Research Article

Bounds on General Randić Index for F -Sum Graphs

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A topological invariant is a numerical parameter associated with molecular graph and plays an imperative role in the study and analysis of quantitative structure activity/property relationships (QSAR/QSPR). The correlation between the entire π -electron energy and the structure of a molecular graph was explored and understood by the first Zagreb index. Recently, Liu et al. (2019) calculated the first general Zagreb index of the F -sum graphs. In the same paper, they also proposed the open problem to compute the general Randić index $R_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} [d_\Gamma(u) \times d_\Gamma(v)]^\alpha$ of the F -sum graphs, where $\alpha \in \mathbb{R}$ and $d_\Gamma(u)$ denote the valency of the vertex u in the molecular graph Γ . Aim of this paper is to compute the lower and upper bounds of the general Randić index for the F -sum graphs when $\alpha \in \mathbb{N}$. We present numerous examples to support and check the reliability as well as validity of our bounds. Furthermore, the results acquired are the generalization of the results offered by Deng et al. (2016), who studied the general Randić index for exactly $\alpha = 1$.

1. Introduction

Suppose the ordered pair $(V(\Gamma), E(\Gamma))$ denotes a finite, simple, and connected molecular graph Γ . The set represented by $V(\Gamma)$ is the vertex set and the set denoted by $E(\Gamma)$, disjoint from $V(\Gamma)$, is the edge set. Vertices of Γ correspond to atoms, whereas edges represent bonding between atoms. For any vertex $v \in V(\Gamma)$, the number of vertices adjacent with v is called the degree of vertex v and is denoted by $d_\Gamma(v)$. The smallest and the largest degree of Γ are symbolized by δ_Γ and Δ_Γ , respectively. Two primary parameters known as the order (total number of vertices) and the size (total number of edges) of graph Γ are denoted by n and e . A path P_k is a simple graph having order k and size $k - 1$ with the property that exactly two vertices have degree 1, and rest of the vertices have degree 2. A cycle C_m is a simple graph with same order and size m in such a way that each vertex has degree 2.

Graph theory is playing a remarkable role in various domains of science, especially in mathematical chemistry,

computer science, and chemical graph theory since the middle of last century. Let Ω be a collection of simple graphs and $\mathbb{R}$ be a set of real numbers; then, a topological index (TI) is considered to be a function $\Phi: \Omega \rightarrow \mathbb{R}$ that associates a graph to a real number. It is worth noting that all the TIs are invariant for the isomorphic structures. To probe and study the chemical, structural, and physical properties of the molecular graphs within the subject of chemical graph theory, several TIs are proposed and intensely investigated. These TIs helped to study the chemical reactivities and physical features such as heat of evaporation and formation, boiling, melting and freezing point, volume of air and vapor pressure, surface tension and density, and critical temperature of the chemical compounds that are involved in the molecular graphs. Moreover, medical behaviors of the drugs, nanomaterials, and crystalline materials which are very important for the chemical industries including pharmaceutical are studied using TIs. For further reading regarding development and applications of TIs, the readers are referred to [1–10].

2. Preliminaries and Background

Some convinced and significant degree-based TIs closely related to our work are defined below.

Definition 1. Let Γ be a molecular graph; then, the first Zagreb index and second Zagreb index are defined as

$$\begin{aligned} M_1(\Gamma) &= \sum_{v \in V(\Gamma)} [d_\Gamma(v)]^2 = \sum_{uv \in E(\Gamma)} [d_\Gamma(u) + d_\Gamma(v)], \\ M_2(\Gamma) &= \sum_{uv \in E(\Gamma)} [d_\Gamma(u) \cdot d_\Gamma(v)]. \end{aligned} \quad (1)$$

Gutman and Trinajstić [11] defined the first and second Zagreb indices to establish the relationship between the entire π -electron energy and a structure of a molecular graph.

Definition 2. Let Γ be a molecular graph; then, the first general Zagreb index (FGZI) is defined as

$$M^\alpha(\Gamma) = \sum_{v \in V(\Gamma)} [d_\Gamma(v)]^\alpha = \sum_{vw \in E(\Gamma)} [d_\Gamma^{\alpha-1}(v) + d_\Gamma^{\alpha-1}(w)], \quad (2)$$

where $\alpha \in \mathbb{R}$, $\alpha \neq 0$, and $\alpha \neq 1$. Li and Zheng [12] provided the idea of FGZI. It is evident that we achieve $M_1(\Gamma)$ (first Zagreb index) and $F(\Gamma)$ (forgotten index) by putting $\alpha = 2$, and $\alpha = 3$ in FGZI, respectively [11, 13].

Definition 3. Let Γ be a molecular graph; then, the general Randić index (GRI) is defined as

$$R_\alpha(\Gamma) = \sum_{vw \in E(\Gamma)} [d_\Gamma(v)d_\Gamma(w)]^\alpha, \quad \alpha \in \mathbb{R}, \alpha \neq 0. \quad (3)$$

Bollobás and Erdős originated the concept of GRI [14]. It is clear that $\alpha = -1/2$ gives the classical Randić connectivity index $R_{-1/2}(\Gamma)$ [15] and $\alpha = 1$ provides second Zagreb index $M_2(\Gamma)$ [11].

Definition 4. Let Γ be a molecular graph; then, the general sum-connectivity index (GSCI) is defined as

$$\chi^\alpha(\Gamma) = \sum_{vw \in E(\Gamma)} [d_\Gamma(v) + d_\Gamma(w)]^\alpha, \quad \alpha \in \mathbb{R}. \quad (4)$$

Zhou and Trinajstić initiated the idea of GSCI [16]. For $\alpha = -1/2$, we attain the classical sum-connectivity index (SCI) $\chi^{-1/2}(\Gamma)$ [17].

Lučić et al. [18] studied and observed that there is good correlation between indices $R_{-1/2}(\Gamma)$ and $\chi^{-1/2}(\Gamma)$ themselves besides their correlation with $E_\pi(\Gamma)$ (π -electron energy) of benzenoid hydrocarbons. For further insight and applications related to all above TIs, the readers are referred to [19–23].

The operations on graphs, in the construction of new graphs, also play an important role in graph theory, where the old graphs are called the factors of the new graph. Cartesian product (binary operation) is an elegant technique to construct a broader network from two base graphs and is

inevitable for design and analysis of networks [24]. In [25], Eliasi and Taeri contrived and constructed the F -sum graphs $(G_1 +_F G_2)$ ($F \in \{S, R, Q, T\}$) by employing the idea of Cartesian product on graphs $F(\Gamma_1)$ and Γ_2 , where Γ_1 and Γ_2 are two simple-connected graphs and $F(\Gamma_1)$ is obtained after applying F on Γ_1 which is elaborated subsequently.

Definition 5. Let Γ be a simple, connected, and finite graph; then, the four significant related graphs can be defined as follows [25, 26]:

- (1) Subdivision graph $S(\Gamma)$ is an expansion of graph Γ by introducing an additional vertex on each edge of Γ .
- (2) Triangle parallel graph $R(\Gamma)$ is derived from $S(\Gamma)$ by joining the solid vertices of the original edges of Γ that are incident with hollow vertices.
- (3) Line superposition graph $Q(\Gamma)$ is obtained from $S(\Gamma)$ by attaching those pairs of new vertices by edges which have common adjacent (solid) vertex.
- (4) Total graph $T(\Gamma)$ is constructed from $S(\Gamma)$ by applying $R(\Gamma)$ and $Q(\Gamma)$, simultaneously.

For more details, see Figure 1. For further insight regarding graph operations, see [27].

Definition 6. Let Γ_1 and Γ_2 be two finite, simple, and connected graphs, F be an operation (one of S, R, Q , and T), and $F(\Gamma)$ be a graph (derived from Γ_1 by employing the operation F) with $V(F(\Gamma_1))$ as vertex set and $E(F(\Gamma_1))$ as edge set. Then, the F -sum graph $\Gamma_1 +_F \Gamma_2$ is a graph with vertex set $V(\Gamma_1 +_F \Gamma_2) = V(F(\Gamma_1)) \times (V(\Gamma_2)) = (V(\Gamma_1) \cup E(\Gamma_1)) \times (V(\Gamma_2))$ such that two vertices (v_1, v_2) and (w_1, w_2) of $V(\Gamma_1 +_F \Gamma_2)$ are adjacent if and only if $[v_1 = w_1 \in V(\Gamma_1) \text{ and } (v_2, w_2) \in E(\Gamma_2)]$ or $[v_2 = w_2 \in V(\Gamma_2) \text{ and } (v_1, w_1) \in E(F(\Gamma_1))]$.

We observe that the graph $\Gamma_1 +_F \Gamma_2$ has $|V(\Gamma_2)|$ copies of the graph $F(\Gamma_1)$ provided that vertices of these copies are labeled with vertices of Γ_2 . In graph $\Gamma_1 +_F \Gamma_2$, the vertices of Γ_1 are referred as solid vertices, whereas the vertices $E(\Gamma_1)$ are referred as hollow vertices. Now join only solid vertices having same label in $F(\Gamma_1)$ such that their adjacency in Γ_2 is preserved. For more clarity, see Figure 2.

Following theorems from basic mathematics are of substantial significance in order to obtain core results.

Theorem 1. Binomial and trinomial theorems provide easy and powerful way in expanding expression involving finite higher powers. The algebraic expressions of binomial and trinomial expansions are described beneath, respectively.

$$(x_1 + x_2)^n = \sum_{i=0}^n \binom{n}{i} x_1^{n-i} x_2^i, \quad (5)$$

$$(x_1 + x_2 + x_3)^n = \sum_{\substack{m,k,l \\ m+k+l=n}} P_{m,k,l} x_1^m x_2^k x_3^l, \quad (6)$$

where $P_{m,k,l} = (m+k+l)!/m!k!l!$.

FIGURE 1: Base graph C_6 along with its derived graphs. FIGURE 2: Graphs P_5 and P_6 along with their F -sum graphs.

Although valency as well as spectral based TIs are current topics of increasing interest for researchers and recently Liu et al [28–30] studied weighted edge corona networks viz a viz spectra of various matrices and valency based indices of Eulerian as well as generalized Sierpinski networks. However, among the valency-based TIs, the Randić index and its variations such as general sum-connectivity, general Randić, harmonic, geometric arithmetic, and atom bond connectivity indices have ample applications in pharmacology and medicinal chemistry [31–33]; for detailed study regarding Randić index, see survey [34]. In [35], Yan et al. computed and analyzed the changes in behavior of Wiener index [36] and enhanced the results to Hosoya polynomial for graph operations presented in Definition 1. In [25], Eliasi and Taeri not only introduced the F -sum graphs but also computed the Wiener index of these graphs. Li et al. [37], Shi [38], and Pan et al. [39] provided bounds on Randić index for

chemical graphs ($d_v \leq 4$), bounds on Randić index for triangle-free graph, and sharp bounds on zeroth order general Randić index for unicyclic graphs with fix diameter, respectively. Ali et al. [40], Jamil et al. [41], and Elumalai et al. [42] computed bounds on zeroth order general Randić index for certain type of graphs. Later on, Deng et al. [43], Imran et al. [44], Liu et al. [45], and Ahmad et al. computed the first Zagreb index and second Zagreb index (general Randić index for exactly $\alpha = 1$) of the F -sum graphs, bounds of several indices of the F -sum graphs, first generalized Zagreb indices of the F -sum graphs, and bounds on general sum-connectivity index for F -sum graphs [46], respectively. Moreover, Liu et al. [45] proposed the open problem to compute the general Randić index for any $\alpha \in \mathcal{R}$. In this paper, we solve this open problem, partially, by computing the lower and upper bounds on general Randić index for the F -sum graphs for any $\alpha \in \mathcal{N}$.

The rest of the paper is put together as follows. Section 2 covers the materials and methods to determine main results and Section 3 includes some applications of the main results. Section 4 covers the conclusion and further directions of the work.

3. Results and Discussion

In this section, the main results regarding general Randić index on the F -sum graphs $\Gamma_1 +_S \Gamma_2$, $\Gamma_1 +_R \Gamma_2$, $\Gamma_1 +_Q \Gamma_2$ and $\Gamma_1 +_T \Gamma_2$, are computed, where Γ_1 and Γ_2 are considered to be finite, simple, and connected graphs. Throughout $n_1 = V(\Gamma_1)$, $n_2 = V(\Gamma_2)$, $e_1 = |E(\Gamma_1)|$, $e_2 = |E(\Gamma_2)|$, $V(S(\Gamma_1)) = n_1 + e_1$, $|E(S(\Gamma_1))| = 2e_1$, $M^0(\Gamma_1) = n_1$, $M^1(\Gamma_1) = 2e_1$, $M^1(\Gamma_2) = 2e_2$, $M^2(\Gamma_1) = M_1(\Gamma_1)$, $M^2(\Gamma_2) = M_1(\Gamma_2)$, $R_1(\Gamma_2) = M_2(\Gamma_2)$, $\chi_0(\Gamma_2) = e_2$, and $\chi_1(\Gamma_1) = M_1(\Gamma_1)$.

Theorem 2. Let Γ_1 and Γ_2 be two simple, finite, and connected graphs. For $\alpha \in \mathcal{N}$, the general Randić index of S -sum graph is $LB_S \leq R_\alpha(\Gamma_1 +_S \Gamma_2) \leq UB_S$, where

$$\begin{aligned}
 LB_S &= \sum_{\substack{m,k,l \\ m+k+l=n}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l} \right] \\
 &\quad + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[R_{\alpha-i}(S(\Gamma_1)) M^i(\Gamma_2) (\delta_{\Gamma_1})^i \right], \\
 UB_S &= \sum_{\substack{m,k,l \\ m+k+l=n}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\Delta_{\Gamma_2})^{2l} \right] \\
 &\quad + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[R_{\alpha-i}(S(\Gamma_1)) M^i(\Gamma_2) (\Delta_{\Gamma_1})^i \right],
 \end{aligned} \tag{7}$$

and $P_{m,k,l} = (m+k+l)!/m!k!l!$. Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity.

Proof. Suppose that $d(v, w) = d_{(\Gamma_1 +_S \Gamma_2)}(v, w)$ denotes the degree of vertex (v, w) in the S -sum graph $\Gamma_1 +_S \Gamma_2$. Then, general Randić index for S -sum graph is calculated as

$$\begin{aligned}
R_\alpha(\Gamma_1 +_S \Gamma_2) &= \sum_{(v_1, w_1)(v_2, w_2) \in E(\Gamma_1 +_S \Gamma_2)} [d(v_1, w_1)d(v_2, w_2)]^\alpha \\
&= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d(v, w_1)d(v, w_2)]^\alpha \\
&\quad + \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(S(\Gamma_1))} [d(v_1, w)d(v_2, w)]^\alpha \\
&= \sum 1 + \sum 2.
\end{aligned} \tag{8}$$

Consider

$$\begin{aligned}
\sum 1 &= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [(d_{\Gamma_1}(v) + d_{\Gamma_2}(w_1))(d_{\Gamma_1}(v) + d_{\Gamma_2}(w_2))]^\alpha \\
&= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d_{\Gamma_1}^2(v) + d_{\Gamma_1}(v)(d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2)) \\
&\quad + d_{\Gamma_2}(w_1)d_{\Gamma_2}(w_2)]^\alpha.
\end{aligned} \tag{9}$$

Using trinomial theorem, we get

$$\sum 1 = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[\sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} d_{\Gamma_1}^{2m}(v) d_{\Gamma_1}^k(v) (d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k (d_{\Gamma_2}(w_1)d_{\Gamma_2}(w_2))^l \right], \tag{10}$$

where $P_{m, k, l} = (m + k + l)!/m!k!l!$.

$$\sum 1 = \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[\left(\sum_{w_1, w_2 \in E(\Gamma_2)} (d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k \right) \left(\sum_{v \in V(\Gamma_1)} d_{\Gamma_1}^{2m+k}(v) \right) (d_{\Gamma_2}(w_1)d_{\Gamma_2}(w_2))^l \right]. \tag{11}$$

Using Definitions 1 and 3 and the fact $\delta_{\Gamma_2}(w) \leq d_{\Gamma_2}(w) \forall w \in V(\Gamma_2)$, we have

$$\begin{aligned}
\sum 1 &\geq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} [M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l}], \\
\sum 2 &= \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(S(\Gamma_1))} [(d(v_1, w)d(v_2, w))]^\alpha \\
&= \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(S(\Gamma_1))} [(d_{S(\Gamma_1)}(v_1) + d_{\Gamma_2}(w))d_{S(\Gamma_1)}(v_2)]^\alpha \\
&= \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(S(\Gamma_1))} [d_{S(\Gamma_1)}(v_1)d_{S(\Gamma_1)}(v_2) + d_{\Gamma_2}(w)d_{S(\Gamma_1)}(v_2)]^\alpha.
\end{aligned} \tag{12}$$

Now applying binomial theorem, we get

$$\begin{aligned}
\sum 2 &= \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(S(\Gamma_1))} \left[\sum_{i=0}^{\alpha} \binom{\alpha}{i} (d_{S(\Gamma_1)}(v_1)d_{S(\Gamma_1)}(v_2))^{\alpha-i} (d_{\Gamma_2}(w)d_{S(\Gamma_1)}(v_2))^i \right] \\
&= \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[\sum_{v_1, v_2 \in E(S(\Gamma_1))} (d_{S(\Gamma_1)}(v_1)d_{S(\Gamma_1)}(v_2))^{\alpha-i} \left(\sum_{w \in V(\Gamma_2)} d_{\Gamma_2}^i(w) \right) d_{S(\Gamma_1)}^i(v_2) \right].
\end{aligned} \tag{13}$$

Using Definitions 5 and 6 and property of smallest degree of graph Γ_1 , we have

$$\sum 2 \geq \sum_{i=0}^{\alpha} \binom{\alpha}{i} [R_{\alpha-i}(S(\Gamma_1)) M^i(\Gamma_2) (\delta_{\Gamma_1})^i]. \tag{14}$$

Substituting the (12) and (14) in (8), we have

$$R_\alpha(\Gamma_1 +_S \Gamma_2) \geq \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l} \right] \\ + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[R_{\alpha-i}(S(\Gamma_1)) M^i(\Gamma_2) (\delta_{\Gamma_1})^i \right] = LB_S. \quad (15)$$

Similarly,

$$R_\alpha(\Gamma_1 +_S \Gamma_2) \leq \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\Delta_{\Gamma_2})^{2l} \right] \\ + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[R_{\alpha-i}(S(\Gamma_1)) M^i(\Gamma_2) (\Delta_{\Gamma_1})^i \right] = UB_S. \quad (16)$$

Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity. This completes the proof. $\square$

Example 1. Let $\Gamma_1 = P_4$, $\Gamma_2 = C_3$, $\alpha = 2$, and $F = S$. Then, $n_1 = M^0(P_4) = 4$, $n_2 = M^0(C_3) = 3$, $e_1 = \chi_0(P_4) = 3$, $e_2 = \chi_0(C_3) = 3$, $\delta_{P_4} = 1$, $\Delta_{P_4} = 2$, $\delta_{C_3} = 2$, and $\Delta_{C_3} = 2$. Moreover, Table 1 contains values of some indices related to certain graphs and is crucial to figure out examples throughout.

Now, we compute lower and upper bound of GRI using formulas derived in Theorem 2.

$$LB_S(P_4 +_S C_3) = \sum_{m+k+l=2} P_{m,k,l} \left[M^{2m+k}(P_4) \chi_k(C_3) (\delta_{\Gamma_2})^{2l} \right] + \sum_{i=0}^2 \binom{2}{i} \left[R_{2-i}(S(P_4)) M^i(C_3) (\delta(P_4))^i \right] \\ = P_{1,1,0} (M(P_4) \chi(C_3)) + P_{1,0,1} (M^2(P_4) \chi_0(C_3) (4)) + P_{0,1,1} (M(P_4) \chi(C_3) (4)) \\ + P_{2,0,0} (M^4(P_4) \chi_0(C_3)) + P_{0,2,0} (M^2(P_4) \chi_2(C_3)) + P_{0,0,2} (M^0(P_4) \chi_0(C_3) (16)) + (R_2(S(P_4)) M^0(C_3)) \\ + 2(R(S(P_4)) M(C_3)) + (R_0(S(P_4)) M^2(C_3)) \\ = 2(18(12) + 10(3)(4) + 6(12)(4)) + 34(3) + 10(48) + 4(3)(16) + 72(3) + 2(20)(6) + 6(12) = 2550. \quad (17)$$

Likewise, $UB_S(P_4 +_S C_3) = 3006$.

To calculate exact value for $R_2(P_4 +_S C_3)$, we require edge partition of graph $P_4 +_S C_3$, which is presented in Table 2.

Now, we calculate exact value of GRI of $P_4 +_S C_3$ for $\alpha = 2$. $R_2(P_4 +_S C_3) = \sum_{vw \in E(P_4 +_S C_3)} (d_{P_4}(v) d_{C_3}(w))^2 = 3006$.

Evidently,

$$LB_S = 2550 \leq R_2(P_4 +_S C_3) = 3006 \leq UB_S = 3006. \quad (18)$$

Additionally, we computed actual values along with corresponding bounds of GRI for various cases, and some are presented in Table 3.

Theorem 3. Let Γ_1 and Γ_2 be two simple, finite, and connected graphs. For $\alpha \in \mathcal{N}$, the general Randić index of R -sum graph is $LB_R \leq R_\alpha(\Gamma_1 +_R \Gamma_2) \leq UB_R$, where

$$LB_R = \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2^{(\alpha+i+1)} M^i(\Gamma_1) M^{(\alpha-i)}(\Gamma_2) \right] + \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} 2^{2m+k} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l} + R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\delta_{\Gamma_1})^k \right], \\ UB_R = \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2^{(\alpha+i+1)} M^i(\Gamma_1) M^{(\alpha-i)}(\Gamma_2) \right] + \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} 2^{2m+k} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\Delta_{\Gamma_2})^{2l} + R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\Delta_{\Gamma_1})^k \right], \quad (19)$$

TABLE 1: Some particular indices of certain graphs.

Indices/graphs	M	M^2	M^3	M^4	M^5	M^6	χ	χ_2	χ_3	R	R_2	R_3
P_4	6	10	18	34	66	130	10	34	118	8	24	80
P_5	8	14	26	50	98	194	14	50	182	12	40	144
C_3	6	12	24	48	96	192	12	48	192	12	48	192
$S(P_4)$							22	82	310	20	72	272
$S(P_5)$										28	104	400

TABLE 2: Edge partition based upon degree of end vertices of graph $P_4 +_S C_3$.

(d_v, d_w)	(2, 3)	(3, 3)	(2, 4)	(4, 4)
$ E $	6	6	12	6

TABLE 3: Few more cases of lower and upper bounds regarding $R_\alpha(\Gamma_1 +_S \Gamma_2)$.

Γ_1	Γ_2	α	$LB_S \leq R_\alpha(\Gamma_1 +_S \Gamma_2) \leq UB_S$
P_4	C_3	3	$31926 \leq 36390 \leq 36390$
P_5	P_4	2	$3274 \leq 3346 \leq 3850$
P_5	P_4	3	$19941 \leq 34834 \leq 40764$

and $P_{m,k,l} = (m+k+l)!/m!k!l!$. Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity.

Proof. Suppose that $d(v, w) = d_{(\Gamma_1 +_R \Gamma_2)}(v, w)$ denotes the degree of vertex (v, w) in the R -sum graph $\Gamma_1 +_R \Gamma_2$. Then, general Randić index for R -sum graph is calculated as

$$\begin{aligned}
R_\alpha(\Gamma_1 +_R \Gamma_2) &= \sum_{\substack{(v_1, w_1)(v_2, w_2) \\ \in E(\Gamma_1 +_R \Gamma_2)}} [d(v_1, w_1)d(v_2, w_2)]^\alpha = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d(v, w_1)d(v, w_2)]^\alpha \\
&\quad + \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(R(\Gamma_1))} [d(v_1, w)d(v_2, w)]^\alpha \\
&= \sum_{w_1, w_2 \in E(\Gamma_2)} [d(v, w_1)d(v, w_2)]^\alpha + \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1, v_2 \in V(\Gamma_1)}} [d(v_1, w)d(v_2, w)]^\alpha + \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} [d(v_1, w)d(v_2, w)]^\alpha \\
&\quad \cdot [d(v_1, w)d(v_2, w)]^\alpha = \sum 3 + \sum 4 + \sum 5, \\
\sum 3 &= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[(d_{R(\Gamma_1)}(v) + d_{\Gamma_2}(w_1))(d_{R(\Gamma_1)}(v) + d_{\Gamma_2}(w_2)) \right]^\alpha = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \\
&\quad \cdot \left[(2d_{\Gamma_1}(v) + d_{\Gamma_2}(w_1))(2d_{\Gamma_1}(v) + d_{\Gamma_2}(w_2)) \right]^\alpha \\
&= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[4d_{\Gamma_1}^2(v) + 2d_{\Gamma_1}(v)(d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2)) + d_{\Gamma_2}(w_1)d_{\Gamma_2}(w_2) \right]^\alpha.
\end{aligned}$$

(20)

Applying trinomial theorem, we get

$$\sum 3 = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[\sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} 4^m d_{\Gamma_1}^{2m}(v) 2^k d_{\Gamma_1}^k(v) (d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k (d_{\Gamma_2}(w_1) d_{\Gamma_2}(w_2))^l \right], \quad (21)$$

where $P_{m, k, l} = (m+k+l)!/m!k!l!$. Now applying summations on the convenient expressions, then replacing with

corresponding formulas, and using smallest degree of graph Γ_2 , we get

$$\begin{aligned} \sum 3 &= \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[2^{2m+k} \left(\sum_{v \in V(\Gamma_1)} d_{\Gamma_1}^{2m+k}(v) \right) \left(\sum_{w_1, w_2 \in E(\Gamma_2)} (d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k (d_{\Gamma_2}(w_1) d_{\Gamma_2}(w_2))^l \right) \right] \\ &\geq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[2^{2m+k} M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l} \right]. \end{aligned} \quad (22)$$

Next sum involves those edges from $R(\Gamma_1)$ whose end vertices are in $V(\Gamma_1)$.

$$\begin{aligned} \sum 4 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1, v_2 \in V(\Gamma_1)}} [d(v_1, w) d(v_2, w)]^\alpha \\ &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1, v_2 \in V(\Gamma_1)}} \left[(d_{R(\Gamma_1)}(v_1) + d_{\Gamma_2}(w)) (d_{R(\Gamma_1)}(v_2) + d_{\Gamma_2}(w)) \right]^\alpha \\ &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1, v_2 \in V(\Gamma_1)}} \left[(2d_{\Gamma_1}(v_1) + d_{\Gamma_2}(w)) (2d_{\Gamma_1}(v_2) + d_{\Gamma_2}(w)) \right]^\alpha \\ &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1, v_2 \in V(\Gamma_1)}} \left[4d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2) + 2d_{\Gamma_2}(w) (d_{\Gamma_1}(v_1) + d_{\Gamma_1}(v_2)) + d_{\Gamma_2}^2(w) \right]^\alpha. \end{aligned} \quad (23)$$

Now applying trinomial theorem, we have

$$\begin{aligned} \sum 4 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(R(\Gamma_1)) \\ v_1, v_2 \in V(\Gamma_1)}} \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left((4d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2))^m 2^k d_{\Gamma_2}^k(w) (d_{\Gamma_1}(v_1) + d_{\Gamma_1}(v_2))^k + d_{\Gamma_2}^{2l}(w) \right) \\ &= \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[\sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(\Gamma_1)} \left((4d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2))^m 2^k d_{\Gamma_2}^k(w) (d_{\Gamma_1}(v_1) + d_{\Gamma_1}(v_2))^k d_{\Gamma_2}^{2l}(w) \right) \right], \end{aligned} \quad (24)$$

$$\begin{aligned} \sum 4 &= \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[2^{2m+k} \left(\sum_{v_1, v_2 \in E(\Gamma_1)} (d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2))^m \right) \left(\sum_{w \in V(\Gamma_2)} d_{\Gamma_2}^{k+2l}(w) \right) (d_{\Gamma_1}(v_1) + d_{\Gamma_1}(v_2))^k \right] \\ &\geq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[2^{2m+k} R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\delta_{\Gamma_1})^k \right]. \end{aligned} \quad (25)$$

Subsequent sum includes those edges from $R(\Gamma_1)$ whose one end vertex is in $V(\Gamma_1)$ while the other is in $V(R(\Gamma_1)) - V(\Gamma_1)$.

$$\begin{aligned}
\sum 5 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} [d(v_1, w) d(v_2, w)]^\alpha \\
&= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} \left[2(d_{R(\Gamma_1)}(v_1) + d_{\Gamma_2}(w)) \right]^\alpha \\
&= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} \left[2(2d_G(v_1) + d_{\Gamma_2}(w)) \right]^\alpha \\
&= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} \left[2d_{\Gamma_2}(w) + 4d_G(v_1) \right]^\alpha \\
&\quad \text{(using binomial theorem)} \\
&= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} \left[\sum_{i=0}^{\alpha} \binom{\alpha}{i} (2d_{\Gamma_2}(w))^{\alpha-i} (4d_G(v_1))^i \right] \\
&= \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2^{(\alpha+i)} \left(\sum_{\substack{v_1 v_2 \in E(R(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(R(\Gamma_1)) - V(\Gamma_1)}} d_G^i(v_1) \right) \left(\sum_{w \in V(\Gamma_2)} d_{\Gamma_2}^{(\alpha-i)}(w) \right) \right] \\
&\geq \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2^{(\alpha+i)} \left(\sum_{w \in V(\Gamma_2)} d_{\Gamma_2}^{(\alpha-i)}(w) \right) 2 \left(\sum_{v_1 \in V(\Gamma_1)} d_G^i(v_1) \right) \right] \geq \sum_{i=0}^{\alpha} \binom{\alpha}{i} [2^{(\alpha+i+1)} M^{(\alpha-i)}(\Gamma_2) M^i(\Gamma_1)].
\end{aligned} \tag{26}$$

Using (22), (25), and (26) in (20), we get

$$\begin{aligned}
R_\alpha(\Gamma_1 +_R \Gamma_2) &\geq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} 2^{2m+k} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l} + R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\delta_{\Gamma_1})^k \right] \\
&\quad + \sum_{i=0}^{\alpha} \binom{\alpha}{i} [2^{(\alpha+i+1)} M^i(\Gamma_1) M^{(\alpha-i)}(\Gamma_2)] = LB_R, R_\alpha(\Gamma_1 +_R \Gamma_2) \\
&\leq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} 2^{2m+k} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\Delta_{\Gamma_2})^{2l} + R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\Delta_{\Gamma_1})^k \right] \\
&\quad + \sum_{i=0}^{\alpha} \binom{\alpha}{i} [2^{(\alpha+i+1)} M^i(\Gamma_1) M^{(\alpha-i)}(\Gamma_2)] = UB_R.
\end{aligned} \tag{27}$$

Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity. This completes the proof. $\square$

Example 2. Let $\Gamma_1 = P_5$, $\Gamma_2 = P_4$, $\alpha = 2$, and $F = R$. Then, $n_1 = M^0(P_5) = 5$, $n_2 = M^0(P_4) = 4$, $e_1 = \chi_0(P_5) = 4$,

$e_2 = \chi_0(P_4) = 3$, $\delta_{P_5} = 1$, $\Delta_{P_5} = 2$, $\delta_{P_4} = 1$, and $\Delta_{P_4} = 2$. Now, we compute lower and upper bound of GRI using formulas derived in Theorem 3.

$$\begin{aligned}
 LB_R(P_5+RP_4) &= \sum_{i=0}^2 \binom{2}{i} \left[2^{(3+i)} M^i(P_5) M^{(2-i)}(P_4) \right] + \sum_{\substack{m,k,l \\ m+k+l=2}} P_{m,k,l} 2^{2m+k} \\
 &\quad \left[M^{2m+k}(P_5) \chi_k(P_4) (\delta_{P_4})^{2l} + R_m(P_5) M^{k+2l}(P_4) (2\delta_{P_5}) \right]^k \\
 &= 8M^0(P_5)M^2(P_4) + 32M(P_5)M(P_4) + 32M^2(P_5)M^0(P_4) + 8P_{1,1,0} (M^3(P_5)\chi(P_4) + 2R(P_5)M(P_4)) \\
 &\quad + 2P_{1,0,1} (M^2(P_5)\chi_0(P_4) + 4R_0(P_5)M^2(P_4)) + 2P_{0,1,1} (4M(P_5)\chi(P_4) + 2R_0(P_5)M^3(P_4)) \\
 &\quad + 16P_{2,0,0} (M^4(P_5)\chi_0(P_4) + R_2(P_5)M^0(P_4)) + 4P_{0,2,0} (M^2(P_5)\chi_2(P_4) + 4R_0(P_5)M^2(P_4)) \\
 &\quad + P_{0,0,2} (16M^0(P_5)\chi_0(P_4) + R_0(P_5)M^4(P_4)), \\
 LB_R(P_5+RP_4) &= 8(5)(10) + 32(8)(10) + 32(14)(4) + 16(26(10) + 12(6)(2)) + 8(14(3)(4) + 12(10)) \\
 &\quad + 4(8(10)(4) + 4(18)(2)) + 16(50(3) + 40(4)) + 4(14(34) + 4(10)(4)) + (5(3)(16) + 4(34)) = 23256.
 \end{aligned} \tag{28}$$

In similar way, we calculate $UB_R(P_5+RP_4) = 28056$.

To compute exact value for $R_2(P_5+RP_4)$, we need edge partition of graph P_5+RP_4 , which is given in Table 4.

Exact value of GRI of P_5+RP_4 for $\alpha = 2$ is given by $R_2(P_5+RP_4) = \sum_{v,w \in E(P_5+RP_4)} (d_{P_5}(v)d_{P_4}(w))^2 = 24592$.

Clearly,

$$23256 \leq R_2(P_5+RP_4) = 24592 \leq 28056. \tag{29}$$

Moreover, we computed actual values along with corresponding bounds of GRI for various cases, and some are presented in Table 5.

Theorem 4. Let Γ_1 and Γ_2 be two simple, finite, and connected graphs. For $\alpha \in \mathcal{N}$, the general Randić index of Q-sum graph is $LB_Q \leq R_\alpha(\Gamma_1+Q\Gamma_2) \leq UB_Q$, where

$$\begin{aligned}
 LB_Q &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) R_l(\Gamma_2) (2\delta_{\Gamma_2})^k \right] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[M^i(\Gamma_2) \chi_\alpha(\Gamma_1) (\delta_{\Gamma_1})^{\alpha-i} \right] + n_2 \chi_\alpha(\Gamma_1) (2\delta_{\Gamma_1})^\alpha, \\
 UB_Q &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) R_l(\Gamma_2) (2\Delta_{\Gamma_2})^k \right] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[M^i(\Gamma_2) \chi_\alpha(\Gamma_1) (\Delta_{\Gamma_1})^{\alpha-i} \right] + n_2 \chi_\alpha(\Gamma_1) (2\Delta_{\Gamma_1})^\alpha,
 \end{aligned} \tag{30}$$

and $P_{m,k,l} = (m+k+l)!/m!k!l!$. Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity.

Proof. Suppose that $d(v, w) = d_{(\Gamma_1+Q\Gamma_2)}(v, w)$ denotes the degree of vertex (v, w) in the Q-sum graph $\Gamma_1+Q\Gamma_2$. Then general Randić index for Q-sum graph is calculated as

TABLE 4: Edge partition based upon degree of end vertices of graph $P_5 +_R P_4$.

(d_v, d_w)	(2, 3)	(2, 4)	(2, 5)	(2, 6)	(3, 4)	(3, 5)	(4, 4)	(4, 6)	(5, 5)	(5, 6)	(6, 6)
$ E $	4	4	12	12	4	4	2	4	4	6	7

TABLE 5: Few more cases of lower and upper bounds regarding $R_\alpha(\Gamma_1 +_R \Gamma_2)$.

Γ_1	Γ_2	α	$LB_R \leq R_\alpha(\Gamma_1 +_R \Gamma_2) \leq UB_R$
P_4	C_3	2	$15696 \leq 18768 \leq 19248$
P_4	C_3	3	$425952 \leq 551232 \leq 589632$
P_5	P_4	3	$526448 \leq 698288 \leq 699904$

$$\begin{aligned}
R_\alpha(\Gamma_1 +_Q \Gamma_2) &= \sum_{(v_1, w_1)(v_2, w_2) \in E(\Gamma_1 +_Q \Gamma_2)} [d(v_1, w_1)d(v_2, w_2)]^\alpha = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d(v, w_1)d(v, w_2)]^\alpha \\
&\quad + \sum_{w \in V(\Gamma_2)} \sum_{v_1, v_2 \in E(Q(\Gamma_1))} [d(v_1, w)d(v_2, w)]^\alpha \\
&= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d(v, w_1)d(v, w_2)]^\alpha + \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(Q(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} [d(v_1, w)d(v_2, w)]^\alpha \\
&\quad + \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1, v_2 \in E(Q(\Gamma_1)) \\ v_1, v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} [d(v_1, w)d(v_2, w)]^{\alpha\alpha} \\
&= \sum 6 + \sum 7 + \sum 8,
\end{aligned} \tag{31}$$

$$\begin{aligned}
\sum 6 &= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d(v, w_1)d(v, w_2)]^\alpha = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[(d_{Q(\Gamma_1)}(v) + d_{\Gamma_2}(w_1))(d_{Q(\Gamma_1)}(v) + d_{\Gamma_2}(w_2)) \right]^\alpha \\
&= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[(d_{\Gamma_1}(v) + d_{\Gamma_2}(w_1))(d_{\Gamma_1}(v) + d_{\Gamma_2}(w_2)) \right]^\alpha, \\
\sum 6 &= \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} [d_{\Gamma_1}^2(v) + d_{\Gamma_1}(v)(d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2)) + d_{\Gamma_2}(w_1)d_{\Gamma_2}(w_2)]^\alpha.
\end{aligned} \tag{32}$$

Applying trinomial theorem, we get

$$\sum 6 = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left[\sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} d_{\Gamma_1}^{2m}(v) d_{\Gamma_1}^k(v) (d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k (d_{\Gamma_2}(w_1)d_{\Gamma_2}(w_2))^l \right], \tag{33}$$

where $P_{m,k,l} = (m+k+l)!/m!k!l!$.

$$\begin{aligned}
 \sum 6 &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[\sum_{v \in V(\Gamma_1)} \sum_{w_1 w_2 \in E(\Gamma_2)} \left((d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k d_{\Gamma_1}^{2m}(v) d_{\Gamma_1}^k(v) (d_{\Gamma_2}(w_1) d_{\Gamma_2}(w_2))^l \right) \right] \\
 &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[\sum_{w_1 w_2 \in E(\Gamma_2)} (d_{\Gamma_2}(w_1) d_{\Gamma_2}(w_2))^l (d_{\Gamma_2}(w_1) + d_{\Gamma_2}(w_2))^k \left[\sum_{v \in V(\Gamma_1)} d_{\Gamma_1}^{2m+k}(v) \right] \right] \geq \\
 &\sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) R_l(\Gamma_2) (2\delta_{\Gamma_2})^k \right].
 \end{aligned} \tag{34}$$

$\sum 7$ involves those edges from $Q(\Gamma_1)$ whose one end vertex is in $V(\Gamma_1)$ and the other is in $V(Q(\Gamma_1)) - V(\Gamma_1)$.

$$\begin{aligned}
 \sum 7 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} [d(v_1, w) d(v_2, w)]^\alpha \\
 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} \left[(d_{Q(\Gamma_1)}(v_1) + d_{\Gamma_2}(w)) d_{Q(\Gamma_1)}(v_2) \right]^\alpha \\
 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} \left[(d_{\Gamma_1}(v_1) + d_{\Gamma_2}(w))^\alpha (d_{Q(\Gamma_1)}(v_2))^\alpha \right].
 \end{aligned} \tag{35}$$

Now applying binomial theorem, we have

$$\begin{aligned}
 \sum 7 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} \left[\sum_{i=0}^{\alpha} \binom{\alpha}{i} (d_{\Gamma_1}(v_1))^{\alpha-i} (d_{\Gamma_2}(w))^i (d_{Q(\Gamma_1)}(v_2)) \right]^\alpha \\
 &= \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left(\sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_1 \in V(\Gamma_1) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} d_{Q(\Gamma_1)}^\alpha(v_2) \left(\sum_{w \in V(\Gamma_2)} d_{\Gamma_2}^i(w) \right) (d_{\Gamma_1}^{\alpha-i}(v_1)) \right).
 \end{aligned} \tag{36}$$

It can easily be observed that $d_{Q(\Gamma_1)}(v_2) = (d_{\Gamma_1}(u_s) + d_{\Gamma_1}(u_t))$ for $v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)$, where v_2 is the vertex inserted into the edge $u_s u_t \in E(\Gamma_1)$. In addition,

$$\sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} d_{Q(\Gamma_1)}(v_2) = 2 \sum_{u_i u_j \in E(\Gamma_1)} (d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_j)).$$

Also, using the fact $\delta_{\Gamma_1}(v) \leq d_{\Gamma_1}(v) \forall v \in V(\Gamma_1)$, we have

$$\sum 7 \geq \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2 \left(\sum_{u_i u_j \in E(\Gamma_1)} (d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_j))^{\alpha} \right) M^i(\Gamma_2) (\delta_{\Gamma_1})^{\alpha-i} \right] = \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2 M^i(\Gamma_2) \chi_{\alpha}(\Gamma_1) (\delta_{\Gamma_1})^{\alpha-i} \right]. \quad (37)$$

Next sum contains those edges from $Q(\Gamma_1)$ whose both end vertices are in $V(Q(\Gamma_1)) - V(\Gamma_1)$.

$$\begin{aligned} \sum 8 &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} [d(v_1, w) d(v_2, w)]^{\alpha} = \sum_{w \in V(\Gamma_2)} \sum_{\substack{v_1 v_2 \in E(Q(\Gamma_1)) \\ v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} \left[d_{Q(\Gamma_1)}(v_1) d_{Q(\Gamma_1)}(v_2) \right]^{\alpha} \\ &= \sum_{w \in V(\Gamma_2)} \sum_{\substack{u_s u_t \in E(\Gamma_1) \\ u_t u_r \in E(\Gamma_1)}} \left[(d_{\Gamma_1}(u_s) + d_{\Gamma_1}(u_t)) (d_{\Gamma_1}(u_t) + d_{\Gamma_1}(u_r)) \right]^{\alpha}, \end{aligned} \quad (38)$$

where v_1 and v_2 are the vertices embedded into the edges $u_s u_t$ and $u_t u_r$ of Γ_1 , respectively.

$$\sum 8 = \sum_{w \in V(\Gamma_2)} \sum_{\substack{u_s u_t \in E(\Gamma_1) \\ u_t u_r \in E(\Gamma_1)}} \left[(d_{\Gamma_1}(u_s) + d_{\Gamma_1}(u_t))^{\alpha} (d_{\Gamma_1}(u_t) + d_{\Gamma_1}(u_r))^{\alpha} \right] \geq n_2 \left[\sum_{u_s u_t \in E(\Gamma_1)} (d_{\Gamma_1}(u_s) + d_{\Gamma_1}(u_t))^{\alpha} (2\delta_{\Gamma_1})^{\alpha} \right] = n_2 \chi_{\alpha}(\Gamma_1) (2\delta_{\Gamma_1})^{\alpha}. \quad (39)$$

Using equations (34)–(39) in (31), we get

$$R_{\alpha}(\Gamma_1 +_Q \Gamma_2) \geq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[M^{2m+k}(\Gamma_1) R_l(\Gamma_2) (2\delta_{\Gamma_2})^k \right] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2 M^i(\Gamma_2) \chi_{\alpha}(\Gamma_1) (\delta_{\Gamma_1})^{\alpha-i} \right] + n_2 \chi_{\alpha}(\Gamma_1) (2\delta_{\Gamma_1})^{\alpha} = LB_Q. \quad (40)$$

Similarly, we have

$$R_{\alpha}(\Gamma_1 +_Q \Gamma_2) \leq \sum_{\substack{m, k, l \\ m+k+l=\alpha}} P_{m, k, l} \left[M^{2m+k}(\Gamma_1) R_l(\Gamma_2) (2\Delta_{\Gamma_2})^k \right] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2 M^i(\Gamma_2) \chi_{\alpha}(\Gamma_1) (\Delta_{\Gamma_1})^{\alpha-i} \right] + n_2 \chi_{\alpha}(\Gamma_1) (2\Delta_{\Gamma_1})^{\alpha} = UB_Q. \quad (41)$$

Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity. This completes the proof. $\square$

Example 3. To compute lower and upper bound of GRI using formulas derived in Theorem 4 for the graphs and corresponding parameters presented in Example 2. we get

$$\begin{aligned}
 UB_Q(P_5+Q P_4) &= \sum_{\substack{m,k,l \\ m+k+l=2}} P_{m,k,l} \left[M^{2m+k}(P_5) R_l(P_4) (2\Delta_{P_4})^k \right] + \sum_{i=0}^2 \binom{2}{i} \left[2M^i(P_4) \chi_\alpha(P_5) (\Delta_{P_5})^{\alpha-i} \right] + n_2 \chi_\alpha(P_5) (2\Delta_{P_5})^\alpha, \\
 UB_Q(P_5+Q P_4) &= P_{2,0,0} (M^4(P_5) R_0(P_4)) + P_{0,2,0} (M^2(P_5) R_0(P_4) (16)) + P_{0,0,2} (M^0(P_5) R_2(P_4)) + P_{1,1,0} (M^3(P_5) R_0(P_4) (4)) \\
 &\quad + P_{1,0,1} (M^2(P_5) R(P_4)) + P_{0,1,1} (M(P_5) R(P_4) (4)) + 2\chi_2(P_5) (4M^0(P_4) + 4M(P_4) + M^2(P_4)) + 64\chi_2(P_5) \\
 &= (50(3) + 14(3)(16) + 5(24)) \\
 &\quad + 2(26(3)(4) + 14(8) + 8(8)(4)) + 100(4(4) + 2(6)(2) + 10) + 64(50) = 10502.
 \end{aligned} \tag{42}$$

In similar way, we calculate $LB_Q(P_5+Q P_4) = 4630$.

To compute exact value for $R_2(P_5+Q P_4)$, we need edge partition of graph $P_5+Q P_4$, and observe 8 edges with end vertex degrees (2, 3), 10 edges with end vertex degrees (3, 3), 26 edges with end vertex degrees (3, 4), and 15 edges with end vertex degrees (4, 4), respectively.

Now, we compute exact value of GRI of $P_5+Q P_4$ for $\alpha = 2$. $R_2(P_5+Q P_4) = \sum_{vw \in E(P_5+Q P_4)} (d_{P_5}(v) d_{P_4}(w))^2 = 8682$.

Obviously,

$$4630 \leq R_2(P_5+Q P_4) = 8682 \leq 10502. \tag{43}$$

Moreover, we computed actual values along with corresponding bounds of GRI for various cases, and some are presented in Table 6.

Theorem 5. Let Γ_1 and Γ_2 be two simple, finite, and connected graphs. For $\alpha \in \mathcal{N}$, the general Randić index of T -sum graph is $LB_T \leq R_\alpha(\Gamma_1+T \Gamma_2) \leq UB_T$, where

$$\begin{aligned}
 LB_T &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\delta_{\Gamma_2})^{2l} + 2^{2m+k} R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\delta_{\Gamma_1})^k \right] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2M^i(\Gamma_2) \chi_\alpha(\Gamma_1) (\delta_{\Gamma_1})^{\alpha-i} \right] \\
 &\quad + n_2 \chi_\alpha(\Gamma_1) (2\delta_{\Gamma_1})^\alpha, \\
 UB_T &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2) (\Delta_{\Gamma_2})^{2l} + 2^{2m+k} R_m(\Gamma_1) M^{k+2l}(\Gamma_2) (2\Delta_{\Gamma_1})^k \right] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} \left[2M^i(\Gamma_2) \chi_\alpha(\Gamma_1) (\Delta_{\Gamma_1})^{\alpha-i} \right] \\
 &\quad + n_2 \chi_\alpha(\Gamma_1) (2\Delta_{\Gamma_1})^\alpha,
 \end{aligned} \tag{44}$$

TABLE 6: Few more cases of lower and upper bounds regarding $R_\alpha(\Gamma_1 +_Q \Gamma_2)$.

Γ_1	Γ_2	α	$LB_Q \leq R_\alpha(\Gamma_1 +_Q \Gamma_2) \leq UB_Q$
P_4	C_3	2	$4266 \leq 5772 \leq 6918$
P_4	C_3	3	$50898 \leq 78636 \leq 96918$
P_5	P_4	3	$43674 \leq 115386 \leq 144422$

and $P_{m,k,l} = (m+k+l)!/m!k!l!$. Equality holds if and only if Γ_1 and Γ_2 are regular graphs with same regularity.

Proof. In total graph, we know $d_{\Gamma_1 +_T \Gamma_2}(v, w) = d_{\Gamma_1 +_R \Gamma_2}(v, w)$ for $v \in V(\Gamma_1)$ and $w \in V(\Gamma_2)$ and $d_{\Gamma_1 +_T \Gamma_2}(v, w) = d_{\Gamma_1 +_Q \Gamma_2}(v, w)$ for $v \in V(T(\Gamma_1)) - V(\Gamma_1)$ and $w \in V(\Gamma_2)$. The lower and upper for total graph can be attained as a direct consequence of Theorems 3 and 4. Moreover, the results and examples illustrated in Theorems 3 and 4 implicate that the bounds provided in Theorem 5 perform significantly well, and hence examples are omitted.

Now, we propose lower and upper bounds of general Randić index of F -sum graphs for $\alpha \in \mathcal{R}$ and following results are intimately tied with generalized binomial and trinomial theorems. $\square$

4. Applications

4.1. Results for Cycles C_a and C_b . Let C_a and C_b be two cycle graphs with vertices a and b , respectively. Then, using Theorems 2–5, the lower and upper bounds of general Randić index of F -sum graphs $C_a +_S C_b$, $C_a +_R C_b$, $C_a +_Q C_b$, and $C_a +_T C_b$, are given as follows:

$$\begin{aligned}
 LB_S = UB_S &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} [ab2^{2m+3k+2l}] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} b^2 2^{2\alpha+1}, \\
 LB_R = UB_R &= \sum_{i=0}^{\alpha} \binom{\alpha}{i} ab2^{2\alpha+i-1} + \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} [ab2^{2m+3k+2l} + b2^{m+4k+2l+1} (1 + (a-2)2^{m-1})], \\
 LB_Q = UB_Q &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} [ab2^{2m+3k+2l}] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} ab2^{3\alpha+1} + ab2^{4\alpha}, \\
 LB_T = UB_T &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} (ab)2^{(2m+4k)} [2^k + 2^{2m+2l}] + \sum_{i=0}^{\alpha} \binom{\alpha}{i} ab2^{3\alpha+1} + ab2^{4\alpha}.
 \end{aligned} \tag{45}$$

Note that lower and upper bounds are equal due to the reason that C_a and C_b are regular graphs with same regularity.

4.2. Results for Paths P_a and P_b . Let P_a and P_b be two path graphs with vertices a and b , respectively. Then, using Theorems 2–5, the lower and upper bounds of general

Randić index of F -sum graphs $P_{a+S}P_b$, $P_{a+R}P_b$, $P_{a+Q}P_b$, and $P_{a+T}P_b$, are given as

$$\begin{aligned}
 LB_S &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[2^{(k+l)} (2 + (a-2)2^{2m+k}) (2 + (b-2)2^l) \right] + \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b-2)2^{i+1}) \right) + b2^{\alpha} \right] (2(3)^{\alpha} + (a-2)2^{2\alpha}), \\
 UB_S &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[2^{(k+l)} (2 + (a-2)2^{2m+k}) (2 + (b-2)2^l) \right] + \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{\alpha-i+1} (2 + (b-2)2^i) \right) + b2^{2\alpha} \right] (2(3)^{\alpha} + (a-2)2^{2\alpha}), \\
 LB_R &= \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b-2)2^{i+1}) \right) + 2^{3m+2k} (2 + (a-2)2^m) \right] + b2^{\alpha} (2(3)^{\alpha} + (a-2)2^{\alpha}) + \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[(2 + (a-2)2^{2m+k}) \right. \\
 &\quad \cdot (2(3)^k + (b-2)2^{2k}) 2^{3m+2k} + (2 + (a-2)2^m) (2 + (b-2)2^{2k+l}) \left. \right], \\
 UB_R &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[2^{2l} (2 + (a-2)2^{2m+k}) (2(3)^k + (b-2)2^{2k}) + 2^{3m+2k} (2 + (a-2)2^m) \right. \\
 &\quad + 2^{3m+3k} (2 + (a-2)2^m) (2 + (b-2)2^{2k+l}) \left. \right] \\
 &\quad + \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{\alpha-i+1} (2 + (b-2)2^i) \right) + 2^{3m+2k} (2 + (a-2)2^m) + b2^{2\alpha} \right] (2(3)^{\alpha} + (a-2)2^{\alpha}), \\
 LB_Q &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[2^{(k+l)} (2 + (a-2)2^{2m+k}) (2 + (b-2)2^l) \right] + \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b-2)2^{i+1}) \right) + b2^{\alpha} \right] (2(3)^{\alpha} + (a-2)2^{2\alpha}), \\
 UB_Q &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[2^{(k+l)} (2 + (a-2)2^{2m+k}) (2 + (b-2)2^l) \right] + \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{\alpha-i+1} (2 + (b-2)2^i) \right) + b2^{2\alpha} \right] \\
 &\quad \cdot (2(3)^{\alpha} + (a-2)2^{2\alpha}), \\
 LB_T &= \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b-2)2^{i+1}) \right) + 2^{3m+2k} (2 + (a-2)2^m) \right] + b2^{\alpha} (2(3)^{\alpha} + (a-2)2^{\alpha}) + \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \\
 &\quad \cdot \left[(2 + (a-2)2^{2m+k}) (2(3)^k + (b-2)2^{2k}) 2^{3m+2k} + (2 + (a-2)2^m) (2 + (b-2)2^{2k+l}) \right], \\
 UB_T &= \sum_{\substack{m,k,l \\ m+k+l=\alpha}} P_{m,k,l} \left[2^{2l} (2 + (a-2)2^{2m+k}) (2(3)^k + (b-2)2^{2k}) + 2^{3m+2k} (2 + (a-2)2^m) \right. \\
 &\quad + 2^{3m+3k} (2 + (a-2)2^m) (2 + (b-2)2^{2k+l}) \left. \right] \\
 &\quad + \left[\left(\sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{\alpha-i+1} (2 + (b-2)2^i) \right) + 2^{3m+2k} (2 + (a-2)2^m) + b2^{2\alpha} \right] (2(3)^{\alpha} + (a-2)2^{\alpha}).
 \end{aligned}$$

(46)

5. Conclusion

For researchers, determining the bounds for pertinent topological index is always intriguing and attractive problem. In [45], Liu et al. proposed an open problem regarding GRI of four operations (F -sum) on graphs. This paper, potentially, addressed and figured out the bounds on GRI for the

F -sum graphs $\Gamma_1+S\Gamma_2$, $\Gamma_1+R\Gamma_2$, $\Gamma_1+Q\Gamma_2$, and $\Gamma_1+T\Gamma_2$ ($\alpha \in \mathbb{N}$) in terms of eminent TIs of their base graphs and graph parameters. Several examples for different combinations of base graphs Γ_1 and Γ_2 along with different parameter α are explored. It can be observed that bounds obtained performed well when compared with exact value. It is worth mentioning that with the help of these four graph

operations, one can construct the molecular graph of his own choice and GRI quantifies information of resulting molecular graph. Computing the bounds of GA-index and ABC-index (variations of GRI) for the F -sum graphs could be an interesting problem for future investigation.

Abbreviation

TI:	Topological index
QSPR:	Quantitative structure property relationships
QSAR:	Quantitative structure activity relationships
GA-Index:	Geometric arithmetic index
FGZI:	First general Zagreb index
ABC-Index:	Atom bond connectivity index
GRI:	General Randić index
SCI:	Sum-connectivity index
GSCI:	General sum-connectivity index.

Data Availability

All data are included within this paper. 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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