) and Yan et al. (2015). It is also investigated that these relationships play an important role in the subject of cheminformatics (Todeschini and Consonni, 2009).

Wiener defined first TI when he was working on the boiling point of paraffin (Wiener, 1947). Classical Zagreb indices was defined in Gutman and Trinajstic (1972) and Gutman et al. (1975). These are very well known and frequently used in the study of chemical graph theory. These are called first Zagreb index ($M_1(G)$) and second Zagreb index ($M_2(G)$). Furtula and Gutman (2015) defined another degree based TI and they called it as third Zagreb index ($M_3(G)$). It was appeared after a long gap, due to that instance, ($M_3(G)$) -index is also known as forgotten index ($F(G)$). At present time, so many TI's have been explored with their properties and they have revolutionized the fruitful results in the study of science especially in the lattest field of cheminformatics that is the combination of three subjects Mathematics, Chemistry and Information Technology (Borovicanin et al., 2017; Das and Gutman, 2004; Liu et al., 2019a, 2019e, 2019f; Shirinivas et al., 2010; Todeschini and Consonni, 2002), Therefore, degree based

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TI's are more studied and well applicabled (Du et al., 2019; Liu et al., 2019b, 2020; Tang et al., 2019).

Recently, Ali and Trinajstic studied the Zagreb connection indices and also checked their capability on thirteen physicochemical properties of octane isomers. They also reported that Zagreb connection indices has better correlation value than classical Zagreb indices (Ali and Trinajstic, 2018). Till now, many work have been started on this descriptor such as Du et al. (2019), defined extremal alkanes to use modified first Zagreb connection index. Ducoffe et al. (2018a, 2018b) presented their work on the 16th cologne-twente workshop on graphs and combinatorial optimization, France, on the topic of extremal graphs with respect to the modified first Zagreb connection index. Shao et al. (2018) studied extremal graphs for alkanes and cycloalkanes under some conditions. Tang et al. (2019) also used Zagreb connection indices and modified first Zagreb connection index to find the new results of the T-sum graphs.

In the computational graph theory, the operations on different graphs have to play an important role in the generalized optimization of graphs (Cvetkocic et al., 1980; Shao et al., 2012). By the use of various operations, a variety of graphs can be developed from the simplest graphs that show as their novel constructed pillars. Supported by this, many researchers have studied the well-frame families of graphs under the subdivision-related operations on graphs. For this ambition, Yan et al. (2007) studied the subdivision-related operations on graphs and computed the Wiener index of the resultant graphs. Eliasi and Taeri (2009) used these operations to develop new sums of graphs. Deng et al. (2016), Akhter and Imran (2017), Shirdel et al. (2013), and Liu et al. (2019c, 2019d) computed the first Zagreb index ($M_1(G)$), second Zagreb index ($M_2(G)$), third Zagreb index ($M_3(G)$), hyper-Zagreb index ($HM(G)$) and computed the exact formulas of first general Zagreb index ($M^{\alpha}(G)$, where α is a real number) of the T-sum graphs and also computed the generalized T_k-sum graphs. Recently, Tang et al. (2019) derived the exact formulas of the Zagreb connection indices $\left(ZC_1(G), ZC_2(G) \& ZC_1^*(G)\right)$ of the T-sum graphs with the help of these subdivision-related operations.

In this paper, we extend the study of Tang et al. (2019), and computed modified Zagreb connection indices such as modified second Zagreb connection index $\left(ZC_2^*(G)\right)$ and modified third Zagreb connection index $\left(ZC_3^*(G)\right)$ of the T-sum graphs $G_1 +_T G_2$ which are achieved by the cartesian product of $T(G_1)$ and G_2, where $T \in \{T_1, T_2\}$, G_1 and G_2 are any connected graphs and $T(G_1)$ is a graph gained after operating the operation T on G_1. Mainly, we included the comparison among the classical Zagreb indices, Zagreb connection indices and modified Zagreb connection indices for the aforsaid family of graphs obtains from alkanes. The current article is framed as follows: Section II presents the preliminary definitions of the classical/novel Zagreb indices, Section III holds the general results and section IV covers the applications and conclusion.

2 Notations and preliminaries

Let $G = (V(G), E(G))$ be a simple and connected graph. The vertex and edge set of G is denoted by V(G) and E(G) respectively. The degree of a vertex b in any graph G is the number of edges incident to a particular vertex. Todeschini and Consonni (2002) defined generalized form of a degree. In particularly,

- Number of incident edges at distance one from b is called simple degree,
- Number of incident edges at distance two from b is called connection number as well as leap degree. For more detail see Ali and Trinajstic (2018) and Naji et al. (2017).

In molecular graph, atom and covalent bond between atoms are represented by vertex and edge respectively. Throughout the study of this paper, we assume that G_1 and G_2 are two connected graphs such that G_1 and G_2 are two connected graphs such that $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, $|E(G_1)| = e_1$ and $|E(G_2)| = e_2$.

Definition 2.1

For a graph G, the first Zagreb index ($M_1(G)$), second Zagreb index ($M_2(G)$) and third Zagreb index ($M_3(G)$) are defined as:

$$M_1(G) = \sum_{b \in V(G)} \left[d_G(b)\right]^2 = \sum_{ab \in E(G)} \left[d_G(a) + d_G(b)\right],$$

$$M_2(G) = \sum_{ab \in E(G)} \left[d_G(a) \times d_G(b)\right] \text{ and}$$

$$M_3(G) = \sum_{b \in V(G)} \left[d_G(b)\right]^3 = \sum_{ab \in V(G)} \left[d_G^2(a) + d_G^2(b)\right].$$

These degree-based indices are defined by Gutman and Trinajstic (1972), Gutman et al., (1975), and Furtula and Gutman (2015). These are continuously used to predict better results in molecular structures such as heat capacity, entropy, acentric factor, absolute value of correlation coefficient and ZE-isomerism (Gutman and Polansky, 1986). These indices also played an important role in the study of QSPR and QSAR (Devillers and Balaban, 1999; Diudea, 2001).

Corresponding to these degree-based TI's, the connection-based TI's are defined in Definition 2.2. For further studies of connection-based TI's (Ali and Trinajstic, 2018; Ducoffe et al., 2018a, 2018b; Naji and Soner, 2018; Naji et al., 2017; Tang et al., 2019).

Definition 2.2

For a graph G, the first Zagreb connection index ($ZC_1(G)$) and second Zagreb connection index ($ZC_2(G)$) are defined as:

$$ZC_1(G)=\sum_{b\in V(G)}\left[\tau_G(b)\right]^2 \text{ and } ZC_2(G)=\sum_{ab\in E(G)}\left[\tau_G(a)\times\tau_G(b)\right].$$

Suppose that $V_0(G)$ be the set of the isolated vertices of the graph G such that $|V_0(G)|= n_0$. In the reference of Doslic et al. (2011), the following relation was derived:

$$\sum_{a\in V(G)\setminus V_0(G)} d_G(a)f\left(d_G(a)\right)=\sum_{ab\in E(G)}\left[f\left(d_G(a)\right)+f\left(d_G(b)\right)\right],$$

where f is defined on the set of degrees of vertex set that is as a real value function of graph G. Ali and Trinajstic (2018) discussed the reality of the following identity on the same pattern:

$$\sum_{a\in V(G)\setminus V_0(G)} d_G(a)g(a)=\sum_{ab\in E(G)}\left[g(a)+g(b)\right],$$

where g has same properties as of f. Moreover, they defined the modified first Zagreb connection index $\left(ZC_1^*(G)\right)$ using $g(a) = \tau_G(a)$ and $g(b) = \tau_G(b)$ in the above equation as

$$ZC_1^*(G)=\sum_{ab\in E(G)}\left[\tau_G(a)+\tau_G(b)\right].$$

Now, if we put $g(a) = d_G(a)\tau_G(b)$ and $g(b) = d_G(b)\tau_G(a)$ or $g(a) = d_G(a)\tau_G(a)$ and $g(b) = d_G(b)\tau_G(b)$ in the above identity, the extended modified Zagreb connection indices are obtained as follows:

Definition 2.3

For a graph G, modified second Zagreb connection index $\left(ZC_2^*(G)\right)$ and modified third Zagreb connection index $\left(ZC_3^*(G)\right)$ are defined as

(a) $$ZC_2^*(G)=\sum_{ab\in E(G)}\left[d_G(a)\tau_G(b)+d_G(b)\tau_G(a)\right].$$

(b) $$ZC_3^*(G)=\sum_{ab\in E(G)}\left[d_G(a)\tau_G(a)+d_G(b)\tau_G(b)\right].$$

Now, we describe the T-sum graphs i.e. subdivision and semi-total point operations on graphs as follow:

- $T_1(G)$ is a graph that is obtained by including a new vertex between each edge of the graph G.
- $T_2(G)$ is a graph that is obtained from $T_1(G)$ by adding the edges between old vertices which are adjacent in G.

The more details of these operations can be found in Harary (1969) and Sampathkumar and Chikkodimath (1973). For further understanding, see Figure 1. The concept of T-sum graphs is defined as in the following definition.

Definition 2.4

For i ϵ {1,2} and T ϵ $\{T_i\}$, assume that G_i are connected graphs and the graph $T(G_1)$ having vertex set $V(T(G_1))$ and edge set $E(T(G_1))$ is happened after operating the operations T on G_1. Then, the graphs $G_1 +_T G_2$ having vertex set $V(G_1 +_T G_2) = V(T(G_1)) \times (V_2) = (V_1 \cup E_1) \times (V_2)$ and edge set $E(G_1 +_T G_2)$ are called T-sum graphs if for $(a_1,b_1)(a_2,b_2) \in E(G_1 +_T G_2)$ either $a_1 = a_2$ in $V(G_1)$ and $b_1b_2 \in E(G_2)$ or $b_1 = b_2$ in $V(G_2)$ and $a_1a_2 \in E(S(G_1))$, where (a_1,b_1), $(a_2,b_2) \in V(G_1 +_T G_2)$. This scheme has been presented according to cartesian product because cartesian product is the best fitted and the most stylish apparatus to construct a large network from a simple graph and is also important for designing as well as exploration of networks (Xu, 2001). For more clearance, see Figures 2 and 3.

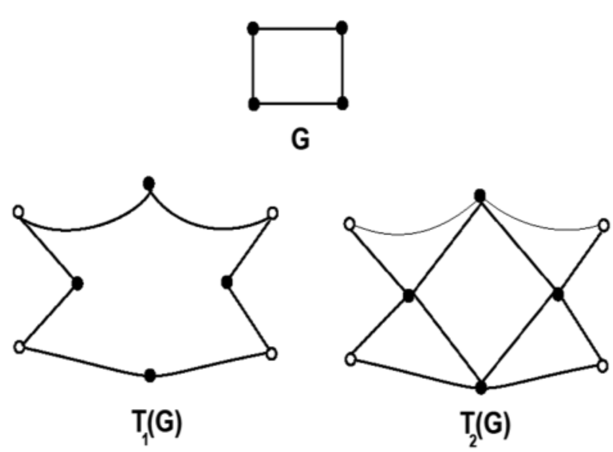

Figure 1: G, $T_1(G)$, $T_2(G)$

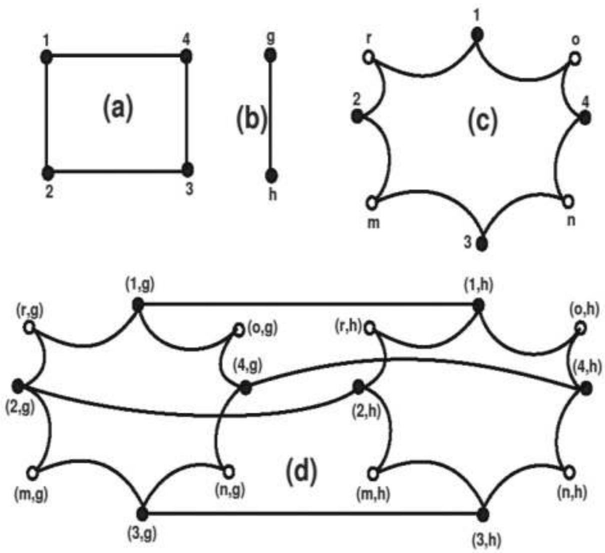

Figure 2: (a) $G_1 \cong C_4$ (b) $G_2 \cong P_2$ (c) $T_1(G_1)$ (d) $G_1 +_T G_2$ iff $T = T_1$

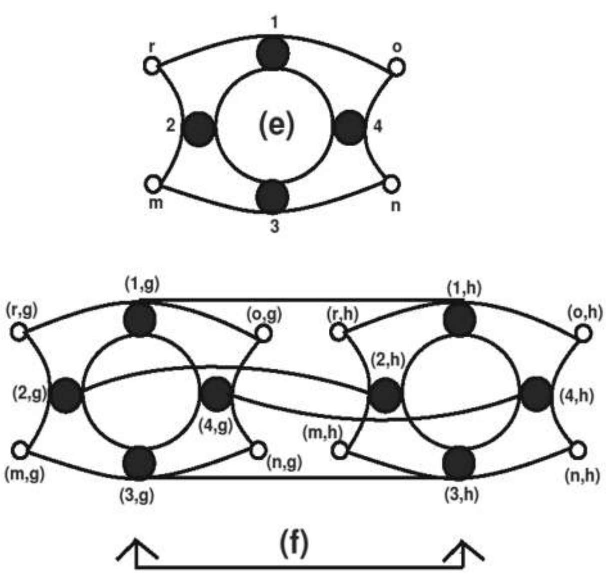

Figure 3: (e) $T_2(G_1)$ (f) $G_1 +_T G_2$ iff $T=T_2$

Definition 2.5

Coefficient of variation (Allan, 2010):

if X is a random variable then a relative measure of dispersion is called coefficient of variation (C.V) in which standard deviation is absolute measure of dispersion. Mathematically, it will be written as:

$$C.V(X) = \frac{S}{\overline{X}} \times 100\%,$$

where,

$$S = \sqrt{\frac{\sum\left(X - \overline{X}\right)^2}{n}}$$

and

$$\overline{X} = \frac{\sum X}{n}$$

are called standard deviation (S) and arithmetic mean $\left(\overline{X}\right)$ for ungroup data. C.V is used to draw the results of at least two commodities or variables.

- All of those commodities which commodity has greater value of $\overline{X}$ is considered more variability among the corresponding or remaining commodities.
- All of those commodities which commodity has less value of C.V is observed more consistent.

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

Lemma 2.1 (Yamaguchi, 2008)

Let G be a connected graph with n vertices and e edges. Then

$$\tau_G(a) + d_G(a) \leq \sum_{b \in N_G(a)} \left(d_G(b)\right),$$

where equality holds if and only if G is a $\{C_3, C_4\}$-free graph.

Lemma 2.2 (Tang et al., 2019)

Let G be a connected and $\{C_3, C_4\}$-free graph with n vertices and e edges. Then,

(i) $\sum_{b \in V(G)} d_G(b) = 2e$,

(ii) $\sum_{b \in VG)} \tau_G(b) = M_1(G) - 2e$.

Lemma 2.3

Let G be a connected and $\{C_3, C_4\}$-free graph with n vertices and e edges. Then,

(i) $d_{T1(G1)}(a) = d_{G2}(b) + \tau_{G2}(b)$,

(ii) $E \mid T_1(G) \mid = 2 \mid E(G) \mid = 2e$,

(iii) $\sum_{ab \in E(T_1(G))} d_{T_1(G)}(b) = 2$ or $d_G(b) = d_{T1(G)}(b) = 2$.

Lemma 2.4

Let G be a connected and $\{C_3, C_4\}$-free graph with n vertices and e edges. Then,

(i) $d_{T2(G)}(a) = 2d_G(a)$,
(ii) $\sum_{ab\in E(T_2(G))} d_{T_2(G)}(b) = 2$ or $d_G(b) = d_{T2(G)}(b) = 2$.

Lemma 2.5

Let G be a connected graph and $G \cong P_n$, then

(i) $ZC_2^*(G) = 8n-22$ if $n \geq 4$,
(ii) $ZC_3^*(G) = 8n-22$ if $n \geq 3$.

For more study, we refer to Naji et al. (2017).

Lemma 2.6 (Deng et al., 2016)

Let G be a connected graph and $G_1 \cong P_m$ and $G_2 \cong P_n$. Also let $\theta_1 = P_m +_{T_1} P_n$ and $\theta_2 = P_m +_{T_2} P_n$, if $m,n \geq 3$. Then,

(i) $M_1(\theta_1) = 20mn - 14m - 18n + 8$ and $M_1(\theta_2) = 40mn - 22m - 44n + 16$,
(ii) $M_2(\theta_1) = 32mn - 32m - 34n + 26$ and $M_2(\theta_2) = 96mn - 78m - 132n + 86$.

Lemma 2.7 (Tang et al., 2019)

Let G be a connected graph and $G_1 \cong P_m$ and $G_2 \cong P_n$.

Also let $\theta_1 = P_m +_{T_1} P_n$ and $\theta_2 = P_m +_{T_2} P_n$, if $m,n \geq 5$. Then,

(i) $ZC_1(\theta_1) = 100mn - 148m - 136n + 172$ and $ZC_1(\theta_2) = 245mn - 332m - 443n + 512$,
(ii) $ZC_2(\theta_1) = 160mn - 274m - 236n + 358$ and $ZC_2(\theta_2) = 588mn - 906m - 1196n + 1628$,
(iii) $ZC_1^*(\theta_1) = 44mn - 50m - 50n + 44$ and $ZC_1^*(\theta_2) = 98mn - 98m - 146n + 112$.

3 Results and discussion

This section consists on the main results.

3.1 Subdivision operation

Let G_1 and G_2 be two connected and $\{C_3,C_4\}$-free graphs. Then, the modified second and third Zagreb connection indices of the T-sum graphs are:

Theorem 3.1

$$ZC_2^*(G_1 +_{T_1} G_2) = n_1 ZC_2^*(G_2) + 2e_1 ZC_1^*(G_2) + n_2 M_3(G_1) + 2n_2 M_2(G_1) + 4e_1 M_2(G_2) + 14e_2 M_1(G_1) + 10e_1 M_1(G_2) + M_1(G_1)M_1(G_2) - 16e_1e_2.$$

Proof

Let $\tau(a,b) = \tau_{G_1+_{T_1}G_2}(a,b)$ be a connection number of the vertex (a,b) in the graph $G_1 +_{T_1} G_2$. Then,

$$ZC_2^*(G_1 +_{T_1} G_2) = \sum_{(a_1,b_1)(a_2,b_2)\in E(G_1+_{T_1}G_2)} \left[d(a_1,b_1)\tau(a_2,b_2) + d(a_2,b_2)\tau(a_1,b_1)\right]$$

$$= \sum_{a\in V(G_1)} \sum_{b_1b_2\in E(G_2)} [d(a,b_1)\tau(a,b_2) + d(a,b_2)\tau(a,b_1)]$$

$$+ \sum_{b\in V(G_2)} \sum_{a_1a_2\in E(T_1(G_1))} \left[d(a_1,b)\tau(a_2,b) + d(a_2,b)\tau(a_1,b)\right].$$

Taking

$$\sum_{a\in V(G_1)} \sum_{b_1b_2\in E(G_2)} \left[d(a,b_1)\tau(a,b_2) + d(a,b_2)\tau(a,b_1)\right]$$

$$= \sum_{a\in V(G_1)} \sum_{b_1b_2\in E(G_2)}$$

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

$$= \sum_{a\in V(G_1)} \sum_{b_1b_2\in E(G_2)} [2d_{G_1}^2(a) + d_{G_1}^2(a)\{d_{G_2}(b_1) + d_{G_2}(b_2)\} + d_{G_1}(a)\{\tau_{G_2}(b_1) + \tau_{G_2}(b_2)\} + d_{G_1}(a) \{d_{G_2}(b_1) + d_{G_2}(b_2)\} + 2d_{G_1}(a)d_{G_2}(b_1)d_{G_2}(b_2) + \{d_{G_2}(b_1)\tau_{G_2}(b_2) + d_{G_2}(b_2)\tau_{G_2}(b_1)\}]$$

$$= 2e_2 M_1(G_1) + M_1(G_1)M_1(G_2) + 2e_1 ZC_1^*(G_2) + 2e_1 M_1(G_2) + 4e_1 M_2(G_2) + n_1 ZC_2^*(G_2).$$

Also taking

$$\sum_{b\in V(G_2)} \sum_{a_1a_2\in E(T_1(G_1))} \left[d(a_1,b)\tau(a_2,b) + d(a_2,b)\tau(a_1,b)\right]$$

$$= \sum_{b\in V(G_2)} \sum_{a_1a_2\in E(G_1)} [[\{d_{G_1}(a_1) + d_{G_2}(b)\}\{d_{G_1}(a_1) + 2d_{G_2}(b) + d_{G_1}(a_2) - 2\} + 2\{d_{G_1}(a_1) + d_{G_1}(a_1) d_{G_2}(b) + \tau_{G_2}(b)\}] + [2\{d_{G_1}(a_2) + d_{G_1}(a_2)d_{G_2}(b) + \tau_{G_2}(b)\} + \{d_{G_1}(a_2) + d_{G_2}(b)\}\{d_{G_1}(a_1) + 2 d_{G_2}(b) + d_{G_1}(a_2) - 2\}]]$$

$$= \sum_{b\in V(G_2)} \sum_{a_1a_2\in E(G_1)} [\{d_{G_1}^2(a_1) + d_{G_1}^2(a_2)\} + 6d_{G_2}(b)\{d_{G_1}(a_1) + d_{G_1}(a_2)\} + 2\{d_{G_1}(a_1)d_{G_1}(a_2)\} + 4d_{G_2}^2(b) - 4d_{G_2}(b) + 4\tau_{G_2}(b)]$$

$$= n_2 M_3(G_1) + 12e_2 M_1(G_1) + 2n_2 M_2(G_1) + 4e_1 M_1(G_2) - 8e_1e_2 + 4e_1[M_1(G_2) - 2e_2]$$

Consequently,

$$ZC_2^*(G_1+_{T_1}G_2)=n_1ZC_2^*(G_2)+2e_1ZC_1^*(G_2)$$
$$+n_2M_3(G_1)+2n_2M_2(G_1)+4e_1M_2(G_2)+14e_2$$
$$M_1(G_1)+10e_1M_1(G_2)+M_1(G_1)M_1(G_2)-16e_1e_2.$$

Theorem 3.2

$$ZC_3^*(G_1+_{T_1}G_2)=n_1ZC_3^*(G_2)+4e_1ZC_1^*(G_2)$$
$$+(n_2+2e_2)M_3(G_1)+2e_1M_3(G_2)+2(e_2+2n_2)$$
$$M_1(G_1)+2e_1M_1(G_2)+3M_1(G_1)M_1(G_2)+8e_1(2e_2-n_2).$$

Proof

$$ZC_3^*(G_1+_{T_1}G_2)=\sum_{(a_1,b_1)(a_2,b_2)\in E(G_1+_{T_1}G_2)}$$
$$[d(a_1,b_1)\tau(a_1,b_1)+d(a_2,b_2)\tau(a_2,b_2)]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[d(a,b_1)\tau(a,b_1)+d(a,b_2)\tau(a,b_2)]$$
$$+\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(T_1(G_1))}[d(a_1,b)\tau(a_1,b)+d(a_2,b)\tau(a_2,b)].$$

Taking

$$\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[d(a,b_1)\tau(a,b_1)+d(a,b_2)\tau(a,b_2)]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}$$
$$[\{d_{G_1}(a)+d_{G_2}(b_1)\}\{d_{G_1}(a)+d_{G_1}(a)d_{G_2}(b_1)+\tau_{G_2}(b_1)\}$$
$$+\{d_{G_1}(a)+d_{G_2}(b_2)\}\{d_{G_1}(a)+d_{G_1}(a)d_{G_2}(b_2)+\tau_{G_2}(b_2)\}]$$
$$=2e_2M_1(G_1)+M_1(G_1)M_1(G_2)+2e_1ZC_1^*(G_2)$$
$$+2e_1M_1(G_2)+2e_1M_3(G_2)+n_1ZC_3^*(G_2).$$

Also taking

$$\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(T_1(G_1))}[d(a_1,b)\tau(a_1,b)+d(a_2,b)\tau(a_2,b)]$$
$$=\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(G_1)}[[\{d_{G_1}(a_1)+d_{G_2}(b)\}\{d_{G_1}(a_1)+d_{G_1}(a_1)d_{G_2}(b)$$
$$+\tau_{G_2}(b)\}+2\{d_{G_1}(a_1)+2d_{G_2}(b)\}+d_{G_1}(a_2)-2\}]$$
$$+[2\{d_{G_1}(a_1)+2d_{G_2}(b)+d_{G_1}(a_2)-2\}$$
$$+\{d_{G_1}(a_2)+d_{G_2}(b)\}\{d_{G_1}(a_2)+d_{G_1}(a_2)d_{G_2}(b)+\tau_{G_2}(b)\}]]$$
$$=n_2M_3(G_1)+2e_2M_3(G_1)+\{M_1(G_2)-2e_2\}M_1(G_1)$$
$$+2e_2M_1(G_1)+M_1(G_2)M_1(G_1)+2e_1$$
$$ZC_1^*(G_2)+4n_2M_1(G_1)+16e_1e_2-8n_2e_1.$$

Consequently,

$$ZC_3^*(G_1+_{T_1}G_2)=n_1ZC_3^*(G_2)+4e_1ZC_1^*(G_2)$$
$$+(n_2+2e_2)M_3(G_1)+2e_1M_3(G_2)+2(e_2+2n_2)$$
$$M_1(G_1)+2e_1M_1(G_2)+3M_1(G_1)M_1(G_2)+8e_1(2e_2-n_2).$$

Semi-total point operation (Tang et al., 2019), or triangle parallel graph (Ahmad et al., 2019)

Let G_1 and G_2 be two connected and $\{C_3,C_4\}$-free graphs. Then, the modified second and third Zagreb connection indices of the T-sum graphs are:

Theorem 3.3

$$ZC_2^*(G_1+_{T_2}G_2)=4n_2ZC_2^*(G_1)+n_1ZC_2^*(G_2)$$
$$+4(3e_2+n_2)ZC_1^*(G_1)+6e_1ZC_1^*(G_2)+2n_2M_3(G_1)$$
$$+4(4e_2+n_2)M_2(G_1)+8e_1M_2(G_2)+10M_1(G_1)M_1(G_2)$$
$$+4e_1M_1(G_2)+2(8e_2-n_2)M_1(G_1)-12e_1e_2.$$

Proof

Let $\tau(a,b)=\tau_{G_1+_{T_2}G_2}(a,b)$ be a connection number of the vertex (a,b) in the graph $G_1+_{T_2}G_2$. Then,

$$ZC_2^*(G_1+_{T_2}G_2)=\sum_{(a_1,b_1)(a_2,b_2)\in E(G_1+_{T_2}G_2)}$$
$$[d(a_1,b_1)\tau(a_2,b_2)+d(a_2,b_2)\tau(a_1,b_1)]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[d(a,b_1)\tau(a,b_2)+d(a,b_2)\tau(a,b_1)]$$
$$+\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(T_2(G_1))}[d(a_1,b)\tau(a_2,b)+d(a_2,b)\tau(a_1,b)].$$

Taking

$$\sum 1=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[d(a,b_1)\tau(a,b_2)+d(a,b_2)\tau(a,b_1)]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[\{2d_{G_1}(a)+d_{G_2}(b_1)\}\{2\tau_{G_1}(a)+\tau_{G_2}(b_2)$$
$$+2d_{G_1}(a)d_{G_2}(b_2)\}+\{2d_{G_1}(a)+d_{G_2}(b_2)\}\{2\tau_{G_1}(a)+\tau_{G_2}(b_1)$$
$$+2d_{G_1}(a)d_{G_2}(b_1)\}]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[8d_G(a)\tau_{G_1}(a)+2d_{G_1}(a)\{\tau_{G_2}(b_1)+\tau_{G_2}(b_2)\}$$
$$+d_{G_1}^2(a)\{d_{G_2}(b_1)+d_{G_2}(b_2)\}+2\tau_{G_1}(a)\{d_{G_2}(b_1)+d_{G_2}(b_2)\}$$
$$+\{d_{G_2}(b_1)\tau_{G_2}(b_2)+d_{G_2}(b_2)\tau_{G_2}(b_1)\}+4d_{G_1}(a)\{d_{G_2}(b_1)d_{G_2}(b_2)\}]$$
$$=8e_2ZC_1^*(G_1)+4e_1ZC_1^*(G_2)+4M_1(G_1)M_1(G_2)$$
$$+2[M_1(G_1)-2e_1]M_1(G_2)+n_1ZC_2^*(G_2)+8e_1M_2(G_2).$$

Also taking

$$\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(T_2(G_1))}\left[d(a_1,b)\tau(a_2,b)+d(a_2,b)\tau(a_1,b)\right]$$
$$=\sum 2+\sum 3$$
$$\sum 2=\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(G_1)}[\{2d_{G_1}(a_1)+d_{G_2}(b)\}\{2\tau_{G_1}(a_2)+\tau_{G_2}(b)$$
$$+\ 2d_{G_1}(a_2)d_{G_2}(b)\}+\{2d_{G_1}(a_2)+d_{G_2}(b)\}\{2\tau_{G_1}(a_1)$$
$$+\ \tau_{G_2}(b)+2d_{G_1}(a_1)d_{G_2}(b)\}]$$

Similarly,

$$\sum 2=4n_2ZC_2^*(G_1)+4e_2ZC_1^*(G_1)+2e_1ZC_1^*(G_2)$$
$$+\ 4M_1(G_1)M_1(G_2)-4e_2M_1(G_1)+16e_2M_2(G_1).$$

And

$$\sum 3=\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(G_1)}[[\{2d_{G_1}(a_1)+d_{G_2}(b)\}\{d_{G_1}(a_1)+d_{G_1}(a_2)$$
$$+\ 2d_{G_2}(b)-1\}+2\{2\tau_{G_1}(a_1)+\tau_{G_2}(b)+2d_{G_1}(a_1)d_{G_2}(b)\}]$$
$$+\ [2\{2\tau_{G_1}(a_2)+\tau_{G_2}(b)+2d_{G_1}(a_2)d_{G_2}(b)\}$$
$$+\ \{2d_{G_1}(a_2)+d_{G_2}(b)\}\{d_{G_1}(a_1)+d_{G_1}(a_2)+2d_{G_2}(b)-1\}]]$$

Similarly,

$$\sum 3=2n_2M_3(G_1)+4n_2M_2(G_1)+20e_2M_1(G_1)$$
$$-2n_2M_1(G_1)+4e_1M_1(G_2)-4e_1e_2$$
$$+4n_2ZC_1^*(G_1)+4e_1[M_1(G_1)-2e_2].$$

Consequently,

$$ZC_2^*(G_1+_{T_2}G_2)=\sum 1+\sum 2+\sum 3$$
$$=4n_2ZC_2^*(G_1)+n_1ZC_2^*(G_2)+4(3e_2+n_2)ZC_1^*(G_1)$$
$$+\ 6e_1ZC_1^*(G_2)+2n_2M_3(G_1)+4(4e_2+n_2)$$
$$M_2(G_1)+8e_1M_2(G_2)+10M_1(G_1)M_1(G_2)$$
$$+\ 4e_1M_1(G_2)+2(8e_2-n_2)M_1(G_1)-12e_1e_2.$$

Theorem 3.4

$$ZC_3^*(G_1+_{T_2}G_2)=n_1ZC_3^*(G_2)+8n_2ZC_3^*(G_1)+16e_2ZC_1^*(G_1)$$
$$+8e_1ZC_1^*(G_2)+4e_1M_3(G_2)+4[4e_2M_3(G_1)$$
$$+e_1M_3(G_2)]+14M_1(G_1)M_1(G_2)$$
$$+4[(n_2-2e_2)M_1(G_1)-e_1M_1(G_2)]$$
$$+4e_1(4e_2-n_2).$$

Proof

$$ZC_3^*(G_1+_{T_2}G_2)=\sum_{(a_1,b_1)(a_2,b_2)\in E(G_1+_{T_2}G_2)}$$
$$\left[d(a_1,b_1)\tau(a_1,b_1)+d(a_2,b_2)\tau(a_2,b_2)\right]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}\left[d(a,b_1)\tau(a,b_1)+d(a,b_2)\tau(a,b_2)\right]$$
$$+\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(T_2(G_1))}\left[d(a_1,b)\tau(a_1,b)+d(a_2,b)\tau(a_2,b)\right].$$

Taking

$$\sum A=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}\left[d(a,b_1)\tau(a,b_1)+d(a,b_2)\tau(a,b_2)\right]$$
$$=\sum_{a\in V(G_1)}\sum_{b_1b_2\in E(G_2)}[\{2d_{G_1}(a)+d_{G_2}(b_1)\}\{2\tau_{G_1}(a)+\tau_{G_2}(b_1)$$
$$+\ 2d_{G_1}(a)d_{G_2}(b_1)\}+\{2d_{G_1}(a)+d_{G_2}(b_2)\}\{2\tau_{G_1}(a)$$
$$+\ \tau_{G_2}(b_2)+2d_{G_1}(a)d_{G_2}(b_2)\}]$$

Similarly,

$$\sum A=8e_2ZC_1^*(G_1)+4e_1ZC_1^*(G_2)+4M_1(G_1)M_1(G_2)$$
$$+\ 2[M_1(G_1)-2e_1]M_1(G_2)+n_1ZC_3^*(G_2)+4e_1M_3(G_2).$$

Also taking

$$\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(T_2(G_1))}\left[d(a_1,b)\tau(a_1,b)+d(a_2,b)\tau(a_2,b)\right]=\sum B+\sum C$$
$$\sum B=\sum_{b\in V(G_2)}\sum_{a_1a_2\in E(G_1)}[\{2d_{G_1}(a_1)+d_{G_2}(b)\}\{2\tau_{G_1}(a_1)+\tau_{G_2}(b)$$
$$+\ 2d_{G_1}(a_1)d_{G_2}(b)\}+\{2d_{G_1}(a_2)+d_{G_2}(b)\}\{2\tau_{G_1}(a_2)$$
$$+\ \tau_{G_2}(b)+2d_{G_1}(a_2)d_{G_2}(b)\}]$$

Similarly,

$$\sum B=4n_2ZC_3^*(G_1)+2[M_1(G_2)-2e_2]M_1(G_1)+8e_2M_3(G_1)$$
$$+\ 4e_2ZC_1^*(G_1)+2e_1ZC_1^*(G_2)+2M_1(G_1)M_1(G_2).$$

And similarly,

$$\sum C=4n_2ZC_3^*(G_1)+2[M_1(G_2)-2e_2]M_1(G_1)$$
$$+\ 8e_2M_3(G_1)+4e_2ZC_1^*(G_1)+2e_1ZC_1^*(G_2)$$
$$+\ 2M_1(G_1)M_1(G_2)+4n_2M_1(G_1)+16e_1e_2-4n_2e_2.$$

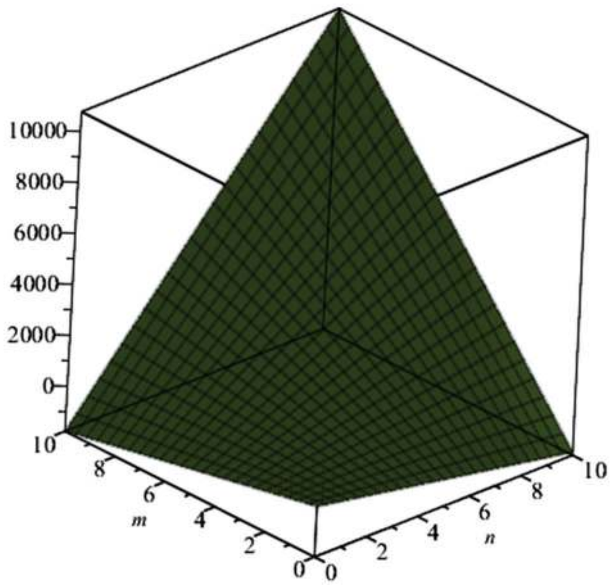

Figure 4: 3D plot of $ZC_2(P_m +_{T_1} P_n)$

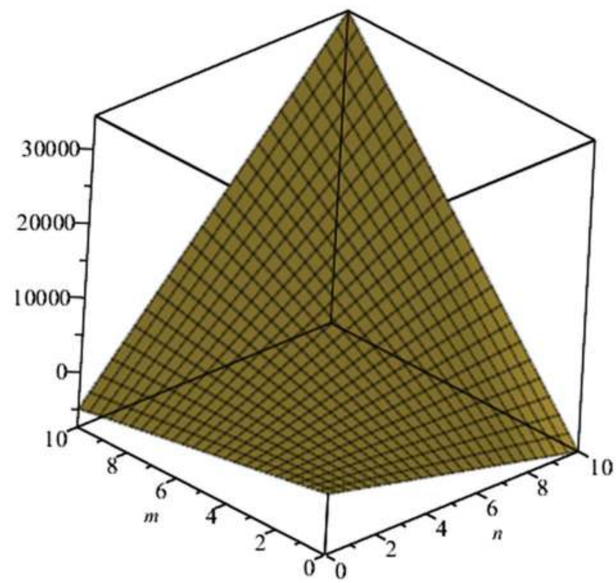

Figure 6: 3D plot of $ZC_2(P_m +_{T_2} P_n)$

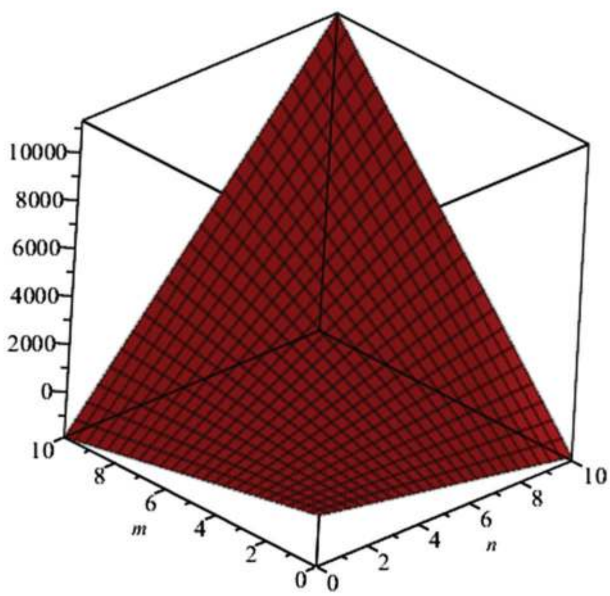

Figure 5: 3D plot of $ZC_3(P_m +_{T_1} P_n)$

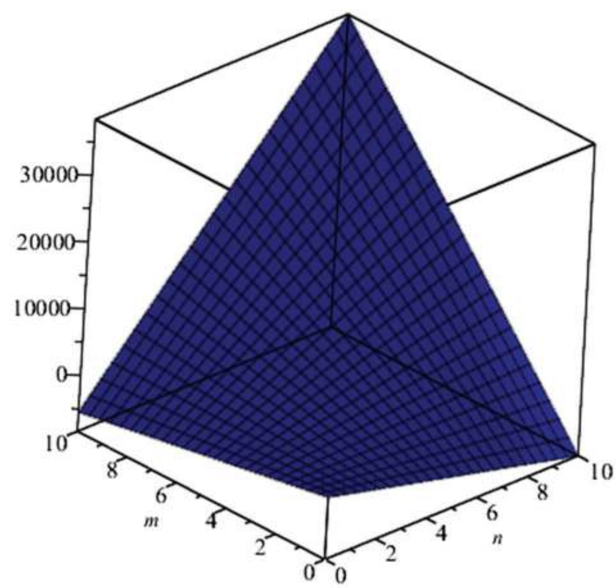

Figure 7: 3D plot of $ZC_3(P_m +_{T_2} P_n)$

Consequently,

$$ZC_3^*(G_1 +_{T_2} G_2) = \sum A + \sum B + \sum C$$

$$\begin{aligned} &= n_1 ZC_3^*(G_2) + 8n_2 ZC_3^*(G_1) + 16e_2 ZC_1^*(G_1) + 8e_1 ZC_1^*(G_2) \\ &+ 4e_1 M_3(G_2) + 4[4e_2 M_3(G_1) + e_1 M_3(G_2)] + 14 M_1(G_1) M_1(G_2) \\ &+ 4[(n_2 - 2e_2) M_1(G_1) - e_1 M_1(G_2)] + 4e_1(4e_2 - n_2) \end{aligned}$$

4 Applications and conclusion

Let $G_1 \cong P_m$ and $G_2 \cong P_n$ be two particular alkanes called by paths. Then, the second and third modified Zagreb connection indices of their T-sum graphs as the consequences of the obtained main results as follows:

1. For $m \geq 3$ and $n \geq 4$, we have $ZC_2^*(P_m +_{T_1} P_n) = 144mn - 198m - 186n + 216$,
2. For $m,n \geq 3$, we have $ZC_3^*(P_m +_{T_1} P_n) = 152mn - 214m - 198n + 244$,
3. For $m,n \geq 3$, we have $ZC_2^*(P_m +_{T_2} P_n) = 476mn - 574m - 820n + 840$,
4. For $m,n \geq 3$, we have $ZC_3^*(P_m +_{T_2} P_n) = 532mn - 646m - 932n + 968$.

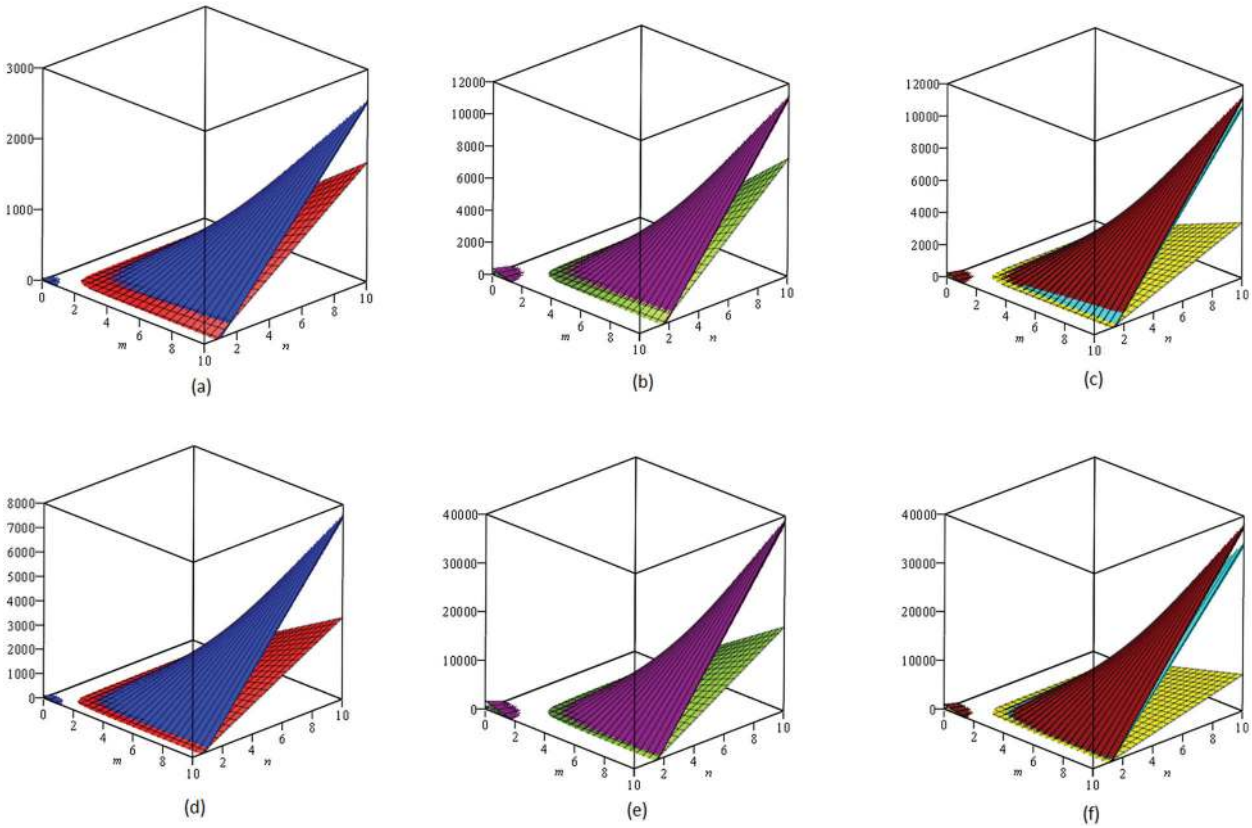

FIGURE 8: (a) 3D plot of $M_1(\theta_1)$ and $M_2(\theta_1)$ are labbled in red and blue graphs, (b) 3D plot of $ZC_1(\theta_1)$ and $ZC_2(\theta_1)$ are labbled in green and purple graphs, (c) 3D plot of $ZC_1(\theta_1)$, $ZC_2(\theta_1)$ and $ZC_3(\theta_1)$ are labbled in golden, ferozi and mehroon graphs, (d) 3D plot of $M_1(\theta_2)$ and $M_2(\theta_2)$ are labbled in red and blue graphs, (e) 3D plot of $ZC_1(\theta_2)$ and $ZC_2(\theta_2)$ are labbled in green and purple graphs, (f) 3D plot of $ZC_1(\theta_2)$, $ZC_2(\theta_2)$ and $ZC_3^*(\theta_2)$ are labbled in golden, ferozi and mehroon graphs

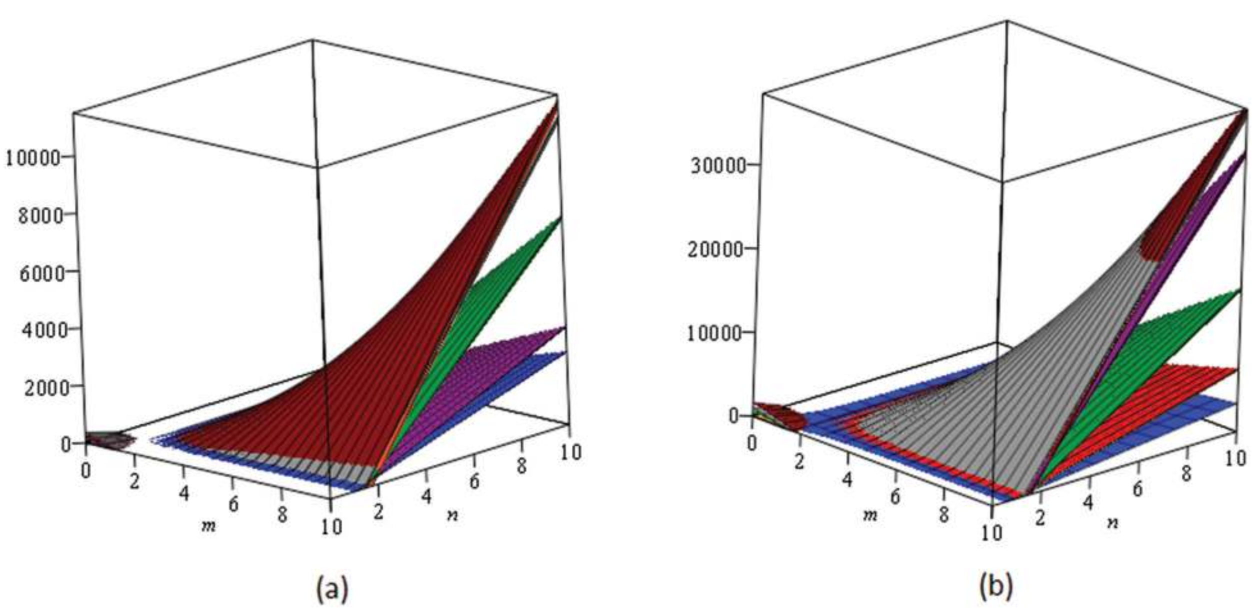

Figure 9: (a) 3D plot of $M_1(\theta_1)$, $M_2(\theta_1)$, $ZC_1(\theta_1)$, $ZC_2(\theta_1)$, $ZC_1(\theta_1)$, $ZC_2(\theta_1)$, and $ZC_3(\theta_1)$are labbled in blue, red, purple, green, orange, gray and mehroon graphs, (b) 3D plot of $M_1(\theta_2)$, $M_2(\theta_2)$, $ZC_1(\theta_2)$, $ZC_2(\theta_2)$, $ZC_1(\theta_2)$, $ZC_2(\theta_2)$, and $ZC_3(\theta_2)$ are labbled in blue, red, green, purple, orange, gray, and mehroon graphs

Table 1: Numeric comparison of the indicated Zagreb indices related to T_1-operation.

(m,n)	$M_1(\theta_1)$	$M_2(\theta_1)$	$ZC_1(\theta_1)$	$ZC_2(\theta_1)$	$ZC_1^*(\theta_1)$	$ZC_2^*(\theta_1)$	$ZC_3^*(\theta_1)$
(5,5)	348	496	1252	1808	644	1896	1984
(5,6)	430	622	1616	2372	814	2430	2546
(5,7)	512	748	1980	2936	984	2964	3108
(5,8)	594	874	2344	3500	1154	3498	3670
(5,9)	676	1000	2708	4064	1324	4032	4232
(5,10)	758	1126	3072	4628	1494	4566	4794
(6,5)	434	624	1604	2334	814	2418	2530
(6,6)	536	782	2068	3058	1028	3096	3244
(6,7)	638	940	2532	3782	1242	3774	3958
(6,8)	740	1098	2996	4506	1456	4452	4672
(6,9)	842	1256	3460	5230	1670	5130	5386
(6,10)	944	1414	3924	5954	1884	5808	6100
(7,5)	520	752	1956	2860	984	2940	3076
(7,6)	642	942	2520	3744	1242	3762	3942
(7,7)	764	1132	3084	4628	1500	4584	4808
(7,8)	886	1322	3648	5512	1758	5406	5674
(7,9)	1008	1512	4212	6396	2016	6228	6540
(7,10)	1130	1702	4776	7280	2274	7050	7406
(8,5)	606	880	2308	3386	1154	3462	3622
(8,6)	712	1102	2972	4430	1456	4428	4640
(8,7)	890	1324	3636	5474	1758	5394	5658
(8,8)	1032	1546	4300	6518	2060	6360	6676
(8,9)	1174	1768	4964	7562	2362	7326	7694
(8,10)	1316	1990	5628	8606	2664	8292	8712
(9,5)	692	1008	2660	3912	1324	3984	4168
(9,6)	872	1262	3424	5116	1670	5094	5338
(9,7)	1016	1516	4188	6320	2016	6204	6508
(9,8)	1178	1770	4952	7524	2362	7314	7678
(9,9)	1340	2024	5716	8728	2708	8424	8848
(9,10)	1502	2278	6480	9932	3054	9534	10018
(10,5)	778	1136	3012	4438	1494	4506	4714
(10,6)	960	1422	3876	5802	1884	5760	6036
(10,7)	1142	1708	4740	7166	2274	7014	7358
(10,8)	1324	1994	5604	8530	2664	8268	8680
(10,9)	1506	2280	6468	9894	3054	9522	10002
(10,10)	1688	2566	7332	11258	3444	10776	11324

4.1 Comparisons with 3D plots

Maple 15 software is used to construct a simple comparison of the classical Zagreb (Lemma 2.6), novel Zagreb connection (Lemma 2.7) and extended modified Zagreb connection (given above) indices related to operations T_1 and T_2 into 3D plots (Figures 4-9).

4.2 Comparisons with numerical values

Tables 1 and 2 are constructed for a simple comparison of the classical Zagreb (Lemma 2.6), novel Zagreb connection (Lemma 2.7) and extended modified Zagreb connection (given above) indices related to operations T_1 and T_2.

Table 2: Numeric comparison of the indicated Zagreb indices related to T_2-operation.

(m,n)	$M_1(\theta_2)$	$M_2(\theta_2)$	$ZC_1(\theta_2)$	$ZC_2(\theta_2)$	$ZC_1^*(\theta_2)$	$ZC_2^*(\theta_2)$	$ZC_3^*(\theta_2)$
(5,5)	686	1436	2762	5818	1342	5770	6378
(5,6)	842	1784	3544	7562	1686	7330	8106
(5,7)	998	2132	4326	9306	2030	8890	9834
(5,8)	1154	2480	5108	11050	2374	10450	11562
(5,9)	1310	2828	5890	12794	2718	12010	13290
(5,10)	1466	3176	6672	14538	3062	13570	15018
(6,5)	864	1838	3655	7852	1734	7576	8392
(6,6)	1060	2282	4682	10184	2176	9612	10652
(6,7)	1256	2726	5709	12516	2618	11648	12912
(6,8)	1452	3170	6736	14848	3060	13684	15172
(6,9)	1648	3614	7763	17180	3502	15720	17432
(6,10)	1844	4058	8790	19512	3944	17756	19692
(7,5)	1042	2240	4548	9886	2126	9382	10406
(7,6)	1278	2780	5820	12806	2666	11894	13198
(7,7)	1514	3320	7092	15726	3206	14406	15990
(7,8)	1750	3860	8364	18646	3746	16918	18782
(7,9)	1986	4400	9636	21566	4286	19430	21574
(7,10)	2222	4940	10908	24486	4826	21942	24366
(8,5)	1220	2642	5441	11920	2518	11188	12420
(8,6)	1496	3278	6958	15428	3156	14176	15744
(8,7)	1772	3914	8475	18936	3794	17164	19068
(8,8)	2048	4550	9992	22444	4432	20152	22392
(8,9)	2324	5186	11509	25952	5070	23140	25716
(8,10)	2600	5822	13026	29460	5708	26128	29040
(9,5)	1398	3044	6334	13954	2910	12994	14434
(9,6)	1714	3776	8096	18050	3646	16458	18290
(9,7)	2030	4508	9858	22146	4382	19922	22146
(9,8)	2346	5240	11620	26242	5118	23386	26002
(9,9)	2662	5972	13382	30338	5854	26850	29858
(9,10)	2978	6704	15144	34434	6590	30314	33714
(10,5)	1576	3446	7227	15988	3302	14800	16448
(10,6)	1932	4274	9234	20672	4136	18740	20836
(10,7)	2288	5102	11241	25356	4970	22680	25224
(10,8)	2644	5930	13248	30040	5804	26620	29612
(10,9)	3000	6758	15255	34724	6638	30560	34000
(10,10)	3356	7586	17262	39408	7472	34500	38388

4.3 Comparisons with line graphs

Now, we close our discussion with the following conclusion:

- In Figures 9a and 9b, we obtain that among all the indices (classical Zagreb indices, Zagreb connection indices and modified Zagreb connection indices), the third modified Zagreb connection index ZC_3^* of $\theta_1 \cong P_m +_{T_1} P_n$ and $\theta_2 \cong P_m +_{T_2} P_n$ are better than the other indices with most upper increasing layer.
- The numerical values of Tables 1 and 2 also present that the third modified Zagreb connection index ZC_3^* of $\theta_1 \cong P_m +_{T_1} P_n$ and $\theta_2 \cong P_m +_{T_2} P_n$ are better than the other indices having larger values.

Table 3: Different values of C.V of the indicated Zagreb indices for both operations T_1 and T_2.

C.V	(θ_1)	(θ_2)
M_1	25.32%	24.76%
M_2	26.53%	25.77%
ZC_1	28.75%	28.31%
ZC_2	29.93%	29.26%
ZC_1^*	27.16%	26.68%
ZC_2^*	28.23%	27.55%
ZC_3^*	28.32%	27.59%

Table 4: Different values of $\overline{X}$ of the indicated Zagreb indices for both operations T_1 and T_2.

$\overline{X}$	(θ_1)	(θ_2)
M_1	553	1076
M_2	811	2306
ZC_1	2162	4717
ZC_2	3218	10178
ZC_1^*	1069	2202
ZC_2^*	3231	9670
ZC_3^*	3389	10698

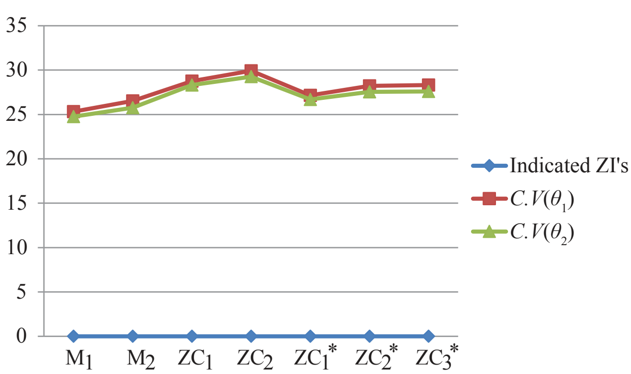

Figure 10: Graph for C.V of the indicated ZI's for both operations T_1 and T_2 based on Table 3

- Figures 10 and 11 statistically prove that M_1 is more consistent and ZC_3^* has better variability than other indicated indices respectively. Moreover, ZC_3^* is averagely consisitent by Figure 10 for both the graphs $\theta_1 \cong P_m +_{T_1} P_n$ and $\theta_2 \cong P_m +_{T_2} P_n$. Additionally by Figures 10 and 11, all the indicated indices of $\theta_2 \cong P_m +_{T_2} P_n$ are more variability and more consisitent than $\theta_1 \cong P_m +_{T_1} P_n$, respectively.

Data availability: The data used to support the findings of this study are cited at relevant places within the text as references.

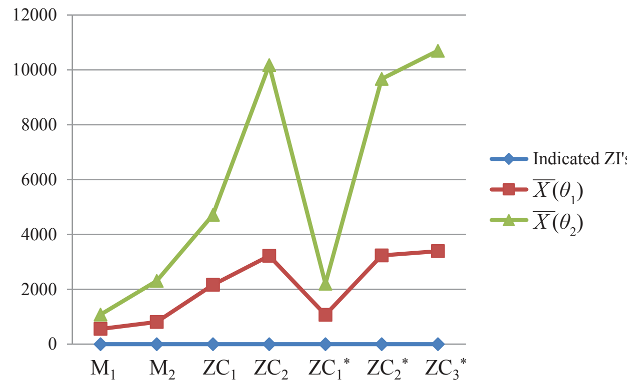

Figure 11: Graph for arithmetic mean (A.M) of the indicated ZI's for both operations based on Table 4

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