Usman Ali, Muhammad Javaid* and Agha Kashif

Modified Zagreb connection indices of the T-sum graphs

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 (TIs) 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 TIs 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 comparison 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 TIs 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 TIs (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 TIs. 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 TIs have been explored with their properties and they have revolutionized the fruitful results in the study of science especially in the latest 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...
TT’s are more studied and well applicable (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 have 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 (Cvetkovic 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 \( H M(G) \) and computed the exact formulas of first general Zagreb index \( M_\alpha(G) \), where \( \alpha \) is a real number) of the T-sum graphs and also computed the generalized \( T \)-sum graphs. Recently, Tang et al. (2019) derived the exact formulas of the Zagreb connection indices \( (Z_{C_1}(G), Z_{C_2}(G) \& Z_{C_3}(G)) \) 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 \( Z_{C_2}(G) \) and modified third Zagreb connection index \( Z_{C_3}(G) \) of the T-sum graphs \( G \), which are achieved by the cartesian product of \( T(G) \) and \( G \), where \( T \in \{ T_1, T_2 \} \), \( G \) and \( G \) are any connected graphs and \( T(G) \) is a graph gained after operating the operation \( T \) on \( G \). Mainly, we included the comparison among the classical Zagreb indices, Zagreb connection indices and modified Zagreb connection indices for the aforesaid 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 \( \left( M_1(G) \right) \), second Zagreb index \( \left( M_2(G) \right) \) and third Zagreb index \( \left( M_3(G) \right) \) are defined as:

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

\[
M_2(G) = \sum_{ab \in E(G)} \left[ d_c(a) \times d_c(b) \right]
\]

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

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 QSAR 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:

\[
ZC_1(G) = \sum_{b \in V(G)} [\tau_c(b)] \quad \text{and} \quad ZC_2(G) = \sum_{ab \in E(G)} [\tau_c(a) \times \tau_c(b)].
\]

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:

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

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:

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

where \( g \) has same properties as \( f \). Moreover, they defined the modified first Zagreb connection index \( (ZC'_1(G)) \) using \( g(a) = \tau_c(a) \) and \( g(b) = \tau_c(b) \) in the above equation as

\[
ZC'_1(G) = \sum_{ab \in E(G)} [\tau_c(a) + \tau_c(b)].
\]

Now, if we put \( g(a) = d_c(a)\tau_c(b) \) and \( g(b) = d_c(b)\tau_c(a) \) or \( g(a) = d_c(a)\tau_c(a) \) and \( g(b) = d_c(b)\tau_c(b) \) 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 \( (ZC'_2(G)) \) and modified third Zagreb connection index \( (ZC'_3(G)) \) are defined as

\[
(a) \quad ZC'_2(G) = \sum_{ab \in E(G)} [d_c(a)\tau_c(b) + d_c(b)\tau_c(a)].
\]

(b) \( ZC'_3(G) = \sum_{ab \in E(G)} [d_c(a)\tau_c(a) + d_c(b)\tau_c(b)]. \)

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 \( i \in \{1,2\} \) and \( T \in \{T_i\} \), assume that \( G_i \) are connected graphs and the graph \( T(G_i) \) having vertex set \( V(T(G_i)) \) and edge set \( E(T(G_i)) \) is happened after operating the operations \( T \) on \( G_i \). Then, the graphs \( G_1 +_T G_2 \) having vertex set \( V(G_1 +_T G_2) = V(T(G_i)) \times (V_i) = (V_i \cup E_i) \times (V_i) \) and edge set \( E(G_1 +_T G_2) \) are called T-sum graphs if for \( (a_i, b_i)(a_j, b_j) \in E(G_1 +_T G_2) \) either \( a_i = a_j \) in \( V(G_i) \) and \( b_i, b_j \in E(G_i) \) or \( b_i = b_j \) in \( V(G_i) \) and \( a_i, a_j \in E(S(G_i)), \) where \( (a_i, b_i), (a_j, b_j) \in V(G_1 +_T G_2). \) 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 cleaart, see Figures 2 and 3.

**Figure 1:** G, T(G), T_i(G)
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:

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

where,

$$S = \sqrt{\frac{1}{n} \sum (X - \bar{X})^2},$$

and

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

are called standard deviation ($S$) and arithmetic mean ($\bar{X}$) 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 $\bar{X}$ 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

$$\tau_c(a) + d_c(a) \leq \sum_{b \in N_G(a)} (d_c(b)),$$

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) $\sum_{b \in N_G(a)} d_c(b) = 2e$,

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

Lemma 2.3

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

(i) $d_{\tau(G)}(a) = d_{\tau(G)}(b) + \tau_{\gamma}(b)$,

(ii) $E | T_1(G)| = 2 | E(G)| = 2e$,

(iii) $\sum_{a \in E_G} d_{\tau(G)}(b) = 2$ or $d_{\tau(G)}(b) = d_{\tau(G)}(b) = 2$.

Lemma 2.4

Let $G$ be a connected and $\{C_3, C_4\}$-free graph with $n$ vertices and $e$ edges. Then,
(i) \( d_{\tau(G)}(a) = 2d_1(a) \),
(ii) \( \sum_{a,b \in E(T(G))} d_{\tau(G)}(b) = 2 \) or \( d_\tau(b) = d_{\tau(G)}(b) = 2 \).

**Lemma 2.5**

Let \( G \) be a connected graph and \( G \equiv P_n \), then

(i) \( ZC^*_1(G) = 8n - 22 \) if \( n \geq 4 \),
(ii) \( ZC^*_1(G) = 8n - 22 \) 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 \( G_i \equiv P_m \) and \( G_j \equiv P_n \).

Also let \( \theta_i = P_m + G_i \) and \( \theta_j = P_n + G_j \), if \( m,n \geq 3 \). Then,

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

**Lemma 2.7 (Tang et al., 2019)**

Let \( G \) be a connected graph and \( G_i \equiv P_m \) and \( G_j \equiv P_n \).

Also let \( \theta_i = P_m + G_i \) and \( \theta_j = P_n + G_j \), if \( m,n \geq 5 \). Then,

(i) \( ZC^*(\theta_i) = 100mn - 148m - 136n + 172 \) and \( ZC^*(\theta_j) = 245mn - 323m - 443n + 512 \),
(ii) \( ZC^*(\theta_i) = 160mn - 274m - 236n + 358 \) and \( ZC^*(\theta_j) = 588mn - 906m - 1196n + 1628 \),
(iii) \( ZC^*_1(\theta_i) = 44mn - 50m - 50n + 44 \) and \( ZC^*_1(\theta_j) = 98mn - 98m - 146n + 112 \).

**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 \( (C_4,C_5) \)-free graphs. Then, the modified second and third Zagreb connection indices of the T-sum graphs are:

**Theorem 3.1**

\[
ZC^*_1(G_1 + \tau, G_2) = n_1ZC^*_1(G_1) + 2eZC^*_1(G_2) + n_1M_1(G_1) + 2n_2M_2(G_1) + 4e_1M_1(G_1) + 14e_2
\]
\[
M_2(G_1) + 10eM_1(G_1) + M_1(G_2)M_1(G_1) - 16e_3e' + 2e_4M_2(G_1)
\]

**Proof**

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

\[
ZC^*_1(G_1 + \tau, G_2) = \sum_{a,b \in E(T(G_1))} [d_\tau(a,b)\tau(a,b) + d_\tau(a,b)\tau(a,b)]
\]
\[
= \sum_{a \in V(G_1), b \in E(G_2)} [d_\tau(a,b)\tau(a,b) + d_\tau(a,b)\tau(a,b)]
\]
\[
\sum_{b \in E(G_2)} [d_\tau(a,b)\tau(a,b) + d_\tau(a,b)\tau(a,b)]
\]

Taking

\[
\sum_{a \in V(G_1), b \in E(G_2)} [d_\tau(a,b)\tau(a,b) + d_\tau(a,b)\tau(a,b)]
\]

Also taking

\[
\sum_{b \in E(G_2)} [d_\tau(a,b)\tau(a,b) + d_\tau(a,b)\tau(a,b)]
\]

Proof
Consequently,
\[ ZC'_3(G_1 + G_2) = n_1ZC'_3(G_1) + 2e_1ZC'_3(G_2) + n_2M_1(G_1) + 2n_2M_1(G_2) + 4e_1M_1(G_1) + 14e_2 \\
+ 10e_2M_1(G_1) + M_1(G_1)M_1(G_2) - 16e_2e_2. \]

**Theorem 3.2**

\[ ZC'_3(G_1 + G_2) = n_1ZC'_3(G_1) + 4e_1ZC'_3(G_1) + (n_1 + 2e_1)M_1(G_1) + 2e_1M_1(G_2) + 2(e_1 + 2n_2) \]
\[ + 2e_2M_1(G_2) + 3M_1(G_1)M_1(G_2) + 8e_2(2e_2 - n_2). \]

**Proof**

\[ ZC'_3(G_1 + G_2) = \sum_{(a, b) \in E(T(G_1))} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ = \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ + \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)]. \]

Taking
\[ \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ = \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ + \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)]. \]

Also taking
\[ \sum_{(a, b) \in E(T(G_1))} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ = \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ + \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)]. \]

\[ \text{Consequently,} \]
\[ ZC'_3(G_1 + G_2) = n_1ZC'_3(G_1) + 4e_1ZC'_3(G_1) + (n_1 + 2e_1)M_1(G_1) + 2e_1M_1(G_2) + 2(e_1 + 2n_2) \]
\[ + 2e_2M_1(G_2) + 3M_1(G_1)M_1(G_2) + 8e_2(2e_2 - n_2). \]

**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 \( \{C_n,C_n\} \)-free graphs. Then, the modified second and third Zagreb connection indices of the T-sum graphs are:

\[ ZC'_3(G_1 + G_2) = 4n_1ZC'_3(G_1) + n_1ZC'_3(G_1) + \]
\[ + 4(3e_1 + n_1)ZC'_3(G_1) + 6e_1ZC'_3(G_1) + 2n_1M_1(G_1) \]
\[ + 8e_2M_1(G_1) + 10M_1(G_1)M_1(G_2) \]
\[ + 4e_1M_1(G_1) + 2(8e_2 - n_2)M_1(G_1) - 12e_1e_2. \]

**Proof**

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

\[ ZC'_3(G_1 + G_2) = \sum_{(a, b) \in V(G_1 + G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ = \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ + \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)]. \]

Taking
\[ \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ = \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)] \]
\[ + \sum_{b \in V(G_2)} [d(a, b)\tau(a, b) + d(a, b)\tau(a, b)]. \]
Also taking
\[
\sum_{b \in V(G_1)} \sum_{a \notin e \notin E(T_1(G_1))} [d(a_1,b_1)\tau(a_2,b_2) + d(a_2,b_2)\tau(a_1,b_1)]
\]
\[= \sum_2 + \sum_3 \]
\[
\sum_2 = \sum_{b \in V(G_1)} \sum_{a \in e \notin E(T_1(G_1))} [(2d_{a_1}(a_1) + d_{b_1}(b_1))[2\tau_{a_1}(a_1) + \tau_{b_1}(b_1)]
\]
\[+ 2d_{a_2}(a_2)\tau_{b_2}(b_2)] + [2d_{a_1}(a_1) + d_{b_1}(b_1)][2\tau_{a_1}(a_1) + \tau_{b_1}(b_1)]
\]
\[+ \tau_{a_1}(b_1) + 2d_{a_2}(a_2)\tau_{b_2}(b_2)]
\]
\[
\sum_3 = \sum_{b \in V(G_1)} \sum_{a \notin e \notin E(T_1(G_1))} [(2d_{a_1}(a_1) + d_{b_1}(b_1))[d_{a_1}(a_1) + d_{b_1}(b_1)]
\]
\[+ 2d_{a_2}(a_2)\tau_{b_2}(b_2) - 1] + [2d_{a_1}(a_1) + \tau_{b_1}(b_1) + 2d_{a_1}(a_1)\tau_{b_1}(b_1)]
\]
\[+ [2d_{a_2}(a_2) + \tau_{b_2}(b_2)] + [2d_{a_2}(a_2) + \tau_{b_2}(b_2)] + [2d_{a_2}(a_2)\tau_{b_2}(b_2) - 1]]
\]

Similarly,
\[
\sum_3 = 2n_1M_1(G_1) + 4n_1M_2(G_1) + 20e_2M_1(G_1)
\]
\[+ 2n_1M_1(G_1) + 4e_2M_2(G_1) - 4e_2
\]
\[+ 4n_1ZC_1(G_1) + 4e_2[M_1(G_1) - 2e_2].
\]

Consequently,
\[
ZC_1(G_1 + G_2) = 1 + 2 + \sum_3
\]
\[= 4n_2ZC_1(G_1) + n_1ZC_1(G_1) + 6e_2ZC_1(G_1)
\]
\[+ 6e_2ZC_1(G_1) + 2n_1M_1(G_1) + 4(e_1 + n_1)
\]
\[M_1(G_1) + 8e_2M_2(G_1) + 10M_1(G_1)M_1(G_1)
\]
\[+ 4e_1M_1(G_1) + 2(8e_2 - n_1)M_1(G_1) - 12e_2.
\]

**Theorem 3.4**
\[
ZC_1(G_1 + G_2) = n_1ZC_1(G_1) + 8n_2ZC_1(G_1) + 16e_2ZC_1(G_1)
\]
\[+ 8e_2ZC_1(G_1) + 4e_1M_1(G_1) + 4[4e_2M_1(G_1)
\]
\[+ e_1M_1(G_1)]M_1(G_1) + 14M_1(G_1)M_1(G_1)
\]
\[+ 4[2(n_2 - 2e_2)M_1(G_1) - e_1M_1(G_1)]
\]
\[+ 4e_1(4e_2 - n_1).
\]

**Proof**
\[
ZC_1(G_1 + G_2) = \sum_{(a_1,b_1) \in G_1 \times G_1} \sum_{(a_2,b_2) \in G_2 \times G_2} [d(a_1,b_1)\tau(a_2,b_2) + d(a_2,b_2)\tau(a_1,b_1)]
\]
\[= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a,b)\tau(a,b) + d(a,b)\tau(a,b)]
\]
\[+ \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a,b)\tau(a,b) + d(a,b)\tau(a,b)]
\]
\[+ \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a,b)\tau(a,b) + d(a,b)\tau(a,b)].
\]

Taking
\[
\sum A = \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [d(a,b)\tau(a,b) + d(a,b)\tau(a,b)]
\]
\[= \sum_{a \in V(G_1)} \sum_{b \in V(G_2)} [(2d_{a_1}(a_1) + d_{b_1}(b_1))[2\tau_{a_1}(a_1) + \tau_{b_1}(b_1)]
\]
\[+ 2d_{a_2}(a_2)\tau_{b_2}(b_2)] + [2d_{a_1}(a_1) + d_{b_1}(b_1)][2\tau_{a_1}(a_1) + \tau_{b_1}(b_1)]
\]
\[+ \tau_{a_1}(b_1) + 2d_{a_2}(a_2)\tau_{b_2}(b_2)]
\]

Similarly,
\[
\sum A = 8e_2[2ZC_1(G_1) + 4e_2ZC_1(G_1) + 4M_1(G_1)M_1(G_2)
\]
\[+ 2[M_1(G_1) - 2e_2]M_1(G_1) + n_1ZC_1(G_1) + 4e_1M_1(G_1).
\]

Also taking
\[
\sum_{b \in V(G_1)} \sum_{a \notin e \notin E(T_1(G_1))} [d(a_1,b_1)\tau(a_2,b_2) + d(a_2,b_2)\tau(a_1,b_1)] = \sum B + \sum C
\]
\[
\sum B = \sum_{b \in V(G_1)} \sum_{a \notin e \notin E(T_1(G_1))} [(2d_{a_1}(a_1) + d_{b_1}(b_1))[2\tau_{a_1}(a_1) + \tau_{b_1}(b_1)]
\]
\[+ 2d_{a_2}(a_2)\tau_{b_2}(b_2)] + [2d_{a_1}(a_1) + d_{b_1}(b_1)][2\tau_{a_1}(a_1) + \tau_{b_1}(b_1)]
\]
\[+ \tau_{a_1}(b_1) + 2d_{a_2}(a_2)\tau_{b_2}(b_2)]
\]

Similarly,
\[
\sum B = 4n_2ZC_1(G_1) + 2[M_1(G_1) - 2e_2]M_1(G_1) + 8e_2M_1(G_1)
\]
\[+ 4e_2ZC_1(G_1) + 2e_2ZC_1(G_2) + 2M_1(G_1)M_1(G_2).
\]

And similarly,
\[
\sum C = 4n_2ZC_1(G_1) + 2[M_1(G_1) - 2e_2]M_1(G_1)
\]
\[+ 8e_2M_1(G_1) + 4e_2ZC_1(G_1) + 2e_2ZC_1(G_2)
\]
\[+ 2M_1(G_1)M_1(G_1) + 4n_2M_1(G_1) + 16e_2 - 4n_1e_2.]
Consequently,

\[ ZC_G(G_1 + G_2) = \sum A + \sum B + \sum C \]

\[ = n[ZC_G(G_1) + 8n_1ZC_G(G_2) + 16e, ZC_G(G_1) + 8e, ZC_G(G_2) + 4e, M_1(G_1) + 4(4e, M_1(G_1) + e, M_1(G_2)] + 14M_1(G_1)M_1(G_2) + 4(n_2 - 2e, M_1(G_1) - e, M_1(G_2)] + 4r_1(4e_1 - n_1) \]

4 Applications and conclusion

Let \( G_1 \equiv P_m \) and \( G_2 \equiv P_n \) 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 \( ZC_{P_m}(P_m + P_n) = 144mn - 198m + 216, \)
2. For \( m, n \geq 3 \), we have \( ZC_{P_m}(P_m + P_n) = 152mn - 214m + 198n + 244, \)
3. For \( m, n \geq 3 \), we have \( ZC_{P_m}(P_m + P_n) = 476mn - 574m + 820n + 840, \)
4. For \( m, n \geq 3 \), we have \( ZC_{P_m}(P_m + P_n) = 532mn - 646m - 932n + 968. \)
**FIGURE 8:** (a) 3D plot of $M_1(\theta)$ and $M_2(\theta)$ are labeled in red and blue graphs, (b) 3D plot of $ZC_1(\theta)$ and $ZC_2(\theta)$ are labeled in green and purple graphs, (c) 3D plot of $ZC_1'(\theta)$, $ZC_2'(\theta)$, and $ZC_3'(\theta)$ are labeled in golden, ferozi and mehroon graphs, (d) 3D plot of $M_1(\theta)$ and $M_2(\theta)$ are labeled in red and blue graphs, (e) 3D plot of $ZC_1(\theta)$ and $ZC_2(\theta)$ are labeled in green and purple graphs, (f) 3D plot of $ZC_1(\theta)$, $ZC_2(\theta)$, and $ZC_3(\theta)$ are labeled in golden, ferozi and mehroon graphs

**Figure 9:** (a) 3D plot of $M_1(\theta)$, $M_2(\theta)$, $ZC_1(\theta)$, $ZC_2(\theta)$, $ZC_3'(\theta)$, $ZC_4(\theta)$, and $ZC_5(\theta)$ are labeled in blue, red, purple, green, orange, gray and mehroon graphs, (b) 3D plot of $M_1(\theta)$, $M_2(\theta)$, $ZC_1(\theta)$, $ZC_2(\theta)$, $ZC_3(\theta)$, $ZC_4(\theta)$, and $ZC_5(\theta)$ are labeled in blue, red, green, purple, orange, gray, and mehroon graphs
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 1: Numeric comparison of the indicated Zagreb indices related to $T_1$-operation.

| $(m,n)$ | $M_1(\theta)$ | $M_2(\theta)$ | $ZC_1(\theta)$ | $ZC_2(\theta)$ | $ZC_1^*(\theta)$ | $ZC_2^*(\theta)$ | $ZC_3^*(\theta)$ |
|---------|---------------|---------------|----------------|----------------|------------------|------------------|------------------|
| (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            |
4.3 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 $\theta_1 \equiv P_m + P_n$ and $\theta_2 \equiv P_n + P_m$ 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 $\theta_1 \equiv P_m + P_n$ and $\theta_2 \equiv P_n + P_m$ are better than the other indices having larger values.

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

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

The third modified Zagreb connection index $ZC^*_3$ of $\theta_1 \equiv P_m + P_n$ and $\theta_2 \equiv P_n + P_m$ 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 $\theta_1 \equiv P_m + P_n$ and $\theta_2 \equiv P_n + P_m$ are better than the other indices having larger values.
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 consistent by Figure 10 for both the graphs $\Theta_1 \cong +_{P_m}T_{n1}$ and $\Theta_2 \cong +_{P_m}T_{n2}$. Additionally, by Figures 10 and 11, all the indicated indices of $\Theta_1 \cong +_{P_m}T_{n2}$ are more variability and more consistent than $\Theta_1 \cong +_{P_m}T_{n1}$, respectively.

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

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

| C.V       | $(\Theta_1)$ | $(\Theta_2)$ |
|-----------|--------------|--------------|
| $M_1$     | 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 $\bar{X}$ of the indicated Zagreb indices for both operations $T_1$ and $T_2$.

| $\bar{X}$ | $(\Theta_1)$ | $(\Theta_2)$ |
|-----------|--------------|--------------|
| $M_1$     | 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.

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

Conflicts of interest: The authors declare that they have no conflicts of interest.

Authors’ contributions: All authors contributed equally to this paper.

Acknowledgments: The authors are thankful to the referees for their supported and helpful comments and suggestions to improve the first version of this paper.

References

Ahmad M., Saeed M., Javaid M., Hussain M., Exact Formula and Improved Bounds for General Sum-Connectivity Index of Graph-Operations. IEEE Access, 2019, 7, 167290-167299.

Akhter S., Imran M., Computing the Forgotten Topological Index of Four Operations on Graphs. AKCE Int. J. Graphs Combinatorics, 2017, 14(1), 70-79.

Ali A., Trinajstic N., A Novel/Old Modification of the First Zagreb Index. Mol. Inform., 2018, 37, 1-7.

Allan G.B., Elementary Statistics: A Step by Step Approach (5th ed.). McGraw-Hill Companies, Inc., 2010, 1-669.

Borovicanin B., Das K.C., Furtula B. Gutman I., Bounds for Zagreb Indices. MATCH-Commun. Math. Co., 2017, 78(1), 17-100.

Cvetkovic D.M., Doob M., Sachs H., Spectra of Graphs: Theory and Application. Academic Press, New York, NY, USA, 1980.

Das K.C., Gutman I., Some Properties of the Second Zagreb Index. MATCH-Commun. Math. Co., 2004, 52, 103-112.

Deng H., Sarala D., Ayyaswamy S.K., Balachandran S., The Zagreb Indices of Four Operations on Graphs. Appl. Math. Comput., 2016, 275, 422-431.

Devillers J., Balaban A.T., Topological Indices and Related Descriptors in QSAR and QSPR. Gordon Breach, Amsterdam, 1999.

Diudea M.V., QSPR/QSAR Studies by Molecular Descriptors. NOVA, New York, 2001.

Doslic T., Furtula B., Graovac A., Gutman I., Moradi S., Yarahmadi Z., MATCH-Commun. Math. Co., 2011, 66, 613-626.

Du Z., Ali A., Trinajstic N., Alkanes with the First Three Maximal/Minimal Modified First Zagreb Connection Indices. Mol. Inform., 2019, 38, 1-9.
