Research Article

Sharp Bounds of First Zagreb Coindex for $F$-Sum Graphs

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Let $G = (V (E), E(G))$ be a connected graph with vertex set $V (G)$ and edge set $E(G)$. For a graph $G$, the graphs $S(G)$, $R(G)$, $Q(G)$, and $T(G)$ are obtained by applying the four subdivisions related operations $S$, $R$, $Q$, and $T$, respectively. Further, for two connected graphs $G_1$ and $G_2$, the graphs $G_1 + SG_2$, $G_1 + RG_2$, $G_1 + QG_2$, and $G_1 + TG_2$ are $F$-sum graphs which are constructed with the help of Cartesian product of $F(G_1)$ and $G_2$, where $F \in \{S, R, Q, T\}$. In this paper, we compute the lower and upper bounds for the first Zagreb coindex of these $F$-sum ($S$-sum, $R$-sum, $Q$-sum, and $T$-sum) graphs in the form of the first Zagreb indices and coincides of their basic graphs. At the end, we use linear regression modeling to find the best correlation among the obtained results for the thirteen physicochemical properties of the molecular structures such as boiling point, density, heat capacity at constant pressure, entropy, heat capacity at constant time, enthalpy of vaporization, acentric factor, standard enthalpy of vaporization, enthalpy of formation, octanol-water partition coefficient, standard enthalpy of formation, total surface area, and molar volume.

1. Introduction

The subject of graph theory is growing and moving into mainstream of mathematics, playing a basic role in various disciplines of science especially in chemistry and computer science. A topological index (TI) is a function from a set of graphs to the set of real numbers that assigns a different numerical value to each graph unless the graphs are isomorphic. Moreover, this numeric value predicts various physical and chemical properties of the involved organic compounds in the molecular graphs such as volume, density, pressure, weight, boiling point, freezing point, vaporization point, heat of formation, and heat of evaporation [1, 2]. TIs are also used to study the quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) and medical behaviors of different drugs in the subject of cheminformatics and pharmaceutical industries, respectively [3–5].

There are various types of TIs based on degree, distance, and polynomial, but degree-based TIs are more studied than others (see the latest survey [6]). Wiener calculated boiling point of paraffin by using a distance-based TI (see [7]). Gutman and Trinajstić defined the TIs known as first and second Zagrebin indices to calculate total $\pi$-electron energy of alternant hydrocarbons [8].

There are different operations on graphs such as joining, deleting, union, intersection, product, complement, switching, and subdivision. These operations on graphs play an important role to obtain the new molecular graphs from the old ones. Yan et al. listed five graphs $L(G)$, $S(G)$, $Q(G)$, $R(G)$, and $T(G)$ with the help of five operations $L$, $S$, $Q$, $R$, and $T$, respectively. They also studied the behavior of Wiener index of graphs under these five decorations (see [4]). Eliasi and Taeri introduced the four subdivision-related operations using the concept of Cartesian product and obtained four sum graphs ($G_{1,2}G_2$, $G_{1,2}G_2$, $G_{1,2}QG_2$, and $G_{1,2}TG_2$). They also computed the Wiener indices of these newly defined $F$-sum graphs (see [9]). Akhtar and Imran calculated the forgotten index [10], Deng et al. [11] computed first and second Zagreb indices, and Liu et al. computed first general Zagreb index of these graphs (see [12]).
Ashrafi et al. computed Zagreb coindices of composite graph operations such as joining, union, disjunction, Cartesian product, corona product, and composition (see [13]). Mansour and Song computed $a$ and $(a, b)$-analogues of Zagreb indices and coindices of graphs [14]. Ashrafi et al. worked on extremal graphs with respect to the Zagreb coindices [15]. Ramane et al. calculated coindices for the transmission- and reciprocal transmission-based graphs (see [16]). Javaid et al. computed the first Zagreb connection index and coindex of some derived graphs [17].

In this paper, we compute the lower and upper bounds for the first Zagreb coindex of $F$-sum ($S$-sum, $R$-sum, $Q$-sum, and $T$-sum) graphs in the form of the first Zagreb indices and coindices of their basic graphs. At the end, the obtained results are also illustrated with the help of the examples of the exact and bounded values for some particular $F$-sum graphs. The reset of the paper is organized as follows: Section 2 includes the basic definitions and notions, Section 3 contains the main results of our work, and Section 4 presents particular examples related to the main results.

2. Preliminaries

Let $G = (V (G), E (G))$ be a connected graph, where $|V (G)|$ is order and $|E (G)|$ is size of the graph $G$. For any vertex $v \in V (G)$, its degree is denoted by $d (v)$ and is defined as number of vertices incident on it. An edge is formed by joining of two vertices $u, v \in V (G)$ denoted by $uv$. The complement of any graph is denoted by $\bar{G}$ and is defined as having same number of vertices as of original graph $G$ but for any two vertices $u$ and $v$, $uv \not\in E (\bar{G})$ iff $uv \in E (G)$. The first and second Zagreb indices $M_1 (G)$ and $M_2 (G)$ of $G$ are defined in [8] as follows:

\[
M_1 (G) = \sum_{v \in V (G)} [d_G (v)]^2 = \sum_{t_1, t_2 \in E (G)} [d_G (t_1) + d_G (t_2)],
\]

\[
M_2 (G) = \sum_{t_1, t_2 \in E (G)} [d_G (t_1)d_G (t_2)].
\]

(1)

The first Zagreb coindex $\overline{M}_1 (G)$ is defined in [15] as follows:

\[
\overline{M}_1 (G) = \sum_{t_1, t_2 \in E (G)} [d_G (t_1) + d_G (t_2)].
\]

(2)

It should be noted that the Zagreb coindices of $G$ run over $E (G)$, but the degrees correspond to $G$. For two connected graphs $G_1$ and $G_2$, the $F$-sum graphs are defined as follows.

Let $G$ be a graph; then,

(i) $S(G)$ is a graph formed by putting one vertex in each edge of $G$.

(ii) $R(G)$ is a graph obtained from $S(G)$ by joining the adjacent vertices of $G$.

(iii) $Q(G)$ is a graph formed from $S(G)$ by joining the pairs of new vertices which are on the adjacent edges of $G$.

(iv) $T(G)$ is formed by applying both operations of $R(G)$ and $Q(G)$ on $S(G)$.

Suppose that $G_1$ and $G_2$ are two connected graphs; then, their $F$-sum graphs are denoted by $G_1 \circ_{1-F} G_2$ and defined with vertex set $|V (G_1 \circ_{1-F} G_2)| = V (G_1) \cup E (G_1) \times V (G_2)$ and edge set as the vertices $(u_1, u_2)$ and $(v_1, v_2)$ of $G_1 \circ_{1-F} G_2$ are joined iff

(i) $u_1 = v_1 \in V (G_1)$ and $u_2 - v_2 \in G_2$.

(ii) $u_2 = v_2 \in V (G_2)$ and $u_1 - v_1 \in F (G_1)$, where $F \in \{S, R, Q, T\}$.

For details, see Figures 1 and 2.

3. Main Results

In this section, we discussed the main results of the first Zagreb coindex on the $F$-sum graphs which will be denoted by simply $\overline{M}^-$.

Theorem 1. Let $G_1$ and $G_2$ be two connected graphs; then, first Zagreb coindex of $G_1 \circ_{1-F} G_2$ is given as

\[
\alpha_1 \leq \overline{M} (G_1 \circ_{1-F} G_2) \leq \alpha_2,
\]

(3)

where

\[
\alpha_1 = 2(n_1^2 e_1^2 - n_2 e_1) + 2(e_1 \overline{e}_2 + e_2 (e_1 + \overline{e}_1)) + n_2 e_1 (n_1 - 2)
\]

\[
\cdot (e_2 + n_2) + (2(e_2 + \overline{e}_2) + n_2)M_1 (G_1) + (n_2 + 2e_2 + 2\overline{e}_2) \overline{M}_1 (G_1)
\]

\[
+ (2e_2 + 2\overline{e}_1)M_1 (G_2) + n_1 + 2(\overline{e}_1 + e_1) \overline{M}_1 (G_2) + 2n_2 e_1 [(2n_2 - 1) + 2(n_2 - 1)(e_2 + n_2)],
\]

\[
\alpha_2 = 2(n_1^2 e_1^2 - n_2 e_1) + 2(e_1 \overline{e}_2 + e_2 (e_1 + \overline{e}_1)) + n_2 e_1 (n_1 - 2)
\]

\[
\cdot (e_2 + n_2) + (2(e_2 + \overline{e}_2) + n_2)M_1 (G_1) + (n_2 + 2e_2 + 2\overline{e}_2) \overline{M}_1 (G_1)
\]

\[
+ (2e_2 + 2\overline{e}_1)M_1 (G_2) + (n_1 + 2(\overline{e}_1 + e_1)) \overline{M}_1 (G_2) + 2e_1 E (S (G_1)) [(n_1 - 2)n_2 (2n_2 - 1) + 2(n_2 - 1)(e_2 + n_2)].
\]
Proof. Using equation (2), we have

\[
\overline{M}(G_1 \times S G_2) = \sum_{(t_1, t_2) \in E(G_1 \times S G_2)} [d(t_1, x_1) + d(t_2, x_2)]a,
\]

\[
\overline{M}(G_1 \times S G_2) = \sum_{t_1, t_2 \in (V(S G_1) - V(G_1))} \sum_{x_1, x_2 \in V G_2} [d(t_1, x_1) + d(t_2, x_2)]
\]

\[
+ \sum_{t_1, t_2 \in V G_1} \sum_{x_1, x_2 \in V G_2} [d(t_1, x_1) + d(t_2, x_2)],
\]

\[
= \sum A + \sum B + \sum C,
\]

\[
\sum A = \sum_{t_1, t_2 \in (V(S G_1) - V(G_1))} \sum_{x_1, x_2 \in V G_2} \left[ d_S(G_1)(t_1) + d_S(G_1)(t_2) \right]
\]

\[
= \sum_{t_1, t_2 \in (V(S G_1) - V(G_1))} \sum_{x_1, x_2 \in V G_2} (2 + 2) = 2(n_2^2 e_1^2 - n_2 e_1),
\]

\[
\sum A = 2(n_2^2 e_1^2 - n_2 e_1),
\]
Figure 2: Graphs $G \cong P_4$, $H \cong P_2$, and $G_tH \cong P_4 \times P_2$. 
\[
\sum B = \sum B_1 + \sum B_2 + \sum B_3 + \sum B_4 + \sum B_5 + \sum B_6,
\]
\[
\sum B_1 = \sum_{t \in V_G, x_1, x_2 \notin E_G} \left[ d(t, x_1) + d(t, x_2) \right]
= \sum_{t \in V_G, x_1, x_2 \notin E_G} \left[ 2d_G(t) + d_G(x_1) + d_G(x_2) \right] = 4e_1 \overline{e}_2 + n_1 \overline{M}_1(G_2),
\]
\[
\sum B_2 = \sum_{x \in V_G, t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x) + d(t_2, x) \right]
= \sum_{x \in V_G, t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x) + d(t_2, x) \right] + \sum_{x \in V_G, t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x) + d(t_2, x) \right]
= \sum_{x \in V_G, t \neq E_G, x_1, x_2 \in E_G} \left[ d_G(t_1) + d_G(t_2) + 2d_G(x) \right] + \sum_{x \in V_G, t \neq E_G, x_1, x_2 \in E_G} \left[ d_G(t_1) + d_G(t_2) + 2d_G(x) \right]
= M_1(G_1)n_2 + 4e_1 \overline{e}_2 + \overline{M}_1(G_1)n_2 + 4 \overline{e}_2 e_2,
\]
\[
\sum B_3 = \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x_1) + d(t_2, x_2) \right]
= \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d_G(t_1) + d_G(t_2) + d_G(x_1) + d_G(x_2) \right] = 2[e_2 M_1(G_1) + e_1 M_1(G_2)],
\]
\[
\sum B_4 = \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x_1) + d(t_2, x_2) \right]
= \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d_G(t_1) + d_G(t_2) + d_G(x_1) + d_G(x_2) \right] = 2[e_2 \overline{M}_1(G_1) + \overline{e}_1 M_1(G_2)],
\]
\[
\sum B_5 = \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x_1) + d(t_2, x_2) \right]
= \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d_G(t_1) + d_G(t_2) + d_G(x_1) + d_G(x_2) \right] = 2[\overline{e}_2 M_1(G_1) + \overline{e}_1 \overline{M}_1(G_2)],
\]
\[
\sum B_6 = \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1, x_1) + d(t_2, x_2) \right]
= \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d_G(t_1) + d_G(t_2) + d_G(x_1) + d_G(x_2) \right] = 2[e_2 M_1(G_1) + e_1 \overline{M}_1(G_2)],
\]
\[
\sum B = 4e_1 \overline{e}_2 + e_2 (e_1 + \overline{e}_1) + (2(e_2 + \overline{e}_2) + n_2) M_1(G_1) + (n_2 (2e_2 + \overline{e}_2)) \overline{M}_1(G_1)
+ 2(e_2 + \overline{e}_2) M_1(G_2) + n_1 + 2(\overline{e}_1 + e_1) \overline{M}_1(G_2),
\]
\[
\sum C = \sum C_1 + \sum C_2 + \sum C_3,
\]
\[
\sum C_1 = \sum_{t \neq E_G, x_1, x_2 \in E_G} \sum_{x \in V_G} \left[ d(t_1, x) + d(t_2, x) \right]
= \sum_{t \neq E_G, x_1, x_2 \in E_G} \sum_{x \in V_G} \left[ d_G(t_1) + d_G(x) + d_G(t_2) \right]
= n_2 \sum_{t \neq E_G, x_1, x_2 \in E_G} \left[ d(t_1) + 2e_1 (n_1 - 2)[e_2 + n_2].
\]
Note that $2e_1 \leq \sum_{i,j \notin E(S(G_1))} (G_1)[d(t_i)] \leq 2e_1$

$(n_1 - 2)E(S(G_1)). \quad t_2 \in V(S(G_1) - V)

$$2n_2e_1(n_1 - 2) + 2e_2e_1(n_1 - 2) + 2n_2e_1(n_1 - 2) \leq \sum C_2 = \sum_{t_1,t_2 \notin E(S(G_1))} \sum_{x_1,x_2 \in V_{G_1}} [d(t_1,x_1) + d(t_2,x_2)]$$

$$= \sum_{t_1,t_2 \notin E(S(G_1))} \sum_{x_1,x_2 \in V_{G_1}} \left[ d_{G_1}(t_1) + d(x_1) + d_{S(G_1)}(t_2) \right].$$

(10)

$= n_2(n_1 - 1) \sum_{t_1,t_2 \notin E(S(G_1))} \sum_{x_1,x_2 \in V_{G_1}} \left[ d_{G_1}(t_1) + d(x_1) + d_{S(G_1)}(t_2) \right].$

Note that $2e_1 \leq \sum_{i,j \notin E(S(G_1))} (G_1)[d(t_i)] \leq 2e_1$

$(n_1 - 2)E(S(G_1)). \quad t_2 \in V(S(G_1) - V(G_1))$

$$2n_2(n_1 - 1)e_1(n_1 - 2) + 2e_2e_1(n_1 - 2)(n_1 - 2) + 2n_2(n_1 - 1)e_1(n_1 - 2) \leq \sum C_2 \leq 2n_2(n_1 - 1)e_1(n_1 - 2)E(S(G_1)),

+ 2e_2e_1(n_1 - 2)(n_1 - 2) + 2n_2(n_1 - 1)e_1(n_1 - 2),

$$\sum C_3 = \sum_{t_1,t_2 \notin E(S(G_1))} \sum_{x_1,x_2 \in V_{G_1}} [d(t_1,x_1) + d(t_2,x_2)] = \sum_{t_1,t_2 \notin E(S(G_1))} \sum_{x_1,x_2 \in V_{G_1}} \left[ d_{G_1}(t_1) + d(x_1) + d_{S(G_1)}(t_2) \right].$$

(11)
Note that \( 2e_1 \leq \sum_{t_1, t_2 \in E(S(G_1))} [d(t_1)] \leq 2e_1 E(S(G_1)). \)

\[
2e_1n_2(n_2 - 1) + 4e_1(n_2 - 1)(e_2 + n_2) \leq \sum C \leq 2e_1n_2(n_2 - 1)E(S(G_1)) + 4e_1(n_2 - 1)(e_2 + n_2).
\]

Consequently,

\[
2e_1n_2(n_2 - 1) + 4e_1(n_2 - 1)(e_2 + n_2) + 2n_2(n_2 - 1)e_1(n_1 - 2) + 2e_1n_1(n_1 - 2) + 2e_2e_1(n_1 - 2) + 2n_2e_1(n_1 - 2) \\
\leq \sum C \leq 2e_1n_2(n_2 - 1)E(S(G_1)) + 4e_1(n_2 - 1)(e_2 + n_2) + 2n_2(n_2 - 1)e_1(n_1 - 2)E(S(G_1)) + 2e_2e_1(n_1 - 2) + 2n_2e_1(n_1 - 2).
\]

By putting the values of \( \sum A + \sum B + \sum C \) in equation (5), we get the required proof.

**Theorem 2.** Let \( G_1 \) and \( G_2 \) be two connected graphs; then, the first Zagreb coindex of \( G_{1+R}G_2 \) is given as

\[
\alpha_1 = 2(n_2^2e_1^2 - n_2e_1) + 4(4e_1^2e_2 + e_2^2e_1) + 2e_1n_2(n_2 - 2)(e_2 + n_2) + (4e_2 + 4e_2^2)M_1(G_1) + 2(e_1 + e_2)M_1(G_2) \\
+ 2(n_2 + 2(e_2 + e_2^2))M_1(G_1) + (n_1 + 2e_1 + 2e_1^2)M_1(G_2) + 2e_1\left[n_2^2(2n_2 - 1) + 2(n_2 - 1)(e_2 + n_2)\right],
\]

\[
\alpha_2 = 2(n_2^2e_1^2 - n_2e_1) + 4(4e_1^2e_2 + e_2^2e_1) + 2e_1n_2(n_2 - 2)(e_2 + n_2) + (4e_2 + 4e_2^2)M_1(G_1) + 2(n_2 + 2(e_2 + e_2^2))M_1(G_1) \\
+ 2(e_1 + e_2)M_1(G_2) + (n_1 + 2e_1 + 2e_1^2)M_1(G_2) + 2E(R(G_1))e_1\left[n_2^2(2n_2 - 1)(n_2 - 2) + 2(n_2 - 1)(e_2 + n_2)\right].
\]

**Proof.** Using equation (2), we have

\[
\overline{M}(G_{1+R}G_2) = \sum_{(t_1, t_2) \in E(G_{1+R}G_2)} [d(t_1, x_1) + d(t_2, x_2)],
\]

\[
\overline{M}(G_{1+R}G_2) = \sum A + \sum B + \sum C.
\]
Using equation (6), we directly have

\[
\begin{align*}
\sum A &= 2(n^2_1 \overline{e}^2_1 - n_2 e_1), \\
\sum B &= \sum B_1 + \sum B_2 + \sum B_3 + \sum B_4 + \sum B_5 + \sum B_6, \\
\sum B_1 &= \sum_{t \in V_{G_1}, x \notin E_{G_1}} \left[ d(t, x_1) + d(t, x_2) \right] \\
&= \sum_{t \in V_{G_1}, x \notin E_{G_1}} \left[ 4d_{(G_1)}(t) + d_{G_1}(x_1) + d_{G_1}(x_2) \right] = 8e_1 \overline{e}^2 + n_1 \overline{M}_{1}(G_2), \\
\sum B_2 &= \sum_{x \in V_{G_1}, t \neq E_{G_1}} \sum_{t_2 \in V_{G_2}} \left[ d(t, x) + d(t_2, x) \right] \\
&= \sum_{x \in V_{G_1}, t \neq E_{G_1}} \sum_{t_2 \in V_{G_2}} \left[ d_{(G_1)}(t) + d_{G_1}(x) + 2d_{G_2}(x) \right] = 2M_{1}(G_1) n_2 + 4e_1 \overline{e}^2, \\
\sum B_3 &= \sum_{t_1, t_2 \in E_{G_1}, x \notin E_{G_2}} \sum_{t_2 \in V_{G_2}} \left[ d(t_1, x_1) + d(t_2, x_2) \right] \\
&= 2 \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \in V_{G_2}} \left[ d_{R}(G_1)(t_1) + d_{G_1}(x_1) + d_{R}(G_1)(t_2) + d_{G_1}(x_2) \right] \\
&= 2 \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \in V_{G_2}} \left[ 2d_{G_1}(t_1) + d_{G_1}(x_1) + 2d_{G_1}(t_2) + d_{G_1}(x_2) \right] = 2[2e_2 M_1(G_1) + e_1 M_1(G_2)], \\
\sum B_4 &= \sum_{t_1, t_2 \notin E_{G_1}, x \notin E_{G_2}} \sum_{t_2 \in V_{G_2}} \left[ d(t_1, x_1) + d(t_2, x_2) \right] \\
&= 2 \sum_{t_1, t_2 \notin E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \in V_{G_2}} \left[ d_{R}(G_1)(t_1) + d_{G_1}(x_1) + d_{R}(G_1)(t_2) + d_{G_1}(x_2) \right] \\
&= 2 \sum_{t_1, t_2 \notin E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \in V_{G_2}} \left[ 2d_{G_1}(t_1) + d_{G_1}(x_1) + 2d_{G_1}(t_2) + d_{G_1}(x_2) \right] = 2[2e_2 M_1(G_1) + e_1 M_1(G_2)], \\
\sum B_5 &= \sum_{t_1, t_2 \in E_{G_1}, x \notin E_{G_2}} \sum_{t_2 \notin E_{G_2}} \left[ d(t_1, x_1) + d(t_2, x_2) \right] \\
&= 2 \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \notin E_{G_2}} \left[ d_{R}(G_1)(t_1) + d_{G_1}(x_1) + d_{R}(G_1)(t_2) + d_{G_1}(x_2) \right] \\
&= 2 \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \notin E_{G_2}} \left[ d_{G_1}(t_1) + d_{G_1}(x_1) + d_{G_1}(t_2) + d_{G_1}(x_2) \right] = 2[2e_2 M_1(G_1) + e_1 M_1(G_2)], \\
\sum B_6 &= \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \notin E_{G_2}} \left[ d(t_1, x_1) + d(t_2, x_2) \right] \\
&= 2 \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \notin E_{G_2}} \left[ d_{R}(G_1)(t_1) + d_{G_1}(x_1) + d_{R}(G_1)(t_2) + d_{G_1}(x_2) \right] \\
&= 2 \sum_{t_1, t_2 \in E_{G_1}, x_1 \notin E_{G_2}} \sum_{t_2 \notin E_{G_2}} \left[ 2d_{G_1}(t_1) + d_{G_1}(x_1) + 2d_{G_1}(t_2) + d_{G_1}(x_2) \right] = 2[2e_2 M_1(G_1) + e_1 M_1(G_2)].
\end{align*}
\]
\[ B = 4(2e_1\overline{e}_2 + 4\overline{e} + e_2\overline{e}_1) + (4e_2 + 4\overline{e}_2)M_1(G_1) + 2(e_1 + \overline{e}_1)M_1(G_2) \]
\[ + 2n_2 + 2(e_2 + \overline{e}_2)M_1(G_1) + (n_1 + 2\overline{e}_1 + 2e_1)M_1(G_2), \]
\[ \sum C = \sum_{t_1, t_2 \in V(R(G_1))} [d(t_1, x_1) + d(t_2, x_2)] \]
\[ = \sum_{t_1, t_2 \not\in E(R(G_1))} \sum_{x \in V(G_2)} [d(t_1, x) + d(t_2, x)] + \sum_{t_1, t_2 \not\in E(R(G_1))} \sum_{x_1, x_2 \not\in V(G_2)} [d(t_1, x_1) + d(t_2, x_2)] \]
\[ + \sum_{t_1, t_2 \in E(R(G_1))} \sum_{x_1, x_2 \in V(G_2)} [d(t_1, x_1) + d(t_2, x_2)] = \sum C_1 + \sum C_2 + \sum C_3, \] (18)

\[ \sum C_1 = \sum_{t_1, t_2 \not\in E(R(G_1))} \sum_{x \in V(G_2)} [d(t_1, x) + d(t_2, x)] \]
\[ = \sum_{t_1, t_2 \not\in E(R(G_1))} \sum_{x \in V(G_2)} [d_{R(G_1)}(t_1) + d(x) + d_{R(G_1)}(t_2)] = \sum_{t_1, t_2 \not\in E(R(G_1))} \sum_{x \in V(G_2)} [d_{R(G_1)}(t_1) + d(x) + 2] \]
\[ = n_2 \sum_{t_1, t_2 \not\in E(R(G_1))} d_{R(G_1)}(t_1) + 2e_2e_1(n_2 - 1) + 2n_2e_1(n_2 - 1). \]
Note that $2e_1 \leq \sum_{t,t_2 \in E(R(G))} d(t_1) \leq 2E(R(G))e_1(n_1 - 2)$.

\[
2n_2e_1 + 2e_2e_1(n_2 - 1) + 2n_2e_1(n_2 - 1) \leq \sum C_1 \leq 2n_2E(R(G))e_1(n_1 - 2) + 2e_2e_1(n_2 - 1) + 2n_2e_1(n_2 - 1),
\]

\[
\sum C_2 = \sum_{t,t_2 \notin E(R(G))} \sum_{(x_1,x_2) \in V_G^2} \left[ d(t_1,x_1) + d(t_2,x_2) \right]
\]

\[
= \sum_{t,t_2 \notin E(R(G))} \sum_{x_1,x_2 \in V_G^2} \left[ d_R(G_1)(t_1) + d(x_1) + d_S(G_1)(t_2) \right]
\]

\[
= \sum_{t,t_2 \notin E(R(G))} \sum_{x_1,x_2 \in V_G^2} \left[ d_R(G_1)(t_1) + d(x_1) + 2 \right]
\]

(19)

\[
= n_2(n_2 - 1) \sum_{t,t_2 \notin E(R(G_1))} d_{RG_1}(t_1) + 2e_2e_1(n_1 - 2)(n_2 - 1)
\]

\[
+ 2n_2(n_2 - 1)e_1(n_1 - 2).
\]

Note that $2e_1 \leq \sum_{t,t_2 \notin E(R(G))} d(t_1) \leq 2E(R(G))e_1(n_1 - 2)$.

\[
2n_2(n_2 - 1)e_1(n_1 - 2) + 2e_2e_1(n_1 - 2)(n_2 - 1) + 2n_2(n_2 - 1)e_1(n_1 - 2)
\]

\[
\leq \sum C_2 \leq 2n_2(n_2 - 1)E(R(G_1))e_1(n_1 - 2)
\]

\[
+ 2e_2e_1(n_1 - 2)(n_2 - 1) + 2n_2(n_2 - 1)e_1(n_1 - 2),
\]

\[
\sum C_3 = \sum_{t,t_2 \notin E(R(G_1))} \sum_{x_1,x_2 \in V_G^2} \left[ d(t_1,x_1) + d(t_2,x_2) \right]
\]

\[
= \sum_{t,t_2 \notin E(R(G))} \sum_{x_1,x_2 \in V_G^2} \left[ d_R(G_1)(t_1) + d(x_1) + d_R(G_1)(t_2) \right] + \sum_{t,t_2 \notin E(R(G))} \sum_{x_1,x_2 \in V_G^2} \left[ d_R(G_1)(t_1) + d(x_1) + 2 \right]
\]

\[
= n_2(n_2 - 1) \sum_{t,t_2 \notin E(R(G_1))} d_R(G_1)(t_1) + 2e_2(n_2 - 1) \sum_{t,t_2 \notin E(R(G_1))} d_R(G_1)(t_1)
\]

\[
+ \sum_{t,t_2 \notin E(R(G))} \sum_{x_1,x_2 \in V_G^2} d_R(G_1)(t_1)
\]

(20)
Note that \( 2e_1 \leq \sum_{t_1, t_2 \in E(G_1)} d(t_1) \leq 4E(R(G_1))e_1 \). So,
\[
d(t_1) \leq 4E(R(G_1))e_1. \tag{21}
\]

Consequently,
\[
2n_2 e_1 + 2e_2 e_1 (n_2 - 1) + 2n_2 e_1 (n_2 - 1) + 2n_2 (n_2 - 1) e_1 (n_1 - 2) + 2e_2 e_1 (n_1 - 2)(n_2 - 1) + 2n_2 (n_2 - 1) e_1 (n_1 - 2) + 2e_2 e_1 (n_1 - 2)(n_2 - 1)
\leq \sum C \leq
2n_2 E(R(G_1))e_1 (n_1 - 2) + 2e_2 e_1 (n_1 - 1) + 2n_2 e_1 (n_1 - 1) + 2n_2 - 1) E(R(G_1))e_1 (n_1 - 2) + 2e_2 e_1 (n_1 - 2)(n_2 - 1)
+ 2n_2 (n_2 - 1) e_1 (n_1 - 2) + 4e_1 [n_2 (n_1 - 1) + 2e_2 (n_2 - 1) + 2n_2 (n_2 - 1)]
\]

By putting the values of \( A + B + C \) in equation (16), we get the required proof. \( \square \) where

\[
\alpha_1 \leq \overline{M}(G_{1 \sqcup} G_2) \leq \alpha_2, \tag{23}
\]

**Theorem 3.** Let \( G_1 \) and \( G_2 \) be two connected graphs; then, first Zagreb coindex of \( G_{1 \sqcup} G_2 \) is given as

\[
\begin{align*}
\alpha_1 &= 4(e_1 \bar{e}_2 + e_2 (e_1 + \bar{e}_1)) + 2(n_2 - 1 + \bar{e}_2)(2e_1 + \bar{e}_1) + 2e_1 (n_1 - 2)(e_2 + 3n_2) + n_2 (2n_2 - 1)e_1 + 2(2e_2 + 3n_2)(n_2 - 1)e_1 + (n_2 + 2e_2 + 2\bar{e}_2)M_1(G_1) + 2(e_1 + \bar{e}_1)\overline{M_1}(G_2), \\
\alpha_2 &= 4(e_1 \bar{e}_2 + e_2 (e_1 + \bar{e}_1)) + e_1 (n_1 - 2)(2e_2 + 3n_2) + 2e_1 (2e_2 + 3n_2)(n_1 - 1) + (n_2 + 2e_2 + 2\bar{e}_2)M_1(G_1) + (n_2 + 2(e_1 + \bar{e}_1)\overline{M_1}(G_1) + 2(e_1 + \bar{e}_1)M_1(G_2) + (n_1 + 2\bar{e}_1 + 2e_1)\overline{M_1}(G_2)
+ n_2 \overline{M_1}(Q(G_1)) + 4((n_2 - 1) + \bar{e}_2)E(Q(G_1))
+ 2n_2^2 E(Q(G_1))e_1 (n_1 - 2) + 2(n_1 - 1 + \bar{e}_2)\overline{M_1}(Q(G_1))\overline{M_1}(Q(G_1)) + 4n_2 e_1 E(Q = (G_1))(n_2 - 1).
\end{align*}
\]

**Proof.** Using equation (2), we have

\[
\overline{M}(G_{1 \sqcup} G_2) = \sum_{(t_1, t_2) \not\in E(G_{1 \sqcup} G_2)} [d(t_1, x) + d(t_2, x)],
\]

\[
\begin{align*}
\overline{M}(G_{1 \sqcup} G_2) &= \sum A + \sum B + \sum C, \\
\sum A &= \sum A_1 + \sum A_2 + \sum A_4 + \sum A_5 + \sum A_6 + \sum A_7, \\
\sum A_1 &= \sum_{t_1, t_2 \not\in E(Q(G_1))} \sum_{x \in V(G_1)} [d(t_1, x) + d(t_2, x)] = n_2 \sum_{t_1, t_2 \not\in E(Q(G_1))} d_{G_2}(t_1) + d_{G_2}(t_2),
\sum A_2 &= \sum_{t_1, t_2 \not\in E(Q(G_1))} \sum_{x \in V(G_2)} [d(t_1, x) + d(t_2, x)] = n_2 \sum_{t_1, t_2 \not\in E(Q(G_1))} d_{G_2}(t_1) + d_{G_2}(t_2),
\sum A_4 &= \sum_{t_1, t_2 \not\in E(Q(G_1))} \sum_{x \in V(G_1)} [d(t_1, x) + d(t_2, x)] = n_2 \sum_{t_1, t_2 \not\in E(Q(G_1))} d_{G_2}(t_1) + d_{G_2}(t_2),
\sum A_5 &= \sum_{t_1, t_2 \not\in E(Q(G_1))} \sum_{x \in V(G_2)} [d(t_1, x) + d(t_2, x)] = n_2 \sum_{t_1, t_2 \not\in E(Q(G_1))} d_{G_2}(t_1) + d_{G_2}(t_2),
\sum A_6 &= \sum_{t_1, t_2 \not\in E(Q(G_1))} \sum_{x \in V(G_1)} [d(t_1, x) + d(t_2, x)] = n_2 \sum_{t_1, t_2 \not\in E(Q(G_1))} d_{G_2}(t_1) + d_{G_2}(t_2),
\sum A_7 &= \sum_{t_1, t_2 \not\in E(Q(G_1))} \sum_{x \in V(G_2)} [d(t_1, x) + d(t_2, x)] = n_2 \sum_{t_1, t_2 \not\in E(Q(G_1))} d_{G_2}(t_1) + d_{G_2}(t_2).
\end{align*}
\)

\( \square \)
Note that $0 \leq \sum_{t_1, t_2 \notin E(Q(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)] \leq M_1(Q(G_1))$, so

$$0 \leq \sum_{t_1, t_2 \in V(Q(G_1))} [d(t_1, x_1) + d(t_2, x_2)]$$

$$= \sum_{t \in V(Q(G_1))} \sum_{x_1, x_2 \notin E_2} [d_{QG_1}(t) + d_{QG_1}(t)] = 2(n_2 - 1) \sum_{t \in V(Q(G_1))} [d_{QG_1}(t)].$$ (26)

Note that $e_1 \leq \sum_{t \in V(Q(G_1))} [d_{QG_1}(t)] \leq 2E(Q(G_1))$, so

$$2(n_2 - 1)e_1 \leq \sum_{t_1, t_2 \in V(Q(G_1))} [d(t_1, x_1) + d(t_2, x_2)]$$

$$= \sum_{t \in V(Q(G_1))} \sum_{x_1, x_2 \notin E_2} [d_{QG_1}(t) + d_{QG_1}(t)] = 2e_1 \sum_{t \in V(Q(G_1))} [d_{QG_1}(t)].$$ (27)

Note that $e_1 \leq \sum_{t \in V(Q(G_1))} [d_{QG_1}(t)] \leq 2E(Q(G_1))$, so

$$2e_1 \leq \sum_{t_1, t_2 \in V(Q(G_1))} [d(t_1, x_1) + d(t_2, x_2)]$$

$$= \sum_{t_1, t_2 \in V(Q(G_1))} \sum_{x_1, x_2 \notin E_2} [d_{QG_1}(t_1) + d_{QG_1}(t_2)] = (n_2 - 1) \sum_{t_1, t_2 \in V(Q(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)].$$ (28)
Note that $e_1 \leq \sum_{t_1, t_2 \in E(Q(G_1))} d_{QG_1}(t_1) + d_{QG_1}(t_2) \leq M_1(Q(G_1))$, so
\[
2(n_2 - 1)e_1 \leq \sum A_3 \leq 2(n_2 - 1)M_1(Q(G_1)),
\]
\[
\sum A_5 = \sum_{t_1, t_2 \in E(Q(G_1)), x_1, x_2 \notin E_{Q_1}} \sum_{t_1, t_2 \in V(Q(G_1) - V(G_1))} [d(t_1, x_1) + d(t_2, x_2)]
\]
\[
= \sum_{t_1, t_2 \in E(Q(G_1)), x_1, x_2 \notin E_{Q_1}} \sum_{t_1, t_2 \in V(Q(G_1) - V(G_1))} [d(t_1, x_1) + d(t_2, x_2)] = 2\bar{e}_2 \sum_{t_1, t_2 \in E(Q(G_1)), t_1, t_2 \in V(Q(G_1) - V(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)].
\]

(29)

Note that $e_1 \leq \sum_{t_1, t_2 \in E(Q(G_1))} d_{QG_1}(t_1) + d_{QG_1}(t_2) \leq M_1(Q(G_1)), so
\[
2\bar{e}_1 \leq \sum A_6 \leq 2\bar{e}_2 M_1(Q(G_1))
\]
\[
\sum A_6 = \sum_{t_1, t_2 \notin E(Q(G_1)), x_1, x_2 \in E_{Q_1}} \sum_{t_1, t_2 \in V(Q(G_1) - V(G_1))} [d(t_1, x_1) + d(t_2, x_2)]
\]
\[
= \sum_{t_1, t_2 \notin E(Q(G_1)), x_1, x_2 \in E_{Q_1}} \sum_{t_1, t_2 \in V(Q(G_1) - V(G_1))} [d(t_1, x_1) + d(t_2, x_2)] = 2(n_2 - 1) \sum_{t_1, t_2 \notin E(Q(G_1)), t_1, t_2 \in V(Q(G_1) - V(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)].
\]

(30)

Note that $\bar{e}_1 \leq \sum_{t_1, t_2 \notin E(Q(G_1)), t_1, t_2 \in V(Q(G_1) - V(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)] \leq M_1(Q(G_1)), so
\[
2(n_2 - 1)\bar{e}_1 \leq \sum A_7 \leq 2(n_2 - 1)\bar{M}_1(Q(G_1)),
\]
\[
\sum A_7 = \sum_{t_1, t_2 \notin E(Q(G_1)), x_1, x_2 \notin E_{Q_1}} \sum_{t_1, t_2 \in V(Q(G_1) - V(G_1))} [d(t_1, x_1) + d(t_2, x_2)]
\]
\[
= \sum_{t_1, t_2 \notin E(Q(G_1)), t_1, t_2 \in V(Q(G_1) - V(G_1))} [d(t_1, x_1) + d(t_2, x_2)] = 2\bar{e}_2 \sum_{t_1, t_2 \notin E(Q(G_1)), t_1, t_2 \in V(Q(G_1) - V(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)].
\]

(31)

Note that $\bar{e}_1 \leq \sum_{t_1, t_2 \notin E(Q(G_1)), t_1, t_2 \in V(Q(G_1) - V(G_1))} [d_{QG_1}(t_1) + d_{QG_1}(t_2)] \leq \bar{M}_1(Q(G_1)), so
\[
2\bar{e}_2 \bar{e}_1 \leq \sum A_7 \leq 2\bar{e}_2 \bar{M}_1(Q(G_1)).
\]

(32)

Consequently,
\[
2(n_2 - 1)e_1 + 2\overline{e}_2 e_1 + 2(n_2 - 1)e_1 + 2\overline{e}_2 e_1 + 2(n_2 - 1)e_1 + 2\overline{e}_2 e_1 \\
\leq \sum A \leq \\
+ n_2 M_1 (Q(G_1)) + 4(n_2 - 1)E(Q(G_1)) + 4\overline{e}_2 E(Q(G_1)) + 2(n_2 - 1)M_1 (Q(G_1)) \\
+ 2\overline{e}_2 M_1 (Q(G_1)) + 2(n_2 - 1)M_1 (Q(G_1)) + 2\overline{e}_2 M_1 (Q(G_1)).
\]

Using equation (8), we directly have

\[
\sum B = 4e_1 \overline{e}_2 + e_2 (e_1 + \overline{e}_1) + (2(e_2 + \overline{e}_2) + n_2)M_1 (G_1) + (n_2 (2e_2 + \overline{e}_2))M_1 (G_1) \\
+ 2(e_2 + \overline{e}_1)M_1 (G_2) + n_1 + 2(\overline{e}_1 + e_1)M_1 (G_2),
\]

\[
\sum C = \sum C_1 + \sum C_2 + \sum C_3,
\]

\[
\sum C_1 = \sum_{t,t_1 \notin E(Q(G_1))} \sum_{x \in V(G_2)} \sum_{t \in E(Q(G_1))} \sum_{t \in E(Q(G_1))} [d(t_1, x) + d(t_2, x)] \\
= n_2 \sum_{t,t_1 \notin E(Q(G_1))} d_{Q(G_1)} (t_1) + 2e_2 e_1 (n_1 - 2) + 3n_2 e_1 (n_1 - 2).
\]

Note that \(2e_1 \leq \sum_{t \in V(G_1)} d_Q \)

\((G_1) (t_1) \leq 2E(Q(G_1)) e_1 (n_1 - 2), \) so

\[
2n_2 e_1 + 2\overline{e}_2 e_1 (n_1 - 2) + 3n_2 e_1 (n_1 - 2) \leq \sum C_1 \leq 2n_2 E(Q(G_1)) e_1 (n_1 - 2) + 2\overline{e}_2 e_1 (n_1 - 2) + 3n_2 e_1 (n_1 - 2).
\]

\[
\sum C_2 = \sum_{t,t_1 \notin E(Q(G_1))} \sum_{x \in V(G_2)} \sum_{t \in E(Q(G_1))} \sum_{t \in E(Q(G_1))} [d(t_1, x) + d(t_2, x)] \\
= n_2 (n_2 - 1) \sum_{t,t_1 \notin E(Q(G_1))} d_{Q(G_1)} (t_1) + (2e_2 + 3n_2) (n_2 - 1)
\]

\[
\sum C_3 = \sum_{t,t_1 \notin E(Q(G_1))} d_{Q(G_1)} (t_1) |.
\]
Note that $2e_1 \leq \sum_{t_1, t_2 \neq E(Q(G_1))} d_Q(G_1)(t_1) \leq 2E(Q(G_1))e_1$, so

$$2e_1n_2(n_2 - 1) + e_1(n_1 - 2)(2e_2 + 3n_2) + 3n_2^2 \leq \sum_{C_2} = \sum_{t_1, t_2 \neq E(Q(G_1))} \sum_{x_1, x_2 \in V(G_1)} [d(t_1, x_1) + d(t_2, x_2)]$$

$$= \sum_{t_1, t_2 \neq E(Q(G_1))} \sum_{x_1, x_2 \in V(G_1)} [d_Q(G_1)(t_1) + d(x_1) + d_Q(G_1)(t_2)]$$

$$= n_2(n_2 - 1) \sum_{t_1, t_2 \neq E(Q(G_1))} d_Q(G_1)(t_1) + 2e_2(n_2 - 1)[(2e_2 + 3n_2) + 3n_2^2]$$

$$+ 3n_2(n_2 - 1) \sum_{t_1, t_2 \neq E(Q(G_1))} d_Q(G_1)(t_1)$$

$$(36)$$

Note that $2E(G_1) \leq \sum_{t_1, t_2 \neq E(Q(G_1))} d_Q(G_1)(t_1) \leq 4E(Q(G_1))e_1$, so

$$4n_2(n_2 - 1)e_1 + (n_2 - 1)(2e_1)(2e_2)(2e_1) + 3n_2^2 \leq \sum_{C_2} = 4n_2(n_2 - 1)Q(E(G_1))e_1 + (n_2 - 1)(2e_1)(2e_2 + 3n_2).$$

$$(37)$$

Consequently,

$$2n_2e_1 + 2e_2e_1(n_1 - 2) + 3n_2e_1(n_1 - 2) + 2e_1n_2(n_2 - 1) + e_1(n_1 - 2)(2e_2 + 3n_2)$$

$$+ 4n_2(n_2 - 1)e_1 + (n_2 - 1)(2e_1)(2e_2)(2e_1) + 3n_2$$

$$\leq \sum_{C_2} = 2n_2E(Q(G_1))e_1(n_1 - 2) + 2e_2e_1(n_1 - 2) + 3n_2e_1(n_1 - 2) + 2E(Q(G_1))e_1(n_1 - 2)[n_2(n_2 - 1) + (2e_2 + 3n_2)(n_2 - 1)]$$

$$+ 4n_2(n_2 - 1)Q(E(G_1))e_1 + (n_2 - 1)(2e_1)(2e_2 + 3n_2).$$

$$(38)$$

By putting the values of $\sum A + \sum B + \sum C$ in equation (25), we get the required proof. □

**Theorem 4.** Let $G_1$ and $G_2$ be two connected graphs; then, first Zagreb coindex of $G_1 \cup G_2$ is given as
Using equation (2), we have
\[ \alpha_1 = 4(2e_1\overline{e}_2 + e_2\overline{e}_1) + e_1(n_1 - 2)(2e_2 + 3n_2) + 2(n_2 + 2(e_2 + \overline{e}_2))M_1(G_1) + 4(e_2 + \overline{e}_2)\overline{M}_1(G_1) + 2(e_1 + \overline{e}_1)M_1(G_2) \]
\[ + (n_1 + 2(\overline{e}_1 + e_1))\overline{M}_1(G_2) + 2((n_2 - 1) + \overline{e}_1)e_1 + (n_2 - 1 + \overline{e}_1)e_1\overline{e}_1 + 2n^2e_1 + e_1(n_2 - 1)[n_2 + 2e_2 + 3n_2], \]
\[ \alpha_2 = 4(2e_1\overline{e}_2 + e_2\overline{e}_1) + e_1(n_1 - 2)(2e_2 + 3n_2) + 2(e_2 + \overline{e}_2)M_1(G_1) + (2n_2 + 4(e_2 + \overline{e}_2))\overline{M}_1(G_1) \]
\[ + 2(e_1 + \overline{e}_1)M_1(G_2) + (n_1 + 2(\overline{e}_1 + e_1))\overline{M}_1(G_2) + n_2\overline{M}_1(T(G_1) + 4((n_2 - 1) + \overline{e}_1)ET(G_1) \]
\[ + (n_2 - 1 + \overline{e}_1)M_1(T(G_1))\overline{M}_1(T(G_1)) + n_2^2E(T(G_1))e_1(n_2 - 1) + 2e_1(2e_2 + 3n_2)(n_2 - 1) \]
\[ + 4n_2e_1ET(G_1)(n_2 - 1) + 2e_1(n_2 - 1)(2e_2 + 3n_2). \]

\[ \text{Proof. Using equation (2), we have} \]
\[ \overline{M}(G_1 + T) \leq \overline{M}(G_2), \quad (39) \]
\[ \text{where} \]
\[ \overline{M}(G_1 + T) = \sum_{(u_1, u_2) \in E(G_1 + T)} [d(u_1, v_1) + d(u_2, v_2)], \]
\[ \overline{M}(G_1 + T) = \sum_{t_1, t_2 \in V(G_1 + T)} \sum_{x_1, x_2 \in V(G_1 + T)} [d(t_1, x_1) + d(t_2, x_2)] + \sum_{t_1, t_2 \in V(G_1 + T)} \sum_{x_1, x_2 \in V(G_1 + T)} [d(t_1, x_1) + d(t_2, x_2)] \]
\[ = \sum A + \sum B + \sum C. \]

Using equations (30) and (17), we directly have
\[ 2(n_2 - 1)e_1 + 2\overline{e}_2e_1 + 2(n_2 - 1)e_1 + 2\overline{e}_3e_1 + 2(n_2 - 1)e_1 + 2\overline{e}_3e_1 \leq \sum A \leq n_2\overline{M}_1(Q(G_1)) + 4(n_2 - 1)E(Q(G_1)) \]
\[ + 4\overline{e}_2E(Q(G_1)) + 2(n_2 - 1)M_1(Q(G_1)) + 2\overline{e}_3M_1(Q(G_1)) \]
\[ + 2(n_2 - 1)\overline{M}_1(Q(G_1)) + 2\overline{e}_3\overline{M}_1(Q(G_1)) \]
\[ \sum B = 4(2e_1\overline{e}_2 + 4\overline{e}_3 + e_2\overline{e}_1) + (4e_2 + 4\overline{e}_2)M_1(G_1) \]
\[ + 2(e_1 + \overline{e}_1)M_1(G_2) + 2n_2 + 2(e_2 + \overline{e}_2)\overline{M}_1(G_1) \]
\[ + (n_1 + 2\overline{e}_1 + 2e_1)\overline{M}_1(G_2). \]

\[ \text{Proof. Using equation (2), we have} \]
\[ \alpha_1 = 4(2e_1\overline{e}_2 + e_2\overline{e}_1) + e_1(n_1 - 2)(2e_2 + 3n_2) + 2(n_2 + 2(e_2 + \overline{e}_2))M_1(G_1) + 4(e_2 + \overline{e}_2)\overline{M}_1(G_1) + 2(e_1 + \overline{e}_1)M_1(G_2) \]
\[ + (n_1 + 2(\overline{e}_1 + e_1))\overline{M}_1(G_2) + 2((n_2 - 1) + \overline{e}_1)e_1 + (n_2 - 1 + \overline{e}_1)e_1\overline{e}_1 + 2n^2e_1 + e_1(n_2 - 1)[n_2 + 2e_2 + 3n_2], \]
\[ \alpha_2 = 4(2e_1\overline{e}_2 + e_2\overline{e}_1) + e_1(n_1 - 2)(2e_2 + 3n_2) + 4(e_2 + \overline{e}_2)M_1(G_1) + (2n_2 + 4(e_2 + \overline{e}_2))\overline{M}_1(G_1) \]
\[ + 2(e_1 + \overline{e}_1)M_1(G_2) + (n_1 + 2(\overline{e}_1 + e_1))\overline{M}_1(G_2) + n_2\overline{M}_1(T(G_1) + 4((n_2 - 1) + \overline{e}_1)ET(G_1) \]
\[ + (n_2 - 1 + \overline{e}_1)M_1(T(G_1))\overline{M}_1(T(G_1)) + n_2^2E(T(G_1))e_1(n_2 - 1) + 2e_1(2e_2 + 3n_2)(n_2 - 1) \]
\[ + 4n_2e_1ET(G_1)(n_2 - 1) + 2e_1(n_2 - 1)(2e_2 + 3n_2). \]
\[
\sum C = \sum C_1 + \sum C_2 + \sum C_3 + \sum_{v \in V_{G_2}} \sum_{t_1, t_2 \in E(T(G_i))} d(t_1, v) + d(t_2, v)
\]
\[
2n_2 \bar{e}_1 + 2e_2 e_1 (n_1 - 2) 3n_2 e_1 (n_1 - 2) \leq \sum C_1 + \sum_{t_1, t_2 \in E(T(G_i))} \sum_{v \in V_{G_2}} (t_1, v) + (t_2, v)
\]
\[
2n_2 (n_2 - 1)e_1 + 2(2e_2 + 3n_2) (n_2 - 1)e_1 (n_1 - 2) \leq \sum C_2 + \sum_{t_1, t_2 \in E(T(G_i))} \sum_{x_1, x_2 \in V_{G_2}} (t_1, x_1) + (t_2, x_2)
\]
\[
2n_2 (n_2 - 1)e_1 + 2(2e_2 + 3n_2) (n_2 - 1)e_1 (n_1 - 2) = \sum C_3 + \sum_{t_1, t_2 \in E(T(G_i))} \sum_{x_1, x_2 \in V_{G_2}} (t_1, x_1) + (t_2, x_2)
\]

Consequently,

\[
2n_2 \bar{e}_1 + 2e_2 e_1 (n_1 - 2) 3n_2 e_1 (n_1 - 2) + 2n_2 (n_2 - 1)e_1 + 2(2e_2 + 3n_2) (n_2 - 1)e_1 (n_1 - 2) + 4n_2 e_1 (n_1 - 2) + 4e_1 (3n_2 (n_2 - 1)) T(E(G_i))
\]
\[
\leq \sum C \leq 2n_2 T(E(G_i)) e_1 (n_1 - 2) + 2e_2 e_1 (n_1 - 2) + 3n_2 e_1 (n_1 - 2) + 2n_2 (n_2 - 1)e_1 (n_1 - 2)
\]
\[
+ 2(2e_2 + 3n_2) (n_2 - 1) T(E(G_i)) e_1 (n_1 - 2) + 8n_2 e_1 (n_2 - 1) T(E(G_i))
\]
\[
+ 8e_1 e_2 (n_2 - 1) T(E(G_i)) + 4e_1 (3n_2 (n_2 - 1)) T(E(G_i)).
\]

By putting the values of \( \sum A + \sum B + \sum C \) in equation (39), we get the required proof. \( \square \)

4. Conclusion

Several topological indices (TIs) have been defined with the help of the graph-theoretic parameters of degree, distance, eccentricity, and eigenvalues, and various results are obtained by different researchers for a large number of molecular structures, graphs, or networks. This popularity is not only due to being the rich mathematical problems of the theory of graphs and networking but also due to the wide range of its applications in different disciplines of sciences, especially in chemistry and computer science such as navigation, combinatorial optimization, pattern recognition, image processing, integer programming, formation of chemical compounds, and discovery of drugs.

In this paper, we have computed bounds for first Zagreb coindex of F–sum graphs such as \( \overline{M}(G_1 G_2), \overline{M}(G_1 \times G_2), \overline{M}(G_1 \circ G_2), \) and \( \overline{M}(G_1 \vee G_2) \) in their general forms. The F-sum graphs obtained by different subdivision operations and Cartesian product of graphs present several families of molecular structures, especially graphs consisting of hexagonal chains.

Table 1 presents the first Zagreb coindex of the Cartesian product of certain path graphs, and Tables 2–5 show the lower and upper bounds of the first Zagreb coindex for the S-sum, R-sum, Q-sum, and T–sum graphs. Now, we compute the linear regression formula to compute correlation between exact values of \( \overline{M}(P_n + P_m) \) and bounded values.
of $F$-sum graphs $(\overline{M}_1(P_n \circ P_m))$. In general, the linear regression formula is expressed as $Y = b_0 + b_1 X$, where $b_0$ is the y-intercept (point of intersection of line and Y-axis) and $b_1$ is slope that describes the line’s direction and inclination.

The linear regression formula of the Cartesian product of paths $Y$ in terms of lower and upper bounds of the $S$-sum graph $(X)$ is $Y = 0 + 1X$ (100 percent correlation between $x$ and $y$ exists with 1 being the value of correlation coefficient) and $Y = 103.9108 + 0.47X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.9993 being the value of correlation coefficient).

The linear regression formula of the Cartesian product of paths $Y$ in terms of lower and upper bounds of the $R$-sum graph $(X)$ is $Y = 96.9504 + 0.6578X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.9982 being the value of correlation coefficient) and $Y = 173.5697 + 0.1731X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.9966 being the value of correlation coefficient).

The linear regression formula of the Cartesian product of paths $Y$ in terms of lower and upper bounds of the $Q$-sum graph $(X)$ is $Y = 305.2811 + 0.5066X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.9851 being the value of correlation coefficient) and $Y = 24.8959 + 0.218X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.9962 being the value of correlation coefficient).

The linear regression formula of the Cartesian product of paths $Y$ in terms of lower and upper bounds of the $T$-sum graph $(X)$ is $Y = 276.3798 + 0.4747X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.9870 being the value of correlation coefficient) and $Y = -565.4512 + 0.3338X$ (a very strong direct relationship between $X$ and $Y$ exists with 0.8784 being the value of correlation coefficient).

Now, we close our discussion with the comment that the molecular structures which are isomorphic to sum graphs ($S$-sum, $R$-sum, $Q$-sum, and $T$-sum) have strong correlation for the thirteen physicochemical properties such as boiling point, density, heat capacity at constant pressure, entropy, heat capacity at constant time, enthalpy of vaporization, acentric factor, standard enthalpy of vaporization, enthalpy of formation, octanol-water partition coefficient, standard enthalpy of formation, total surface area, and molar volume.

### Data Availability

All data are included within this article. However, the reader may contact the corresponding author for more details of the data.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

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