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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, $G_{1+F}G_2$ 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 Trinajsti defined the TIs known as first and second Zagreb indices to calculate total π-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 ($G_{1+S}G_2$, $G_{1+R}G_2$, $G_{1+Q}G_2$, and $G_{1+T}G_2$). 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)-analogs 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 coincides of their basic graphs. At the end, the obtained results are also illustrated with the help of the examples of the exact and bonded 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 $\overline{G}$ and is defined as having same number of vertices as of original graph G but for any two vertices u and v, $uv \in E(\overline{G})$ iff $uv \notin E(G)$. The first and second Zagreb indices $M_1(G)$ and $M_2(G)$ of G are defined in [8] as follows:

$$M_1(G) = \sum_{t \in V(G)} [d_G(t)]^2 = \sum_{t_1 t_2 \in E(G)} [d_G(t_1) + d_G(t_2)],$$
$$M_2(G) = \sum_{t_1 t_2 \in E(G)} [d_G(t_1) d_G(t_2)]. \tag{1}$$

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

$$\overline{M}_1(G) = \sum_{t_1 t_2 \notin E(G)} [d_G(t_1) + d_G(t_2)]. \tag{2}$$

It should be noted that the Zagreb coindices of G run over $E(\overline{G})$, 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 $G_{1+F}G_2$ and defined with vertex set $|V(G_{1+S}G_2)| = V(G_1) \cup E(G_1) \times V(G_2)$ and edge set as the vertices (u_1, u_2) and (v_1, v_2) of $G_{1+F}G_2$ are joined iff

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

(ii) $u_2 = v_2 \in V(G_2)$ and $u_1 \sim v_1 \in F(G_1)$, 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 M^-.

Theorem 1. *Let G_1 and G_2 be two connected graphs; then, first Zagreb coindex of $G_{1+S}G_2$ is given as*

$$\alpha_1 \le \overline{M}(G_{1+s}G_2) \le \alpha_2, \tag{3}$$

where

$$\begin{aligned}
\alpha_1 &= 2\left(n_2^2 e_1^2 - n_2 e_1\right) + 2\left(e_1 \overline{e_2} + e_2\left(e_1 + \overline{e_1}\right)\right) + n_2 e_1 (n_1 - 2) \\
&\quad \cdot (e_2 + n_2) + \left(2(e_2 + \overline{e}_2) + n_2\right) M_1(G_1) + (n_2 + 2e_2 + 2\overline{e}_2)\overline{M}_1(G_1) \\
&\quad + (2e_2 + 2\overline{e}_1) M_1(G_2) + n_1 + 2(\overline{e}_1 + e_1)\overline{M}_1(G_2) + 2n_2 e_1 \left[(2n_2 - 1) + 2(n_2 - 1)(e_2 + n_2)\right], \\
\alpha_2 &= 2\left(n_2^2 e_1^2 - n_2 e_1\right) + 2\left(e_1 \overline{e_2} + e_2\left(e_1 + \overline{e_1}\right)\right) + n_2 e_1 (n_1 - 2) \\
&\quad \cdot (e_2 + n_2) + \left(2(e_2 + \overline{e}_2) + n_2\right) M_1(G_1) + (n_2 + 2e_2 + 2\overline{e}_2)\overline{M}_1(G_1) \\
&\quad + (2e_2 + 2\overline{e}_1) M_1(G_2) + (n_1 + 2(\overline{e}_1 + e_1))\overline{M}_1(G_2) + 2e_1 E(S(G_1))\left[(n_1 - 2) n_2 (2n_2 - 1) + 2(n_2 - 1)(e_2 + n_2)\right].
\end{aligned} \tag{4}$$

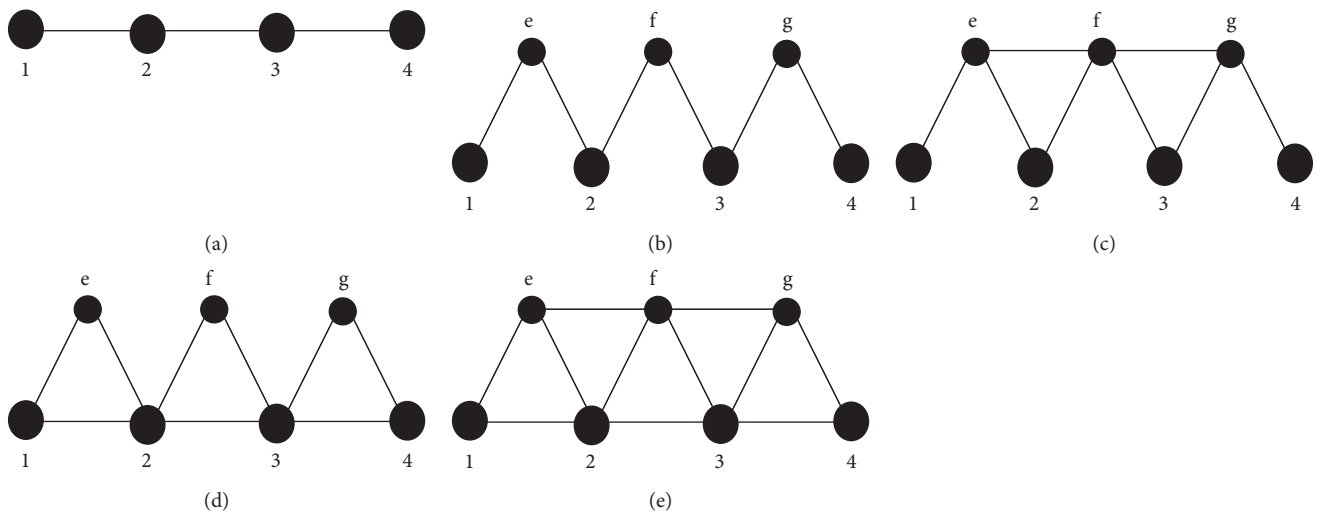

Figure 1: (a) $G \cong P_4$, (b) $S(G) \cong S(P_4)$, (c) $Q(G) \cong (P_4)$, (d) $R(G) \cong R(P_4)$, and (e) $T(G) \cong T(P_4)$.

Proof. Using equation (2), we have

$$\begin{aligned}
\overline{M}(G_{1+S}G_2) &= \sum_{(t_1,t_2)(x_1,x_2) \notin E(G_{1+S}G_2)} [d(t_1,x_1) + d(t_2,x_2)]a, \\
\overline{M}(G_{1+S}G_2) &= \sum_{t_1,t_2 \in (V(SG_1)-V(G_1))} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)] \\
&\quad + \sum_{t_1,t_2 \in V_{G_1}} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)] \\
&\quad \sum_{\substack{t_1,t_2 \in V(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)], \\
&= \sum A + \sum B + \sum C,
\end{aligned} \tag{5}$$

$$\begin{aligned}
\sum A &= \sum_{t_1,t_2 \in V(S(G_1)-V(G_1))} \sum_{x_1,x_2 \in V_{G_2}} \left[d_{S(G_1)}(t_1) + d_{S(G_1)}(t_2)\right] \\
&= \sum_{t_1,t_2 \in V(S(G_1)-V(G_1))} \sum_{x_1,x_2 \in V_{G_2}} (2+2) = 2\left(n_2^2 e_1^2 - n_2 e_1\right), \\
\sum A &= 2\left(n_2^2 e_1^2 - n_2 e_1\right),
\end{aligned} \tag{6}$$

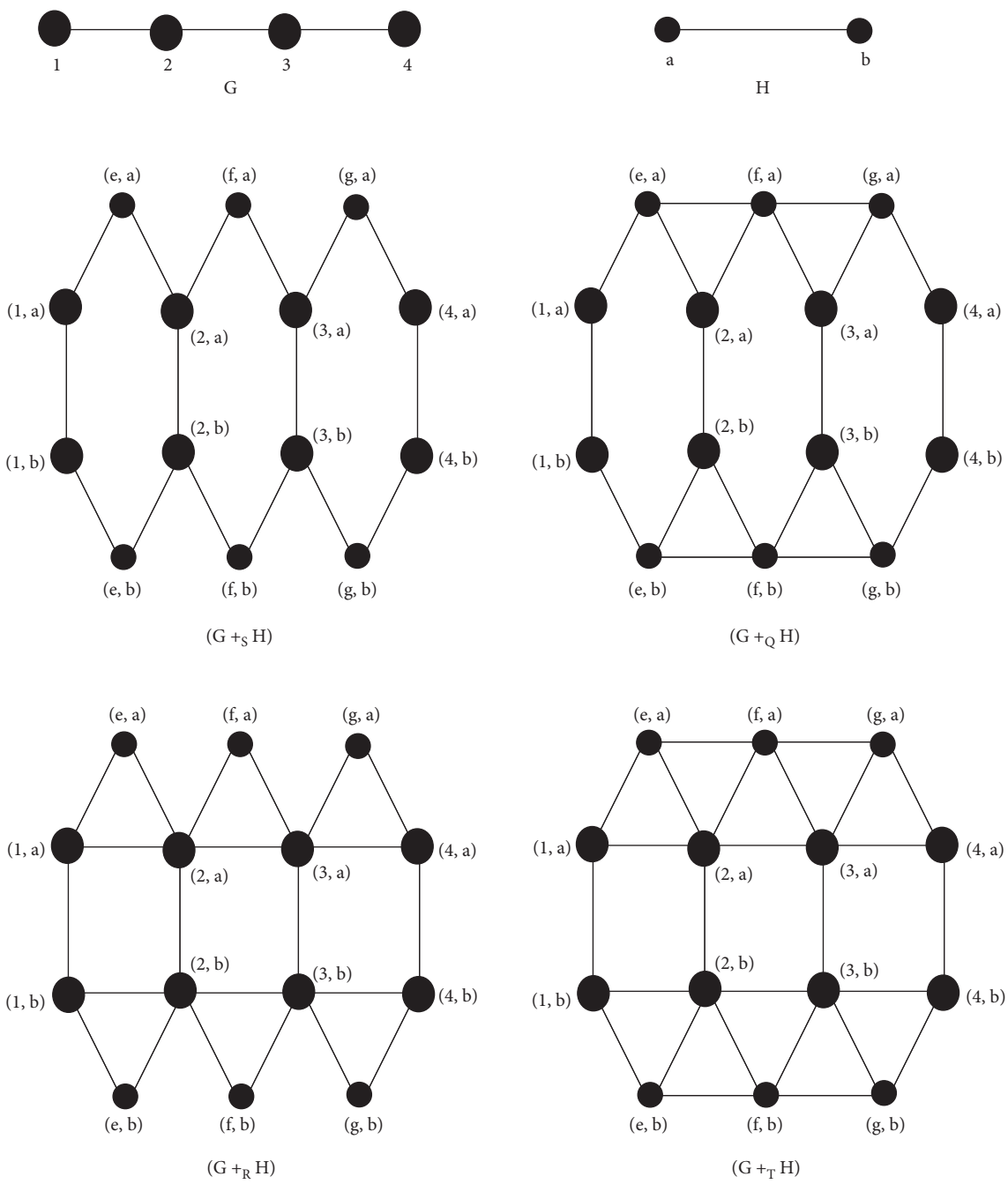

Figure 2: Graphs $G \cong P_4$, $H \cong P_2$, and $G_{+F}H \cong P_{4+F}P_2$.

$$
\begin{aligned}
\sum B &= \sum B_1 + \sum B_2 + \sum B_3 + \sum B_4 + \sum B_5 + \sum B_6,\\
\sum B_1 &= \sum_{t\in V_{G_1}} \sum_{x_1x_2\notin E_{G_2}} [d(t,x_1)+d(t,x_2)]\\
&= \sum_{t\in V_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[2d_{G_1}(t)+d_{G_2}(x_1)+d_{G_2}(x_2)\right] = 4e_1\overline{e_2}+n_1\overline{M_1}(G_2),\\
\sum B_2 &= \sum_{x\in V_{G_2}} \sum_{t_1,t_2\in V_{G_1}} [d(t_1,x)+d(t_2,x)]\\
&= \sum_{x\in V_{G_2}} \sum_{t_1t_2\in E_{G_1}} [d(t_1,x)+d(t_2,x)] + \sum_{x\in V_{G_2}} \sum_{t_1t_2\notin E_{G_1}} [d(t_1,x)+d(t_2,x)]\\
&= \sum_{x\in V_{G_2}} \sum_{t_1t_2\in E_{G_1}} \left[d_{G_1}(t_1)+d_{G_1}(t_2)+2d_{G_2}(x)\right] + \sum_{x\in V_{G_2}} \sum_{t_1t_2\notin E_{G_1}} \left[d_{G_1}(t_1)+d_{G_1}(t_2)+2d_{G_2}(x)\right]\\
&= M_1(G_1)n_2+4e_1e_2+\overline{M_1}(G_1)n_2+4\overline{e_1}e_2,\\
\sum B_3 &= \sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\in E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\
&= \sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[d_{G_1}(t_1)+d_{G_2}(x_1)+d_{G_1}(t_2)+d_{G_2}(x_2)\right] = 2[e_2M_1(G_1)+e_1M_1(G_2)].\\
\sum B_4 &= \sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\in E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\
&= \sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[d_{G_1}(t_1)+d_{G_2}(x_1)+d_{G_1}(t_2)+d_{G_2}(x_2)\right] = 2[e_2\overline{M_1}(G_1)+\overline{e_1}M_1(G_2)],\\
\sum B_5 &= \sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\
&= \sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d_{G_1}(t_1)+d_{G_2}(x_1)+d_{G_1}(t_2)+d_{G_2}(x_2)\right] = 2[\overline{e_2}\overline{M_1}(G_1)+\overline{e_1}\overline{M_1}(G_2)],\\
\sum B_6 &= \sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\
&= \sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d_{G_1}(t_1)+d_{G_2}(x_1)+d_{G_1}(t_2)+d_{G_2}(x_2)\right] = 2[\overline{e}_2M_1(G_1)+e_1\overline{M_1}(G_2)],
\end{aligned}
\tag{7}
$$

$$
\begin{aligned}
\sum B = {}& 4e_1\overline{e}_2+e_2(e_1+\overline{e}_1)+(2(e_2+\overline{e}_2)+n_2)M_1(G_1)+(n_2(2e_2+\overline{e}_2))\overline{M}_1(G_1)\\
&+2(e_2+\overline{e}_1)M_1(G_2)+n_1+2(\overline{e}_1+e_1)\overline{M}_1(G_2),
\end{aligned}
\tag{8}
$$

$$
\begin{aligned}
\sum C &= \sum C_1 + \sum C_2 + \sum C_3,\\
\sum C_1 &= \sum_{\substack{t_1t_2\notin E(S(G_1))\\ t_1\in V(G_1)\\ t_2\in V(S(G_1)-V(G_1))}} \sum_{x\in V_{G_2}} [d(t_1,x)+d(t_2,x)],\\
&= \sum_{\substack{t_1t_2\notin E(S(G_1))\\ t_1\in V(G_1)\\ t_2\in V(S(G_1)-V(G_1))}} \sum_{x\in V_{G_2}} \left[d_{G_1}(t_1)+d(x)+d_{S(G_1)}(t_2)\right]\\
&= n_2 \sum_{\substack{t_1t_2\notin E(S(G_1))\\ t_1\in V(G_1)\\ t_2\in V(S(G_1)-V(G_1))}} d(t_1)+2e_1(n_1-2)[e_2+n_2].
\end{aligned}
\tag{9}
$$

Note that $2e_1 \le \sum_{\substack{t_1t_2 \notin E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V}} (G_1))[d(t_1)] \le 2e_1 (n_1-2)E(S(G_1))$.

$$2n_2e_1(n_1-2)+2e_2e_1(n_1-2)+2n_2e_1(n_1-2) \le \sum C_1 \le 2n_2e_1(n_1-2)E(S(G_1))+2e_2e_1(n_1-2)+2n_2e_1(n_1-2),$$

$$\begin{aligned}\sum C_2 &= \sum_{\substack{t_1t_2 \notin E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1,x_1)+d(t_2,x_2)] \\ &= \sum_{\substack{t_1t_2 \notin E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} \left[d_{G_1}(t_1)+d(x_1)+d_{S(G_1)}(t_2)\right], \\ &= n_2(n_2-1) \sum_{\substack{t_1t_2 \notin E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V(G_1))}} \cdot \left[d_{G_1}(t_1)\right] + 2e_2e_1(n_1-2)(n_2-1)+2n_2(n_2-1)e_1(n_1-2).\end{aligned} \tag{10}$$

Note that $2e_1 \le \sum_{\substack{t_1t_2 \notin E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V(G_1))}} [d(t_1)] \le 2e_1 (n_1-2)\ E(S(G_1))$.

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

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

$$\sum C_3 = \sum_{\substack{t_1t_2 \in E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V*(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1,x_1)+d(t_2,x_2)] = \sum_{\substack{t_1t_2 \in E(S(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(S(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} \left[d_{G_1}(t_1)+d(x_1)+d_{S(G_1)}(t_2)\right]$$

$$= n_2(n_2-1) \sum_{\substack{t_1t_2 \in E(S(G_1)) \\ t_1 \in V(G_1) t_2 \in V(S(G_1)-V(G_1))}} [d(t_1)] + 2e_2(n_1-2)| \sum_{\substack{t_1t_2 \in E(S(G_1)) \\ t_1 \in V(G_1) t_2 \in V(S(G_1)-V(G_1))}} d(t_1)| + 2n_2(n_2-1)|$$

$$\sum_{\substack{t_1t_2 \in E(S(G_1)) \\ t_1 \in V(G_1) t_2 \in V}} (S(G_1)-G_1)d(t_1)|. \tag{11}$$

Note that $2e_1 \leq \sum_{\substack{t_1t_2 \in E(S(G_1)) \\ t_1 \in V(G_1) t_2 \in V(S(G_1) - V(G_1))}} [d(t_1)] \leq 2e_1 E(S(G_1))$.

$$2e_1n_2(n_2-1) + 4e_1(n_2-1)(e_2+n_2) \leq \sum C_3 \leq 2e_1n_2(n_2-1)E(S(G_1)) + 4e_1(n_2-1)(e_2+n_2). \tag{12}$$

Consequently,

$$\begin{aligned} &2e_1n_2(n_2-1) + 4e_1(n_2-1)(e_2+n_2) + 2n_2(n_2-1)e_1(n_1-2)+ \\ &\quad 2e_2e_1(n_1-2)(n_2-1) + 2n_2(n_2-1)e_1(n_1-2) + 2n_2e_1(n_1-2) + 2e_2e_1(n_1-2) + 2n_2e_1(n_1-2) \\ &\leq \sum C \leq \\ &\quad 2e_1n_2(n_2-1)E(S(G_1)) + 4e_1(n_2-1)(e_2+n_2) + 2n_2(n_2-1)e_1(n_1-2)E(S(G_1))+ \\ &\quad 2e_2e_1(n_1-2)(n_2-1) + 2n_2(n_2-1)e_1(n_1-2) + n_2e_1(n_1-2)E(S(G_1)) + 2e_2e_1(n_1-2) + 2n_2e_1(n_1-2). \end{aligned} \tag{13}$$

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, first Zagreb coindex of $G_{1+R}G_2$ is given as*

$$\alpha_1 \leq \overline{M}(G_{1+R}G_2) \leq \alpha_2, \tag{14}$$

where

$$\begin{aligned} \alpha_1 &= 2\left(n_2^2e_1^2 - n_2e_1\right) + 4(4e_1\overline{e}_2 + e_2\overline{e}_1) + 2e_1n_2(n_1-2)(e_2+n_2) + (4e_2+4\overline{e}_2)M_1(G_1) + 2(e_1+\overline{e}_1)M_1(G_2) \\ &\quad + 2(n_2 + 2(e_2+\overline{e}_2))\overline{M}_1(G_1) + (n_1 + 2\overline{e}_1 + 2e_1)\overline{M}_1(G_2) + 2e_1\left[n_2^2(2n_2-1) + 2(n_2-1)(e_2+n_2)\right], \\ \alpha_2 &= 2\left(n_2^2e_1^2 - n_2e_1\right) + 4(4e_1\overline{e}_2 + e_2\overline{e}_1) + 2e_1n_2(n_1-2)(e_2+n_2) + (4e_2+4\overline{e}_2)M_1(G_1) + 2(n_2 + 2(e_2+\overline{e}_2))\overline{M}_1(G_1) \\ &\quad + 2(e_1+\overline{e}_1)M_1(G_2) + (n_1 + 2\overline{e}_1 + 2e_1)\overline{M}_1(G_2) + 2E(R(G_1))e_1\left[n_2^2(2n_2-1)(n_1-2) + 2(n_2-1)(e_2+n_2)\right]. \end{aligned} \tag{15}$$

Proof. Using equation (2), we have

$$\begin{aligned} \overline{M}(G_{1+R}G_2) &= \sum_{(t_1,t_2)(x_1,x_2) \notin E(G_{1+R}G_2)} [d(t_1,x_1) + d(t_2,x_2)], \\ \overline{M}(G_{1+R}G_2) &= \sum A + \sum B + \sum C. \end{aligned} \tag{16}$$

Using equation (6), we directly have

$$
\begin{aligned}
\sum A &= 2\left(n_2^2 e_1^2 - n_2 e_1\right),\\
\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}} \sum_{x_1x_2\notin E_{G_2}} \left[d(t,x_1) + d(t,x_2)\right]\\
&= \sum_{t\in V_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[4d_{(G_1)}(t) + d_{G_2}(x_1) + d_{G_2}(x_2)\right] = 8e_1\overline{e_2} + n_1\overline{M_1}(G_2),\\
\sum B_2 &= \sum_{x\in V_{G_2}} \sum_{t_1,t_2\in V_{G_1}} \left[d(t_1,x) + d(t_2,x)\right]\\
&= \sum_{x\in V_{G_2}} \sum_{t_1t_2\notin E_{G_1}} \left[d(t_1,x) + d(t_2,x)\right] = \sum_{x\in V_{G_2}} \sum_{(t_1t_2)\notin E_{G_1}} \left[d_{R(G_1)}(t_1) + d_{R(G_1)}(t_2) + 2d_{G_2}(x)\right]\\
&= \sum_{x\in V_{G_2}} \sum_{(t_1t_2)\notin E_{G_1}} \left[2d_{(G_1)}(t_1) + 2d_{(G_1)}(t_2) + 2d_{G_2}(x)\right] = \left[2\overline{M_1}(G_1)n_2 + 4\overline{e_1}e_2\right],\\
\sum B_3 &= \sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[d(t_1,x_1) + d(t_2,x_2)\right]\\
&= 2\left[\sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[d_{R(G_1)}(t_1) + d_{G_2}(x_1) + d_{R(G_1)}(t_2) + d_{G_2}(x_2)\right]\right.\\
&= 2\left[\sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[2d_{(G_1)}(t_1) + d_{G_2}(x_1) + 2d_{(G_1)}(t_2) + d_{G_2}(x_2)\right]\right. = 2\left[2e_2M_1(G_1) + e_1M_1(G_2)\right],\\
\sum B_4 &= \sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[d(t_1,x_1) + d(t_2,x_2)\right]\\
&= 2\left[\sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[d_{R(G_1)}(t_1) + d_{G_2}(x_1) + d_{R(G_1)}(t_2) + d_{G_2}(x_2)\right]\right.\\
&= 2\left[\sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\in E_{G_2}} \left[2d_{(G_1)}(t_1) + d_{G_2}(x_1) + 2d_{(G_1)}(t_2) + d_{G_2}(x_2)\right]\right. = 2\left[2e_2\overline{M_1}(G_1) + \overline{e_1}M_1(G_2)\right],\\
\sum B_5 &= \sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d(t_1,x_1) + d(t_2,x_2)\right]\\
&= 2\left[\sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d_{R(G_1)}(t_1) + d_{G_2}(x_1) + d_{R(G_1)}(t_2) + d_{G_2}(x_2)\right]\right]\\
&= 2\left[\sum_{t_1t_2\notin E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d_{(G_1)}(t_1) + d_{G_2}(x_1) + d_{(G_1)}(t_2) + d_{G_2}(x_2)\right]\right. = 2\left[2\overline{e_2}\,\overline{M_1}(G_1) + \overline{e_1}\,\overline{M_1}(G_2)\right],\\
\sum B_6 &= \sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d(t_1,x_1) + d(t_2,x_2)\right]\\
&= 2\left[\sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[d_{R(G_1)}(t_1) + d_{G_2}(x_1) + d_{R(G_1)}(t_2) + d_{G_2}(x_2)\right]\right.\\
&= 2\left[\sum_{t_1t_2\in E_{G_1}} \sum_{x_1x_2\notin E_{G_2}} \left[2d_{(G_1)}(t_1) + d_{G_2}(x_1) + 2d_{(G_1)}(t_2) + d_{G_2}(x_2)\right]\right. = 2\left[2\overline{e}_2M_1(G_1) + e_1\overline{M}_1(G_2)\right],
\end{aligned}
\tag{17}
$$

$$\sum B = 4\left(2e_1\overline{e}_2 + 4\overline{e} + e_2\overline{e}_1\right) + \left(4e_2 + 4\overline{e}_2\right)M_1\left(G_1\right) + 2\left(e_1 + \overline{e}_1\right)M_1\left(G_2\right)$$
$$+ 2n_2 + 2\left(e_2 + \overline{e}_2\right)\overline{M}_1\left(G_1\right) + \left(n_1 + 2\overline{e}_1 + 2e_1\right)\overline{M}_1\left(G_2\right),$$
$$\sum C = \sum_{\substack{t_1,t_2\in V\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} \left[d\left(t_1,x_1\right) + d\left(t_2,x_2\right)\right]$$
$$= \sum_{\substack{t_1t_2\notin E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} \sum_{x\in V_{G_2}} \left[d\left(t_1,x\right) + d\left(t_2,x\right)\right] + \sum_{\substack{t_1t_2\notin E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(RG_1-V\left(G_1\right)\right)}} \sum_{x_1,x_2\in V_{G_2}} \left[d\left(t_1,x_1\right) + d\left(t_2,x_2\right)\right]$$
$$+ \sum_{\substack{t_1t_2\in E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} \sum_{x_1,x_2\in V_{G_2}} \left[d\left(t_1,x_1\right) + d\left(t_2,x_2\right)\right] = \sum C_1 + \sum C_2 + \sum C_3, \tag{18}$$

$$\sum C_1 = \sum_{\substack{t_1t_2\notin E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} \sum_{x\in V_{G_2}} \left[d\left(t_1,x\right) + d\left(t_2,x\right)\right]$$
$$= \sum_{\substack{t_1t_2\notin E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} \sum_{x\in V_{G_2}} \left[d_{R\left(G_1\right)}\left(t_1\right) + d\left(x\right) + d_{R\left(G_1\right)}\left(t_2\right)\right] = \sum_{\substack{t_1t_2\notin E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} \sum_{x\in V_{G_2}} \left[d_{R\left(G_1\right)}\left(t_1\right) + d\left(x\right) + 2\right]$$
$$= n_2 \sum_{\substack{t_1t_2\notin E\left(R\left(G_1\right)\right)\\ t_1\in V\left(G_1\right)\\ t_2\in V\left(R\left(G_1\right)-V\left(G_1\right)\right)}} d_{RG_1}\left(t_1\right) + 2e_2e_1\left(n_2-1\right) + 2n_2e_1\left(n_2-1\right).$$

Note that $2e_1 \le \sum_{t_1t_2 \notin E(R(G_1))t_1 \in V(G_1)t_2 \in V(S(G_1)-V(G_1))} [d(t_1)] \le 2E(R(G_1))e_1(n_1-2)$.

$$
\begin{aligned}
2n_2e_1 + 2e_2e_1(n_2-1) + 2n_2e_1(n_2-1) \le \sum C_1 &\le 2n_2E(R(G_1))e_1(n_1-2) + 2e_2e_1(n_2-1) + 2n_2e_1(n_2-1),\\
\sum C_2 &= \sum_{\substack{t_1t_2 \notin E(R(G_1))\\ t_1 \in V(G_1)\\ t_2 \in V(R(G_1)-V(G_1))}} \sum_{(x_1,x_2)\in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)]\\
&= \sum_{\substack{t_1t_2 \notin E(R(G_1))\\ t_1 \in V(G_1)\\ t_2 \in V(R(G_1)-V(G_1))}} \sum_{x_1,x_2\in V_{G_2}} \left[d_{R(G_1)}(t_1) + d(x_1) + d_{S(G_1)}(t_2)\right]\\
&= \sum_{\substack{t_1t_2 \notin E(R(G_1))\\ t_1 \in V(G_1)\\ t_2 \in V(R(G_1)-V(G_1))}} \sum_{x_1,x_2\in V_{G_2}} \left[d_{R(G_1)}(t_1) + d(x_1) + 2\right]\\
&= n_2(n_2-1) \sum_{\substack{t_1t_2 \notin E(R(G_1))\\ t_1 \in V(G_1)t_2 \in V(R(G_1)-V(G_1))}} d_{RG_1}(t_1) + 2e_2e_1(n_1-2)(n_2-1)\\
&\quad + 2n_2(n_2-1)e_1(n_1-2).
\end{aligned}
\tag{19}
$$

Note that $2e_1 \le \sum_{t_1t_2 \notin E(R(G_1))t_1 \in V(G_1)t_2 \in V(S(G_1)-V(G_1))} [d(t_1)] \le 2E(R(G_1))e_1(n_1-2)$.

$$
\begin{aligned}
&2n_2(n_2-1)e_1(n_1-2) + 2e_2e_1(n_1-2)(n_2-1) + 2n_2(n_2-1)e_1(n_1-2)\\
&\le \sum C_2 \le 2n_2(n_2-1)E(R(G_1))e_1(n_1-2)\\
&\quad + 2e_2e_1(n_1-2)(n_2-1) + 2n_2(n_2-1)e_1(n_1-2),\\
\sum C_3 &= \sum_{\substack{t_1t_2 \in E(R(G_1))\\ t_1 \in V(G_1)\\ t_2 \in V(R(G_1)-V(G_1))}} \sum_{x_1,x_2\in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)]\\
&= \sum_{\substack{t_1t_2 \in E(R(G_1))\\ t_1 \in V(G_1)\\ t_2 \in V(R(G_1)-V(G_1))}} \sum_{(x_1,x_2)\in V_{G_2}} \left[d_{R(G_1)}(t_1) + d(x_1) + d_{R(G_1)}(t_2)\right] + \sum_{\substack{t_1t_2 \in E(R(G_1))\\ t_1 \in V(G_1)\\ t_2 \in V(R(G_1)-V(G_1))}} \left[d_{R(G_1)}(t_1) + d(x_1) + 2\right]\\
&= n_2(n_2-1) \sum_{\substack{t_1t_2 \in E(R(G_1))\\ t_1 \in V(G_1)t_2 \in V(R(G_1)-V(G_1))}} d_{R(G_1)}(t_1) + 2e_2(n_2-1)\left|\sum_{\substack{t_1t_2 \in E(R(G_1))\\ t_1 \in V(G_1)t_2 \in V(R(G_1)-V(G_1))}} d_{R(G_1)}(t_1)\right|\\
&\quad + 2n_2(n_2-1)\left|\sum_{\substack{t_1t_2 \in E(R(G_1))\\ t_1 \in V(G_1)t_2 \in V(R(G_1)-V(G_1))}} d_{R(G_1)}(t_1)\right|.
\end{aligned}
\tag{20}
$$

Note that $2e_1 \le \sum_{\substack{t_1t_2 \in E(R(G_1)) \\ t_1 \in V(G_1) t_2 \in V(S(G_1) - V(G_1))}} d(t_1) \le 4E(R(G_1))e_1$. So,

$$4e_1[n_2(n_2-1) + 2e_2(n_2-1) + 2n_2(n_2-1)] \le \sum C_3 \le 4e_1E(R(G_1))[n_2(n_2-1) + 2e_2(n_2-1) + 2n_2(n_2-1)]. \tag{21}$$

Consequently,

$$\begin{aligned} &2n_2e_1 + 2e_2e_1(n_2-1) + 2n_2e_1(n_2-1) + 2n_2(n_2-1)e_1(n_1-2) + 2e_2e_1(n_1-2)(n_2-1) \\ &\quad + 2n_2(n_2-1)e_1(n_1-2) + 4e_1[n_2(n_2-1) + 2e_2(n_2-1) + 2n_2(n_2-1)] \\ &\le \sum C \le \\ &\quad 2n_2E(R(G_1))e_1(n_1-2) + 2e_2e_1(n_2-1) + 2n_2e_1(n_2-1) + 2n_2(n_2-1)E(R(G_1))e_1(n_1-2) + 2e_2e_1(n_1-2)(n_2-1) \\ &\quad + 2n_2(n_2-1)e_1(n_1-2) + 4e_1E(R(G_1))[n_2(n_2-1) + 2e_2(n_2-1) + 2n_2(n_2-1)] \end{aligned} \tag{22}$$

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

Theorem 3. *Let G_1 and G_2 be two connected graphs; then, first Zagreb coindex of $G_{1+Q}G_2$ is given as*

$$\alpha_1 \le \overline{M}\left(G_{1+Q}G_2\right) \le \alpha_2, \tag{23}$$

where

$$\begin{aligned} \alpha_1 &= 4(e_1\overline{e}_2 + e_2(e_1 + \overline{e}_1)) + 2(n_2 - 1 + \overline{e}_2)(2e_1 + \overline{e}_1) + 2e_1(n_1-2)(e_2 + 3n_2) + n_2(2n_2-1)e_1 \\ &\quad + 2(2e_2 + 3n_2)(n_2-1)e_1 + (n_2 + 2e_2 + 2\overline{e}_2)M_1(G_1) + 2(e_2 + \overline{e}_2) \\ &\quad \overline{M}_1(G_1) + 2(e_1 + \overline{e}_1)M_1(G_2) + (n_1 + 2\overline{e}_1 + 2e_1)\overline{M}_1(G_2), \\ \alpha_2 &= 4(e_1\overline{e}_2 + e_2(e_1 + \overline{e}_1)) + e_1(n_1-2)(2e_2 + 3n_2) + 2e_1(2e_2 + 3n_2)(n_2-1) + (n_2 + 2e_2 + 2\overline{e}_2)M_1(G_1) \\ &\quad + (n_2 + 2(e_2 + \overline{e}_2))\overline{M}_1(G_1) + 2(e_1 + \overline{e}_1)M_1(G_2) + (n_1 + 2\overline{e}_1 + 2e_1)\overline{M}_1(G_2) \\ &\quad + n_2\overline{M}_1(Q(G_1)) + 4((n_2-1) + \overline{e_2})E(Q(G_1)) \\ &\quad + 2n_2^2E(Q(G_1))e_1(n_1-2) + 2(n_2 - 1 + \overline{e_2})M_1(Q(G_1))\overline{M}_1(Q(G_1)) + 4n_2e_1E(Q = (G_1))(n_2-1). \end{aligned} \tag{24}$$

Proof. Using equation (2), we have

$$\begin{aligned} \overline{M}\left(G_{1+Q}G_2\right) &= \sum_{(t_1,t_2)(x_1,x_2) \notin E(G_{1+Q}G_2)} [d(t_1,x_1) + d(t_2,x_2)], \\ \overline{M}\left(G_{1+Q}G_2\right) &= \sum A + \sum B + \sum C, \\ \sum A &= \sum A_1 + \sum A_2 + \sum A_3 + \sum A_4 + \sum A_5 + \sum A_6 + \sum A_7, \\ \sum A_1 &= \sum_{\substack{t_1t_2 \notin E(Q(G_1)) \\ t_1,t_2 \in V(Q(G_1) - V(G_1))}} \sum_{x \in V_{G_2}} [d(t_1,x) + d(t_2,x)] = n_2 \sum_{\substack{t_1t_2 \notin E(Q(G_1)) \\ t_1,t_2 \in V(Q(G_1) - V(G_1))}} \left[d_{QG_1}(t_1) + d_{QG_1}(t_2)\right]. \end{aligned} \tag{25}$$

Note that $0 \le \sum_{\substack{t_1t_2 \notin E(Q(G_1)) \\ t_1, t_2 \in V(Q(G_1) - V(G_1))}} [d_{QG_1}(t_1) + d_{QG_1}(t_2)] \le \overline{M}_1(Q(G_1))$, so

$$\begin{aligned} 0 &\le \sum A_1 \le n_2 \overline{M}_1(Q(G_1)) \\ \sum A_2 &= \sum_{t \in V(Q(G_1) - V(G_1))} \sum_{x_1x_2 \in E_{G_2}} [d(t, x_1) + d(t, x_2)] \\ &= \sum_{t \in V(Q(G_1) - V(G_1))} \sum_{x_1x_2 \in E_{G_2}} \left[d_{QG_1}(t) + d_{QG_1}(t)\right] = 2(n_2 - 1) \sum_{t \in V(Q(G_1) - (G_1))} \left[d_{QG_1}(t)\right]. \end{aligned} \tag{26}$$

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

$$\begin{aligned} 2(n_2 - 1)e_1 &\le \sum A_2 \le 4(n_2 - 1)E(Q(G_1)), \\ \sum A_3 &= \sum_{t \in V(Q(G_1) - V(G_1))} \sum_{x_1x_2 \notin E_{G_2}} [d(t, x_1) + d(t, x_2)] \\ &= \sum_{t \in V(Q(G_1) - V(G_1))} \sum_{x_1x_2 \notin E_{G_2}} \left[d_{QG_1}(t) + d_{QG_1}(u)\right] = 2\overline{e_2} \sum_{t \in V(Q(G_1) - (G_1))} \left[d_{QG_1}(u)\right]. \end{aligned} \tag{27}$$

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

$$\begin{aligned} 2\overline{e_2}e_1 &\le \sum A_3 \le 4\overline{e_2}E(Q(G_1)), \\ \sum A_4 &= \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1, t_2 \in V(Q(G_1) - V(G_1))}} \sum_{x_1x_2 \in E_{G_2}} [d(t_1, x_1) + d(t_2, x_2)] \\ &= \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1, t_2 \in V(Q(G_1) - V(G_1))}} \sum_{x_1x_2 \in E_{G_2}} [d(t_1, x_1) + d(t_2, x_2)] = 2(n_2 - 1) \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1, t_2 \in V(Q(G_1) - V(G_1))}} \left[d_{QG_1}(t_1) + d_{QG_1}(t_2)\right]. \end{aligned} \tag{28}$$

Note that $e_1 \le \sum_{\substack{t_1t_2\in E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} [d_{QG_1}(t_1)+d_{QG_1}(t_2)] \le M_1(Q(G_1))$, so

$$2(n_2-1)e_1 \le \sum A_4 \le 2(n_2-1)M_1(Q(G_1)),$$

$$\begin{aligned}\sum A_5 &= \sum_{\substack{t_1t_2\in E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \sum_{x_1x_2\notin E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\ &= \sum_{\substack{t_1t_2\in E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \sum_{x_1x_2\notin E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)] = 2\overline{e_2} \sum_{\substack{t_1t_2\in E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \left[d_{QG_1}(t_1)+d_{QG_1}(t_2)\right].\end{aligned} \tag{29}$$

Note that $e_1 \le \sum_{\substack{t_1t_2\in E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} [d_{QG_1}(t_1)+d_{QG_1}(t_2)] \le M_1(Q(G_1))$, so

$$2\overline{e_2}e_1 \le \sum A_5 \le 2\overline{e_2}M_1(Q(G_1))$$

$$\begin{aligned}\sum A_6 &= \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \sum_{x_1x_2\in E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\ &= \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \sum_{x_1x_2\in E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)] = 2(n_2-1) \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \left[d_{QG_1}(t_1)+d_{QG_1}(t_2)\right].\end{aligned} \tag{30}$$

Note that $\overline{e}_1 \le \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} [d_{QG_1}(t_1)+d_{QG_1}(t_2)] \le \overline{M}_1(Q(G_1))$, so

$$2(n_2-1)\overline{e}_1 \le \sum A_6 \le 2(n_2-1)\overline{M}_1(Q(G_1)),$$

$$\begin{aligned}\sum A_7 &= \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \sum_{x_1x_2\notin E_{G_2}} [d(t_1,x_1)+d(t_2,x_2)]\\ &= \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} [d(t_1,x_1)+d(t_2,x_2)] = 2\overline{e_2} \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} \left[d_{QG_1}(t_1)+d_{QG_1}(t_2)\right].\end{aligned} \tag{31}$$

Note that $\overline{e}_1 \le \sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1,t_2\in V(Q(G_1)-V(G_1))}} [d_{QG_1}(t_1)+d_{QG_1}(t_2)] \le \overline{M}_1(Q(G_1))$, so

$$2\overline{e_2}\overline{e}_1 \le \sum A_7 \le 2\overline{e_2}\overline{M}_1(Q(G_1)). \tag{32}$$

Consequently,

$$\begin{aligned}
&2(n_2-1)e_1+2\overline{e_2}e_1+2(n_2-1)e_1+2\overline{e_2}e_1+2(n_2-1)\overline{e}_1+2\overline{e_2}\overline{e}_1\\
&\quad\le\sum A\le\\
&\quad+n_2\overline{M}_1(Q(G_1))+4(n_2-1)E(Q(G_1))+4\overline{e_2}E(Q(G_1))+2(n_2-1)M_1(Q(G_1))\\
&\quad+2\overline{e_2}M_1(Q(G_1))+2(n_2-1)\overline{M}_1(Q(G_1))+2\overline{e_2}\overline{M}_1(Q(G_1)).
\end{aligned}\tag{33}$$

Using equation (8), we directly have

$$\begin{aligned}
\sum B&=4e_1\overline{e}_2+e_2(e_1+\overline{e}_1)+(2(e_2+\overline{e}_2)+n_2)M_1(G_1)+(n_2(2e_2+\overline{e}_2))\overline{M}_1(G_1)\\
&\quad+2(e_2+\overline{e}_1)M_1(G_2)+n_1+2(\overline{e}_1+e_1)\overline{M}_1(G_2),\\
\sum C&=\sum C_1+\sum C_2+\sum C_3,\\
\sum C_1&=\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}\ \sum_{x\in V_{G_2}}[d(t_1,x)+d(t_2,x)]=\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}\ \sum_{x\in V_{G_2}}\left[d_{G_1}(t_1)+d(x)+d_{Q(G_1)}(t_2)\right]\\
&=n_2\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}d_{Q(G_1)}(t_1)+2e_2e_1(n_1-2)+3n_2e_1(n_1-2).
\end{aligned}\tag{34}$$

Note that $2e_1\le\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}d_{Q(G_1)}(t_1)\le 2E(Q(G_1))e_1(n_1-2)$, so

$$\begin{aligned}
2n_2e_1+2e_2e_1(n_1-2)+3n_2e_1(n_1-2)&\le\sum C_1\le 2n_2E(Q(G_1))e_1(n_1-2)+2e_2e_1(n_1-2)+3n_2e_1(n_1-2),\\
\sum C_2&=\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}\ \sum_{(x_1,x_2)\in V_{G_2}}[d(t_1,x_1)+d(t_2,x_2)]\\
\sum C_2&=\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}\ \sum_{x_1,x_2\in V_{G_2}}\left[d_{Q(G_1)}(t_1)+d(x_1)+d_{Q(G_1)}(t_2)\right]\\
&=n_2(n_2-1)\sum_{\substack{t_1t_2\notin E(Q(G_1))\\ t_1\in V(G_1)\\ t_2\in V(Q(G_1)-V(G_1))}}d_{Q(G_1)}(t_1)+(2e_2+3n_2)(n_2-1)|\\
&\quad\sum_{t_1t_2\notin E(Q(G_1))}d_{Q(G_1)}(t_1)|.
\end{aligned}\tag{35}$$

Note that $2e_1 \leq \sum_{\substack{t_1t_2 \notin E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} d_{Q(G_1)}(t_1) \leq 2E(Q(G_1))e_1(n_1-2)$, so

$$2e_1n_2(n_2-1)+e_1(n_1-2)[(2e_2+3n_2)(n_2-1)] \leq \sum C_2 \leq 2E(Q(G_1))e_1(n_1-2)[n_2(n_2-1)+(2e_2+3n_2)(n_2-1)]$$

$$\begin{aligned}
\sum C_3 &= \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1,x_1)+d(t_2,x_2)] \\
&= \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} \left[d_{Q(G_1)}(t_1)+d(x_1)+d_{Q(G_1)}(t_2)\right] \\
&= n_2(n_2-1) \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} d_{Q(G_1)}[(t_1)] + 2e_2(n_2-1)| \\
&\quad \cdot \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} d_{Q(G_1)}(t_1)| \\
&\quad + 3n_2(n_2-1)| \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} d_{Q(G_1)}[(t_1)]|.
\end{aligned} \tag{36}$$

Note that $2E(G_1) \leq \sum_{\substack{t_1t_2 \in E(Q(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(Q(G_1)-V(G_1))}} d_{Q(G_1)}[(t_1)] \leq 4E(Q(G_1))e_1$, so

$$4n_2(n_2-1)e_1+(n_2-1)(2e_1)(2e_2(2e_1)+3n_2) \leq \sum C_3 \leq 4n_2(n_2-1)Q(E(G_1))e_1+(n_2-1)(2e_1)(2e_2+3n_2). \tag{37}$$

Consequently,

$$\begin{aligned}
&2n_2e_1+2e_2e_1(n_1-2)+3n_2e_1(n_1-2)+2e_1n_2(n_2-1)+e_1(n_1-2)[(2e_2+3n_2)(n_2-1)] \\
&\quad +4n_2(n_2-1)e_1+(n_2-1)(2e_1)(2e_2(2e_1)+3n_2) \\
&\leq \sum C \leq \\
&\quad 2n_2E(Q(G_1))e_1(n_1-2)+2e_2e_1(n_1-2)+3n_2e_1(n_1-2)+2E(Q(G_1))e_1(n_1-2)[n_2(n_2-1)+(2e_2+3n_2)(n_2-1)] \\
&\quad +4n_2(n_2-1)Q(E(G_1))e_1+(n_2-1)(2e_1)(2e_2+3n_2).
\end{aligned} \tag{38}$$

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 $G_{1+T}G_2$ is given as*

$$\alpha_1 \le \overline{M}(G_{1+T}G_2) \le \alpha_2, \tag{39}$$

where

$$\begin{aligned}
\alpha_1 &= 4(2e_1\overline{e}_2 + e_2\overline{e}_1) + e_1(n_1-2)(2e_2+3n_2) + 2(n_2 + 2(e_2+\overline{e}_2))M_1(G_1) + 4(e_2+\overline{e}_2)\overline{M}_1(G_1) + 2(e_1+\overline{e}_1)M_1(G_2) \\
&\quad + (n_1 + 2(\overline{e}_1 + e_1))\overline{M}_1(G_2) + 2((n_2-1)+\overline{e_2})e_1 + (n_2 - 1 + \overline{e_2})e_1\overline{e}_1 + 2n_2^2e_1 + 2e_1(n_2-1)[n_2+2e_2+3n_2], \\
\alpha_2 &= 4(2e_1\overline{e}_2 + e_2\overline{e}_1) + e_1(n_1-2)(2e_2+3n_2) + 4(e_2+\overline{e}_2)M_1(G_1) + (2n_2 + 4(e_2+\overline{e}_2))\overline{M}_1(G_1) \\
&\quad + 2(e_1+\overline{e}_1)M_1(G_2) + (n_1 + 2(\overline{e}_1+e_1))\overline{M}_1(G_2) + n_2\overline{M}_1T(G_1) + 4((n_2-1)+\overline{m_2})ET(G_1) \\
&\quad + (n_2 - 1 + \overline{m_2})M_1(T(G_1))\overline{M}_1(T(G_1)) + n_2^2E(T(G_1))e_1(n_2-1) + 2e_1(2e_2+3n_2)(n_2-1) \\
&\quad + 4n_2e_1ET(G_1)(n_2-1) + 2e_1(n_2-1)(2e_2+3n_2).
\end{aligned} \tag{40}$$

Proof. Using equation (2), we have

$$\begin{aligned}
\overline{M}(G_{1+T}G_2) &= \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_{1+T}G_2)} [d(u_1,v_1) + d(u_2,v_2)], \\
\overline{M}(G_{1+T}G_2) &= \sum_{t_1,t_2\in V(T(G_1)-V(G_1))} \sum_{x_1,x_2\in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)] + \sum_{t_1,t_2\in V_{G_1}} \sum_{x_1,x_2\in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)] \\
&\quad + \sum_{t_1,t_2\in V(T(G_1)-V(G_1))} \sum_{x_1,x_2\in V_{G_2}} [d(t_1,x_1) + d(t_2,x_2)] \\
&= \sum A + \sum B + \sum C.
\end{aligned} \tag{41}$$

Using equations (30) and (17), we directly have

$$\begin{aligned}
2(n_2-1)e_1 + 2\overline{e_2}e_1 + 2(n_2-1)e_1 + 2\overline{e_2}e_1 + 2(n_2-1)\overline{e}_1 + 2\overline{e_2}\overline{e}_1 \le \sum A \le &+ n_2\overline{M}_1(Q(G_1)) + 4(n_2-1)E(Q(G_1)) \\
&+ 4\overline{e_2}E(Q(G_1)) + 2(n_2-1)M_1(Q(G_1)) + 2\overline{e_2}M_1(Q(G_1)) \\
&+ 2(n_2-1)\overline{M}_1(Q(G_1)) + 2\overline{e_2}\overline{M}_1(Q(G_1)) \\
\sum B = &\ 4(2e_1\overline{e}_2 + 4\overline{e} + e_2\overline{e}_1) + (4e_2 + 4\overline{e}_2)M_1(G_1) \\
&+ 2(e_1+\overline{e}_1)M_1(G_2) + 2n_2 + 2(e_2+\overline{e}_2)\overline{M}_1(G_1) \\
&+ (n_1 + 2\overline{e}_1 + 2e_1)\overline{M}_1(G_2).
\end{aligned} \tag{42}$$

Now, we find

$$\begin{aligned}
\sum C &= \sum C_1 + \sum C_2 + \sum C_3 \\
\sum C_1 &= \sum_{\substack{t_1t_2 \notin E(T(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(T(G_1)-V(G_1))}} \sum_{v \in V_{G_2}} [d(t_1, v) + d(t_2, v)] \\
2n_2\overline{e}_1 + 2e_2e_1(n_1-2)3n_2e_1(n_1-2) &\le \sum C_1 \le 2n_2T(E(G_1))e_1(n_1-2) + 2e_2e_1(n_1-2) + 3n_2e_1(n_1-2) \\
\sum C_2 &= \sum_{\substack{t_1t_2 \notin E(T(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(T(G_1)-V(G_1))}} \sum_{(x_1,x_2) \in V_{G_2}} [d(t_1, x_1) + d(t_2, x_2)] \\
2n_2(n_2-1)e_1 + 2(2e_2+3n_2)(n_2-1)e_1(n_1-2) &\le \sum C_2 \le 2n_2(n_2-1)E(T(G_1))e_1(n_1-2)a \\
&\quad + 2(2e_2+3n_2)(n_2-1)T(E(G_1))e_1(n_1-2), \\
\sum C_3 &= \sum_{\substack{t_1t_2 \in E(T(G_1)) \\ t_1 \in V(G_1) \\ t_2 \in V(T(G_1)-V(G_1))}} \sum_{x_1,x_2 \in V_{G_2}} [d(t_1, x_1) + d(t_2, x_2)] \\
&\quad 4n_2e_1(n_2-1) + 4e_1e_2(n_2-1) + 4e_1(3n_2(n_2-1))T(E(G_1)) \\
&\le \sum C_3 \le 8n_2e_1(n_2-1)T(E(G_1)) \\
&\quad + 8e_1e_2(n_2-1)T(E(G_1)) + 4e_1(3n_2(n_2-1))T(E(G_1)).
\end{aligned} \tag{43}$$

Consequently,

$$\begin{aligned}
&2n_2\overline{e}_1 + 2e_2e_1(n_1-2) + 3n_2e_1(n_1-2) + 2n_2(n_2-1)e_1 + 2(2e_2+3n_2)(n_2-1)e_1(n_1-2) + 4n_2e_1(n_2-1) + 4e_1e_2(n_2-1) \\
&\quad + 4e_1(3n_2(n_2-1))T(E(G_1)) \\
&\le \sum C \le \\
&\quad 2n_2T(E(G_1))e_1(n_1-2) + 2e_2e_1(n_1-2) + 3n_2e_1(n_1-2) + 2n_2(n_2-1)E(T(G_1))e_1(n_1-2) \\
&\quad + 2(2e_2+3n_2)(n_2-1)T(E(G_1))e_1(n_1-2) + 8n_2e_1(n_2-1)T(E(G_1)) \\
&\quad + 8e_1e_2(n_2-1)T(E(G_1)) + 4e_1(3n_2(n_2-1))T(E(G_1)).
\end{aligned} \tag{44}$$

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

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 $\overline{M}(G_{1+S}G_2)$, $\overline{M}(G_{1+R}G_2)$, $\overline{M}(G_{1+Q}G_2)$, and $\overline{M}(G_{1+T}G_2)$ 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 $(\overline{M}_1(P_n + P_m))$ and bounded values

Table 1: Exact value of first Zagreb coindex for Cartesian product of path graphs.

Cartesian product of paths	Exact value of $\overline{M_1}$
$P_2 \otimes P_2$	36
$P_3 \otimes P_3$	374
$P_4 \otimes P_4$	1748
$P_5 \otimes P_5$	4853

Table 2: Bounds of first Zagreb coindex for S-sum graph.

S-sum graphs	Lower bound of $\overline{M_1}$	Upper bound of $\overline{M_1}$
$P_{2+S}P_2$	36	40
$P_{3+S}P_3$	374	534
$P_{4+S}P_4$	1748	3284
$P_{5+S}P_5$	4853	10176

Table 3: Bounds of first Zagreb coindex for R-sum graph.

R-sum graphs	Lower bound of $\overline{M_1}$	Upper bound of $\overline{M_1}$
$P_{2+R}P_2$	36	44
$P_{3+R}P_3$	510	1430
$P_{4+R}P_4$	2208	7584
$P_{5+R}P_5$	7314	27442

Table 4: Bounds of first Zagreb coindex for Q-sum graph.

Q-sum operation	Lower bound of $\overline{M_1}$	Upper bound of $\overline{M_1}$
$P_{2+Q}P_2$	36	92
$P_{3+Q}P_3$	470	2500
$P_{4+Q}P_4$	1756	6708
$P_{5+Q}P_5$	9166	22409

Table 5: Bounds of first Zagreb coindex for T-sum graph.

T-sum operation	Lower bound of $\overline{M_1}$	Upper bound of $\overline{M_1}$
$P_{2+T}P_2$	38	118
$P_{3+T}P_3$	556	4370
$P_{4+T}P_4$	2004	10488
$P_{5+T}P_5$	9842	12807

of F-sum graphs ($\overline{M}_1(P_{n_F} + P_m)$). In general, the linear regression formula is expressed as $Y = b_0 + b_1X$, 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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