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 \( \pi \)-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 \( \Gamma \). 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 \( \Gamma \). 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 \( \Gamma \) 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 \( \Gamma \) are symbolized by \( \delta_\Gamma \) and \( \Delta_\Gamma \), respectively. Two primary parameters known as the order (total number of vertices) and the size (total number of edges) of graph \( \Gamma \) 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 \( \Omega \) 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 $\Gamma$ be a molecular graph; then, the first Zagreb index and second Zagreb index are defined as

\[
M_1(\Gamma) = \sum_{v \in V(\Gamma)} [d_v(v)]^2 = \sum_{vw \in E(\Gamma)} [d_v(u) + d_v(v)],
\]

\[
M_2(\Gamma) = \sum_{v \in V(\Gamma)} [d_v(u) \cdot d_v(v)].
\]  

(1)

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

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

\[
M^\alpha(\Gamma) = \sum_{v \in V(\Gamma)} [d_v(v)]^\alpha = \sum_{v \in V(\Gamma)} [d_v^{-1}(v) + d_v^{-1}(w)],
\]  

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 $\Gamma$ be a molecular graph; then, the general Randić index (GRI) is defined as

\[
R_\alpha(\Gamma) = \sum_{v \in V(\Gamma)} [d_v(v)d_v(v)]^\alpha, \quad \alpha \in \mathbb{R}, \alpha \neq 0.
\]  

(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 $\Gamma$ be a molecular graph; then, the general sum-connectivity index (GSCI) is defined as

\[
\chi^\alpha(\Gamma) = \sum_{v \in V(\Gamma)} [d_v(v) + d_v(w)]^\alpha, \quad \alpha \in \mathbb{R}.
\]  

(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 $E_n(\Gamma)$ ($\pi$-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 $(G_1 +_FG_2)$ $(F \in \{S, R, Q, T\})$ by employing the idea of Cartesian product on graphs $F(\Gamma_1)$ and $\Gamma_2$, where $\Gamma_1$ and $\Gamma_2$ are two simple-connected graphs and $F(\Gamma_i)$ is obtained after applying $F$ on $\Gamma_i$ which is elaborated subsequently.

Definition 5. Let $\Gamma$ 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 $\Gamma$ by introducing an additional vertex on each edge of $\Gamma$.
2. Triangle parallel graph $R(\Gamma)$ is derived from $S(\Gamma)$ by joining the solid vertices of the original edges of $\Gamma$ 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 $\Gamma_1$ and $\Gamma_2$ 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 $\Gamma_1$ 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 $\Gamma_1 +_FG_2$ is a graph with vertex set $\{V(\Gamma_1) + V(\Gamma_2)\} \times \{(V(\Gamma_1)) \times (V(\Gamma_2)) = (V(\Gamma_1) \cup E(F(\Gamma_1))) \times (V(\Gamma_2))\}$ such that two vertices $(v_1, v_2)$ and $(w_1, w_2)$ of $V(\Gamma_1) +_FG_2$ are adjacent if and only if $[v_1 = w_1 \in V(\Gamma_1)$ and $(v_2, w_2) \in E(F(\Gamma_2))]$ or $[v_2 = w_2 \in V(\Gamma_2)$ and $(v_1, v_1) \in E(F(\Gamma_1))]$.

We observe that the graph $\Gamma_1 +_FG_2$ has $|V(\Gamma_1)|$ copies of the graph $F(\Gamma_1)$ provided that vertices of these copies are labeled with vertices of $\Gamma_1$. In graph $\Gamma_1 +_FG_2$, the vertices of $\Gamma_1$ are referred as solid vertices, whereas the vertices $E(F(\Gamma_1))$ are referred as hollow vertices. Now join only solid vertices having same label in $F(\Gamma_1)$ such that their adjacency in $F_2$ 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.

\[
(x_1 + x_2)^n = \sum_{i=0}^{n} \binom{n}{i} x_1^{n-i} x_2^i,
\]

(5)

\[
(x_1 + x_2 + x_3)^n = \sum_{m+k+l=n} P_{m,k,l} x_1^m x_2^k x_3^l,
\]

(6)

where $P_{m,k,l} = (m + k + l)!/m!k!l!$. 
The graph $Q(C_6)$

The graph $R(C_6)$

The graph $T(C_6)$

**Figure 1:** Base graph $C_6$ along with its derived graphs.

The graph $P_1$

The graph $P_4 + S C_3$

The graph $P_4 + Q C_3$

The graph $P_4 + R C_3$

The graph $P_4 + T C_3$

**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 for $F$-sum graphs [46], respectively. Moreover, Liu et al. [45] proposed the open problem to compute the general Randić index for any $\alpha \in \mathbb{R}$. 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 $\alpha \in \mathbb{N}$.

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 $\Gamma_1 +_f \Gamma_2$, $\Gamma_1 +_g \Gamma_2$, $\Gamma_1 +_Q \Gamma_2$ and $\Gamma_1 +_T \Gamma_2$, are computed, where $\Gamma_1$ and $\Gamma_2$ are considered to be finite, simple, and connected graphs. Throughout $n_1 = V(\Gamma_1)$, $n_2 = V(\Gamma_2)$, $e_1 = |E(\Gamma_1)|$, $e_2 = |E(\Gamma_2)|$, $V(S(\Gamma_1)) = n_1 + e_1$, $|E(S(\Gamma_1))| = 2e_1$, $M^0(\Gamma_1) = n_1$, $M^1(\Gamma_1) = 2e_1$, $M^2(\Gamma_1) = M_1(\Gamma_1)$, $M^2(\Gamma_2) = M_1(\Gamma_2)$, $R(\Gamma_2) = M_2(\Gamma_2)$, $\chi(\Gamma_1) = e_2$, and $\chi(\Gamma_2) = M_1(\Gamma_1)$.

**Theorem 2.** Let $\Gamma_1$ and $\Gamma_2$ be two simple, binary, and connected graphs. For $\alpha \in \mathbb{N}$, the general Randić index of $S$-sum graph is $LB_S \leq R_\alpha(\Gamma_{1+s}\Gamma_2) \leq UB_S$, where

\[
LB_S = \sum_{m,k,l=n} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2)(\delta_{\Gamma_1})^{2l} \right]
+ \sum_{i=0}^{\alpha} \left(\binom{\alpha}{i} R_{\alpha-i}(S(\Gamma_1)) M^l(\Gamma_2) (\sigma_{\Gamma_1})^{2i} \right),
\]

\[
UB_S = \sum_{m,k,l=n} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1) \chi_k(\Gamma_2)(\Delta_{\Gamma_1})^{2l} \right]
+ \sum_{i=0}^{\alpha} \left(\binom{\alpha}{i} R_{\alpha-i}(S(\Gamma_1)) M^l(\Gamma_2) (\sigma_{\Gamma_1})^{2i} \right),
\]

and $P_{m,k,l} = (m + k + l)! / m!k!l!$. Equality holds if and only if $\Gamma_1$ and $\Gamma_2$ are regular graphs with same regularity.

**Proof.** Suppose that $d(v,w) = d(\Gamma_1,\Gamma_2)(v,w)$ 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
\[ R_{\alpha}(\Gamma_1 + \Gamma_2) = \sum_{(v_1, w_1)(v_2, w_2) \in E(\Gamma_1 + \Gamma_2)} [d(v_1, w_1)d(v_2, w_2)]^\alpha \]
\[ = \sum_{v \in V(\Gamma_1)} \sum_{w, v \in E(\Gamma_1)} [d(v, w_1)d(v, w)]^\alpha \]
\[ + \sum_{w \in V(\Gamma_1) \cap \delta(\Gamma_1)} \sum_{v \in E(\delta(\Gamma_1))} [d(v, \omega)]^\alpha \]
\[ = \sum 1 + \sum 2. \tag{8} \]

Consider
\[ \sum 1 = \sum_{v \in V(\Gamma_1 \cap \delta(\Gamma_1))} \sum_{w \in E(\Gamma_1)} \left[ P_{m,k,l}d_{\alpha}^{2m}(v)d_{\alpha}^{k}(\delta_{\Gamma_1}(v))d_{\alpha}^{l}(\delta_{\Gamma_1}(v))^2 \right]. \tag{10} \]

where \( P_{m,k,l} = \frac{(m + k + l)!}{m!k!l!} \).

Using Definitions 1 and 3 and the fact \( \delta_{\Gamma_1}(w) \leq d_{\Gamma_1}(w) \) \( \forall w \in V(\Gamma_2) \), we have
\[ \sum 1 \geq \sum_{m,k,l} P_{m,k,l} \left[ \sum_{w \in E(\Gamma_1)} (d_{\Gamma_1}(w_1) + d_{\Gamma_1}(w_2))^k (d_{\Gamma_1}(w_1)d_{\Gamma_1}(w_2))^l \right]. \tag{11} \]

Using trinomial theorem, we get
\[ \sum 2 = \sum_{v \in V(\Gamma_1) \cap \delta(\Gamma_1)} \sum_{w \in E(\delta(\Gamma_1))} [d(v, \omega)d(v, \omega)]^\alpha \]
\[ = \sum_{v \in V(\Gamma_1) \cap \delta(\Gamma_1)} \sum_{w \in E(\delta(\Gamma_1))} \left[ d_{\delta(\Gamma_1)}(v_1) + d_{\delta(\Gamma_1)}(v_2) \right]^\alpha \]
\[ = \sum_{v \in V(\Gamma_1) \cap \delta(\Gamma_1)} \sum_{w \in E(\delta(\Gamma_1))} \left[ d_{\delta(\Gamma_1)}(v_1)d_{\delta(\Gamma_1)}(v_2) + d_{\delta(\Gamma_1)}(v_1)d_{\delta(\Gamma_1)}(v_2) \right]. \tag{12} \]

Now applying binomial theorem, we get
\[ \sum 2 \geq \sum_{i=0}^{a} \left( \begin{array}{c} a \\ i \end{array} \right) \sum_{v \in V(\Gamma_1) \cap \delta(\Gamma_1)} \left[ d_{\delta(\Gamma_1)}(v_1)d_{\delta(\Gamma_1)}(v_2) \right]^{a-i} \left[ d_{\delta(\Gamma_1)}(v_1)d_{\delta(\Gamma_1)}(v_2) \right]^i. \tag{13} \]

Using Definitions 5 and 6 and property of smallest degree of graph \( \Gamma_1 \), we have
\[ \sum 2 \geq \sum_{i=0}^{a} \left( \begin{array}{c} a \\ i \end{array} \right) \left[ R_{\alpha}(\Lambda(1))M_{\Gamma_2}(\delta_{\Gamma_1}) \right]. \tag{14} \]
Substituting the (12) and (14) in (8), we have
\[
R_a(\Gamma_1 \ast \Gamma_2) \geq \sum_{m,k,l=a} P_{m,k,l} \left[ M^{2m+2k-1} \cdot (\Gamma_1)_{m,k,l} (\Gamma_2)_{m,k,l} (\delta_{\Gamma_1})^{2l} \right] + \sum_{i=0}^a \left( \frac{\alpha}{i} \right) \left[ R_{a-i} (S(\Gamma_1)) M^i (\Gamma_2) (\delta_{\Gamma_1})^i \right] = LB_a.
\]
Similarly,
\[
R_a(\Gamma_1 \ast \Gamma_2) \leq \sum_{m,k,l=a} P_{m,k,l} \left[ M^{2m+2k-1} \cdot (\Gamma_1)_{m,k,l} (\Gamma_2)_{m,k,l} (\Delta_{\Gamma_1})^{2l} \right] + \sum_{i=0}^a \left( \frac{\alpha}{i} \right) \left[ R_{a-i} (S(\Gamma_1)) M^i (\Delta_{\Gamma_1})^i \right] = UB_a.
\]
Equality holds if and only if \( \Gamma_1 \) and \( \Gamma_2 \) are regular graphs with same regularity. This completes the proof.

**Example 1.** Let \( \Gamma_1 = P_4, \Gamma_2 = C_3, \alpha = 2, \) and \( F = S. \) Then, \( n_1 = M^0 (P_4) = 4, \) \( n_2 = M^0 (C_3) = 3, \) \( e_1 = \chi_0 (P_4) = 3, \) \( e_2 = \chi_0 (C_3) = 3, \) \( \delta_{\Gamma_1} = 1, \) \( \Delta_{\Gamma_1} = 2, \) \( \delta_{\Gamma_2} = 2, \) and \( \Delta_{\Gamma_2} = 2. \) 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.

\[
LB_a(P_4 \ast C_3) = \sum_{m+k+l=2} P_{m,k,l} \left[ M^{2m+2k-1} \cdot (P_4)_{m,k,l} (C_3) (\delta_{\Gamma_1})^{2l} \right] + \sum_{i=0}^2 \left( \frac{\alpha}{i} \right) \left[ R_{2-i} (S(P_4)) M^i (C_3) (\delta(P_4)) \right] = 2 (18 (12) + 10 (3) (4) + 6 (12) (4)) + 34 (3) + 10 (48) + 4 (3) (16) + 72 (3) + 2 (20) (6) + 6 (12) = 2550.
\]

Likewise, \( UB_a(P_4 \ast C_3) = 3006. \)

To calculate exact value for \( R_a(P_4 \ast C_3), \) we require edge partition of graph \( P_4 \ast C_3, \) which is presented in Table 2.

Now, we calculate exact value of GRI of \( P_4 \ast C_3 \) for \( \alpha = 2. \) \( R_a(P_4 \ast C_3) = \sum_{x \in E(P_4 \ast C_3)} (d_{P_4} (x) d_{C_3} (x))^2 = 3006. \)

Evidently,
\[
LB_a = 2550 \leq R_a(P_4 \ast C_3) = 3006 \leq UB_a = 3006.
\]

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

**Theorem 3.** Let \( \Gamma_1 \) and \( \Gamma_2 \) be two simple, finite, and connected graphs. For \( \alpha \in N, \) the general Randić index of R-sum graph is \( LB_R \leq R_a(\Gamma_1 \ast \Gamma_2) \leq UB_R, \) where
\[
LB_R = \sum_{i=0}^a \left( \frac{\alpha}{i} \right) \left[ 2^{\alpha + i + 1} M^i (\Gamma_1) M^{(\alpha - i)} (\Gamma_2) \right] + \sum_{m,k,l=a} P_{m,k,l} 2^{2m+2k} \left[ M^{2m+2k-1} \cdot (\Gamma_1)_{m,k,l} (\delta_{\Gamma_1})^{2l} + R_m (\Gamma_1) M^{k+2l} (\Gamma_2) \right] \cdot (2\delta_{\Gamma_1})^k,
\]
\[
UB_R = \sum_{i=0}^a \left( \frac{\alpha}{i} \right) \left[ 2^{\alpha + i + 1} M^i (\Gamma_1) M^{(\alpha - i)} (\Gamma_2) \right] + \sum_{m,k,l=a} P_{m,k,l} 2^{2m+2k} \left[ M^{2m+2k-1} \cdot (\Gamma_1)_{m,k,l} (\Delta_{\Gamma_1})^{2l} + R_m (\Gamma_1) M^{k+2l} (\Gamma_2) \right] \cdot (2\Delta_{\Gamma_1})^k.
\]
Table 1: Some particular indices of certain graphs.

| Indices/graphs | $M$ | $M^2$ | $M^3$ | $M^4$ | $M^5$ | $M^6$ | $\chi$ | $\chi_2$ | $\chi_3$ | $R$ | $R_2$ | $R_3$ |
|----------------|------|-------|-------|-------|-------|-------|-------|--------|--------|-----|------|------|
| $P_4$          | 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  |
| $C_7$          | 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 $P_4 + _5 C_3$.

| $(d_1, d_2)$ | $(2, 3)$ | $(3, 3)$ | $(2, 4)$ | $(4, 4)$ |
|-------------|----------|----------|----------|----------|
| $|E|$         | 6        | 6        | 12       | 6        |

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

| $\Gamma_1$ | $\Gamma_2$ | $\alpha$ | $LB_\alpha \leq R_\alpha(\Gamma_1 + _\alpha \Gamma_2) \leq UB_\alpha$ |
|------------|------------|----------|-----------------------------------------------|
| $P_4$      | $C_3$      | 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 $\Gamma_1$ and $\Gamma_2$ are regular graphs with same regularity.

Proof. Suppose that $d(v, w) = d_{[\Gamma_1 + _\alpha \Gamma_2]}(v, w)$ 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

$$R_\alpha (\Gamma_1 + _\alpha \Gamma_2) = \sum_{(v_1, w_1) \in E(\Gamma_1), (v_2, w_2) \in E(\Gamma_2)} [d(v_1, w_1) d(v_2, w_2)]^\alpha = \sum_{v \in V(\Gamma_1)} \sum_{w \in V(\Gamma_2)} [d(v, w_1) d(v, w_2)]^\alpha$$

$$+ \sum_{w \in V(\Gamma_1)} \sum_{v \in V(\Gamma_2)} [d(v_1, w) d(v_2, w)]^\alpha$$

$$= \sum_{v \in V(\Gamma_1)} \sum_{w \in V(\Gamma_2)} [d(v, w_1) d(v, w_2)]^\alpha + \sum_{v \in V(\Gamma_1)} \sum_{w \in V(\Gamma_2)} [d(v_1, w) d(v_2, w)]^\alpha + \sum_{v \in V(\Gamma_1)} \sum_{w \in V(\Gamma_2)} [d(v_1, w) d(v_2, w)]^\alpha$$

$$\cdot [d(v, w) d(v, w)]^\alpha = \sum 3 + \sum 4 + \sum 5,$$

$$\sum 3 = \sum_{v \in V(\Gamma_1)} \sum_{w \in V(\Gamma_2)} \left[ \left( d_{\Gamma_1}(v) + d_{\Gamma_2}(w_1) \right) \left( d_{\Gamma_1}(v) + d_{\Gamma_2}(w_2) \right) \right]^\alpha$$

$$\cdot \left[ \left( 2d_{\Gamma_1}(v) + d_{\Gamma_1}(w_1) \right) \left( 2d_{\Gamma_1}(v) + d_{\Gamma_2}(w_1) \right) \right]^\alpha$$

$$= \sum_{v \in V(\Gamma_1)} \sum_{w \in V(\Gamma_2)} \left[ 4d_{\Gamma_1}^2(v) + 2d_{\Gamma_1}(v) d_{\Gamma_1}(w_1) + d_{\Gamma_2}(w_1) \right] ^\alpha$$

Applying trinomial theorem, we get

$$\text{(20)}$$
\[
\sum 3 = \sum_{v \in V(\Gamma_1)} \sum_{w_1, w_2 \in E(\Gamma_1)} \left[ \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} 4^m d_{\Gamma_1}^m(v) 2^k d_{\Gamma_1}^k(v) \left( d_{\Gamma_1}(w_1) + d_{\Gamma_1}(w_2) \right)^k \right],
\]

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 \( \Gamma_2 \), we get

\[
\sum 3 = \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} \left[ 2^{2m+k} \left( \sum_{v \in V(\Gamma_1)} d_{\Gamma_1}^{2m+k}(v) \right) \left( \sum_{w_1, w_2 \in E(\Gamma_1)} \left( d_{\Gamma_1}(w_1) + d_{\Gamma_1}(w_2) \right)^k \right) \right]
\geq \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} \left[ 2^{2m+k} M^{2m+k}(\Gamma_1) \delta_{\Gamma_1}^k(2\delta_{\Gamma_1})^k \right].
\]

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

\[
\sum 4 = \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in E(\Gamma_1)} \left[ d(v_1, w_1) d(v_2, w_2) \right]^a
\]

\[
= \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in E(\Gamma_1)} \left[ \left( d_{R(\Gamma_1)}(v_1) + d_{\Gamma_1}(w_1) \right) \left( d_{R(\Gamma_1)}(v_2) + d_{\Gamma_1}(w_2) \right) \right]^a
\]

\[
= \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in E(\Gamma_1)} \left[ 2d_{\Gamma_1}(v_1) + d_{\Gamma_1}(w_1) \right] \left[ 2d_{\Gamma_1}(v_2) + d_{\Gamma_1}(w_2) \right]^a
\]

\[
= \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in E(\Gamma_1)} \left[ 4d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2) + 2d_{\Gamma_1}(w_1) d_{\Gamma_1}(v_1) + d_{\Gamma_1}(v_1) + d_{\Gamma_1}(w_2) \right]^a.
\]

Now applying trinomial theorem, we have

\[
\sum 4 = \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in E(\Gamma_1)} \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} \left( 4d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2) \right)^m 2^k d_{\Gamma_1}^k(v) \left( d_{\Gamma_1}(w_1) + d_{\Gamma_1}(w_2) \right) + d_{\Gamma_1}^{2l}(w)
\]

\[
= \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} \left[ \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in E(\Gamma_1)} \left( 4d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2) \right)^m 2^k d_{\Gamma_1}^k(v) \left( d_{\Gamma_1}(w_1) + d_{\Gamma_1}(w_2) \right) + d_{\Gamma_1}^{2l}(w) \right],
\]

\[
\sum 4 = \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} \left[ 2^{2m+k} \left( \sum_{v_1, v_2 \in E(\Gamma_1)} \left( d_{\Gamma_1}(v_1) d_{\Gamma_1}(v_2) \right)^m \right) \left( \sum_{w \in V(\Gamma_1)} d_{\Gamma_1}^{2l}(w) \right) \left( d_{\Gamma_1}(v_1) + d_{\Gamma_1}(v_2) \right)^k \right]
\geq \sum_{m,k,l \atop m+k+l=a} P_{m,k,l} \left[ 2^{2m+k} R_m(\Gamma_1) M^{2k+2l}(\Gamma_2)(2\delta_{\Gamma_1})^k \right].
Subsequent sum includes those edges from $R(\Gamma_1)$ whose one end vertex is in $V(\Gamma_1)$ while the other is in $V(R(\Gamma_1)) - V(\Gamma_1)$.

\[
\sum 5 = \sum_{\omega \in V(\Gamma_2)} \sum_{\nu, \nu' \in E(R(\Gamma_1)) \cap (V(\Gamma_1) \cup V(\Gamma_1) - V(\Gamma_1))} \left[ d(\nu, \omega)d(\nu', \omega) \right]^a
\]

\[
= \sum_{\omega \in V(\Gamma_2)} \sum_{\nu, \nu' \in E(R(\Gamma_1)) \cap (V(\Gamma_1) \cup V(\Gamma_1) - V(\Gamma_1))} \left[ 2 \left( d_{R(\Gamma_1)}(\nu) + d_{R(\Gamma_1)}(\nu') \right) \right]^a
\]

\[
= \sum_{\omega \in V(\Gamma_2)} \sum_{\nu, \nu' \in E(R(\Gamma_1)) \cap (V(\Gamma_1) \cup V(\Gamma_1) - V(\Gamma_1))} \left[ 2 \left( 2d_G(\nu) + d_{R(\Gamma_1)}(\nu) \right) \right]^a
\]

\[
= \sum_{\omega \in V(\Gamma_2)} \sum_{\nu, \nu' \in E(R(\Gamma_1)) \cap (V(\Gamma_1) \cup V(\Gamma_1) - V(\Gamma_1))} \left[ 2d_{R(\Gamma_1)}(\nu) + 4d_G(\nu) \right]^a
\]

(using binomial theorem)

\[
= \sum_{\omega \in V(\Gamma_2)} \sum_{\nu, \nu' \in E(R(\Gamma_1)) \cap (V(\Gamma_1) \cup V(\Gamma_1) - V(\Gamma_1))} \left[ \sum_{i=0}^{a} \binom{a}{i} \left( 2d_{R(\Gamma_1)}(\nu) \right)^i \left( 4d_G(\nu) \right)^{a-i} \right]
\]

\[
= \sum_{\omega \in V(\Gamma_2)} \sum_{\nu, \nu' \in E(R(\Gamma_1)) \cap (V(\Gamma_1) \cup V(\Gamma_1) - V(\Gamma_1))} \left[ \sum_{i=0}^{a} \binom{a}{i} \left( 2d_{R(\Gamma_1)}(\nu) \right)^i \left( 4d_G(\nu) \right)^{a-i} \right]
\]

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

\[
R_\alpha(\Gamma_1 \ast_R \Gamma_2) \geq \sum_{\alpha \in \mathbb{N}^{k+\ell}} \sum_{m,k,l} P_{m,k,l} 2^{2m+k} \left[ M^{2m+k}(\Gamma_1)M^{k}(\delta_{\Gamma_1})^{2\ell} + R_m(\Gamma_1)M^{k+2\ell}(\Gamma_2)(2\delta_{\Gamma_1})^k \right]
\]

\[
+ \sum_{i=0}^{a} \binom{a}{i} \left[ 2 \left( a+i+1 \right) M(\Gamma_1)M^{\alpha-i}(\Gamma_2) \right] = LB_R, \quad R_\alpha(\Gamma_1 \ast_R \Gamma_2)
\]

\[
\leq \sum_{\alpha \in \mathbb{N}^{k+\ell}} \sum_{m,k,l} P_{m,k,l} 2^{2m+k} \left[ M^{2m+k}(\Gamma_1)M^{k}(\Delta_{\Gamma_1})^{2\ell} + R_m(\Gamma_1)M^{k+2\ell}(\Gamma_2)(2\Delta_{\Gamma_1})^k \right]
\]

\[
+ \sum_{i=0}^{a} \binom{a}{i} \left[ 2 \left( a+i+1 \right) M(\Gamma_1)M^{\alpha-i}(\Gamma_2) \right] = UB_R.
\]
Partition of graph

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.

Equality holds if and only if $\Gamma_1$ and $\Gamma_2$ are regular graphs with same regularity. This completes the proof. □

In similar way, we calculate $UB_Q(P_5 +_RP_4) = 28056$. 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 $R_2(P_5 +_RP_4)$ for $\alpha = 2$ is given by

$$\text{LB}_R(P_5 +_RP_4) = \sum_{v,w \in (P_5 +_RP_4)} (d_{P_5}(v) \cdot d_{P_4}(w))^2 = 24592.$$  

Clearly,

$$23256 \leq R_2(P_5 +_RP_4) = 24592 \leq 28056. \quad (29)$$

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

Theorem 4. Let $\Gamma_1$ and $\Gamma_2$ be two simple, finite, and connected graphs. For $\alpha \in \mathcal{N}$, the general Randić index of Q-sum graph is $\text{LB}_Q \leq \text{R}_Q(\Gamma_1 +_Q \Gamma_2) \leq \text{UB}_Q$, where

$$\text{LB}_Q = \sum_{m,k,l \geq \alpha} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1)R_1(\Gamma_2)(2\delta_{\Gamma_1})^k + \sum_{\alpha \leq i \leq \alpha} \chi_{\alpha}(\Gamma_1)(2\Delta_{\Gamma_1})^a \right],$$

$$\text{UB}_Q = \sum_{m,k,l \geq \alpha} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1)R_1(\Gamma_2)(2\Delta_{\Gamma_1})^k + \sum_{\alpha \leq i \leq \alpha} \chi_{\alpha}(\Gamma_1)(2\Delta_{\Gamma_1})^a \right],$$

and $P_{m,k,l} = (m + k + l)!/m!k!l!$. Equality holds if and only if $\Gamma_1$ and $\Gamma_2$ 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 $\langle v,w \rangle$ in the Q-sum graph $\Gamma_1 +_Q \Gamma_2$. Then general Randić index for Q-sum graph is calculated as

$$e_2 = \chi_0(P_4) = 3, \delta_{P_5} = 1, \Delta_{P_5} = 2, \delta_{P_4} = 1, \Delta_{P_4} = 2.$$
Applying trinomial theorem, we get

$$\sum 6 = \sum_{v \in V(\Gamma_1)} \sum_{u_1, u_2 \in E(\Gamma_1)} \left[ P_{m,k,l} d_{m}^{(3m)}(v) \left( d_{r_1}(u_1) + d_{r_2}(u_2) \right)^k \left( d_{r_3}(u_1) d_{r_4}(u_2) \right)^l \right]$$
where \( P_{m,k,l} = (m + k + l)!/m!k!l! \).

\[
\sum_6 = \sum_{m,k,l} P_{m,k,l} \left[ \sum_{v \in V(\Gamma_2)} \sum_{w_1, w_2 \in E(\Gamma_2)} \left( (d_{\Gamma_1}(w_1) + d_{\Gamma_2}(w_2))^k d_{\Gamma_1}^m(v) d_{\Gamma_2}^k(v) (d_{\Gamma_1}(w_1) d_{\Gamma_2}(w_2))^l \right) \right]
\]

\[
= \sum_{m,k,l} P_{m,k,l} \left[ \sum_{v_1, v_2 \in V(\Gamma_1)} \sum_{v \in V(\Gamma_1)} \left( (d_{\Gamma_1}(v_1) + d_{\Gamma_2}(v))^k (d_{\Gamma_1}(w_1) + d_{\Gamma_2}(w_2))^l \right) \right] \geq \sum_{v \in V(\Gamma_1)} \left( \sum_{d_{\Gamma_1}(v)} \right)^k. \tag{34}
\]

\[
\sum_7 \text{ involves those edges from } Q(\Gamma_1) \text{ whose one end vertex is in } V(\Gamma_1) \text{ and the other is in } V(Q(\Gamma_1)) - V(\Gamma_1).
\]

\[
\sum_7 = \sum_{v_1, v_2 \in V(\Gamma_1)} \sum_{v \in V(\Gamma_1)} \left[ d(v_1, w) d(v_2, w) \right]^\alpha
\]

\[
= \sum_{v_1, v_2 \in V(\Gamma_1)} \sum_{v \in V(\Gamma_1)} \left[ (d_{Q(\Gamma_1)}(v_1) + d_{\Gamma_2}(v))^\alpha d_{Q(\Gamma_1)}(v_2) \right]^\alpha \tag{35}
\]

Now applying binomial theorem, we have

\[
\sum_7 = \sum_{v_1, v_2 \in V(\Gamma_1)} \sum_{v \in V(\Gamma_1)} \left[ \sum_{i=0}^\alpha \binom{\alpha}{i} (d_{\Gamma_1}(v_1))^\alpha-i (d_{\Gamma_2}(v))^i (d_{Q(\Gamma_1)}(v_2))^\alpha \right]^\alpha \tag{36}
\]

\[
= \sum_{i=0}^\alpha \binom{\alpha}{i} \left[ \sum_{v \in V(\Gamma_1)} \sum_{v_1, v_2 \in V(\Gamma_1)} \sum_{v_1 \in V(\Gamma_1)} \sum_{v_2 \in V(\Gamma_1)} (d_{\Gamma_1}(v_1))^{\alpha-i} (d_{\Gamma_2}(v))^i (d_{Q(\Gamma_1)}(v_2))^\alpha \right]^{\alpha-i} (d_{\Gamma_2}(v))^i (d_{Q(\Gamma_1)}(v_2))^\alpha \right] \tag{36}
\]
It can easily be observed that $d_{Q(\Gamma)}(v_2) = (d_{r_1}(u_r) + d_{r_1}(u))$ for $v_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)$, where $v_2$ is the vertex inserted into the edge $u_ru_t \in E(\Gamma_1)$. In addition, $\sum_{v_1, v_2 \in V(Q(\Gamma_1))} d_{Q(\Gamma)}(v_2) = 2\sum_{u_ru_t \in E(\Gamma_1)} (d_{r_1}(u_r) + d_{r_1}(u_t))$.

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

\[
\sum_{i=0}^{\alpha} \left( \begin{array}{c} \alpha \\ i \end{array} \right) \left( \sum_{u_r, u_t \in E(\Gamma_1)} (d_{r_1}(u_r) + d_{r_1}(u_t))^a \right) M'(\Gamma_1)(\delta_{\Gamma_1})^{a-i} \right] = \sum_{i=0}^{\alpha} \left( \begin{array}{c} \alpha \\ i \end{array} \right) \left[ 2M'(\Gamma_1)x(\Gamma_1)(\delta_{\Gamma_1})^{a-i} \right].
\] (37)

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

\[
\sum_{v_1, v_2 \in V(Q(\Gamma_1)) \setminus V(\Gamma_1)} |d(v_1, w)d(v_2, w)|^a = \sum_{v_1, v_2 \in V(Q(\Gamma_1)) \setminus V(\Gamma_1)} \left[ d_{Q(\Gamma_1)}(v_1)d_{Q(\Gamma_1)}(v_2) \right]^a = \sum_{v_1, v_2 \in V(Q(\Gamma_1)) \setminus V(\Gamma_1)} \left[ 2M'(\Gamma_1)x(\Gamma_1)(\delta_{\Gamma_1})^{a-i} \right].
\] (38)

where $v_1$ and $v_2$ are the vertices embedded into the edges $u_ru_t$ and $u_tu_r$ of $\Gamma_1$, respectively.

\[
\sum_{i=0}^{\alpha} \left( \begin{array}{c} \alpha \\ i \end{array} \right) \left[ (d_{r_1}(u_r) + d_{r_1}(u_t))^a (d_{r_1}(u_r) + d_{r_1}(u_t))^a \right] \geq n_2 \sum_{u_r, u_t \in E(\Gamma_1)} (d_{r_1}(u_r) + d_{r_1}(u_t))^a (2\delta_{\Gamma_1})^a = n_2x(\Gamma_1)(2\delta_{\Gamma_1})^a.
\] (39)

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

\[
R_a(\Gamma_1 + Q\Gamma_2) \geq \sum_{m+k=l=a} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1)R_l(\Gamma_2)(2\Delta_{\Gamma_2})^k \right] + \sum_{i=0}^{\alpha} \left( \begin{array}{c} \alpha \\ i \end{array} \right) \left[ 2M'(\Gamma_1)x(\Gamma_1)(\delta_{\Gamma_1})^{a-i} \right] + n_2x(\Gamma_1)(2\delta_{\Gamma_1})^a = LB_{Q_a}.
\] (40)

Similarly, we have

\[
R_a(\Gamma_1 + Q\Gamma_2) \leq \sum_{m+k=l=a} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1)R_l(\Gamma_2)(2\Delta_{\Gamma_2})^k \right] + \sum_{i=0}^{\alpha} \left( \begin{array}{c} \alpha \\ i \end{array} \right) \left[ 2M'(\Gamma_1)x(\Gamma_1)(\Delta_{\Gamma_1})^{a-i} \right] + n_2x(\Gamma_1)(2\Delta_{\Gamma_1})^a = UB_{Q_a}.
\] (41)
Equality holds if and only if $\Gamma_1$ and $\Gamma_2$ are regular graphs with same regularity. This completes the proof. 

\[ UB_Q(P_5+QP_4) = \sum_{m,k,l} P_{m,k,l} \left[ M^{2m+k}(P_5)R_l(P_4)(2\Delta_{P_4})^k \right] + \sum_{i=0}^{\frac{a}{i}} \left( \begin{array}{c} 2 \\ i \end{array} \right) \left[ 2M^r(P_4)\chi_\alpha(P_5)(\Delta_{P_4})^{a-i} \right] + n_2\chi_\alpha(P_5)(2\Delta_{P_4})^a, \]

\[ UB_Q(P_5+QP_4) = P_{2,0,0}(M^4(P_5)R_0(P_4)) + P_{0,2,0}(M^2(P_5)R_0(P_4)) + P_{0,0,2}(M^0(P_5)R_0(P_4)) \]

\[ + P_{1,0,1}(M^2(P_5)R(P_4)) + P_{0,1,1}(M(P_5)R(P_4)) + 2\chi_2(P_3)(4M^0(P_4) + 4M(P_4) + M^2(P_4)) + 64\chi_2(P_5) \]

\[ = (50(3) + 14(3)(16) + 5(24)) \]

\[ + 2(26(3)(4) + 14(8) + 8(8)(4)) + 100(4(4) + 2(6)(2) + 10) + 64(50) = 10502. \]

\[ UB_T = \sum_{m,k,l} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1)\chi_\alpha(\Gamma_2)(\Delta_{\Gamma_1})^{2l} + 2^{m+k}M^{k+2l}(\Gamma_2)(2\Delta_{\Gamma_1})^k \right] + \sum_{i=0}^{\alpha} \left( \begin{array}{c} a \\ i \end{array} \right) \left[ 2M^r(\Gamma_2)\chi_\alpha(\Gamma_1)(\Delta_{\Gamma_1})^{a-i} \right] + n_2\chi_\alpha(\Gamma_1)(2\Delta_{\Gamma_1})^a, \]

\[ UB_T = \sum_{m,k,l} P_{m,k,l} \left[ M^{2m+k}(\Gamma_1)\chi_\alpha(\Gamma_2)(\Delta_{\Gamma_1})^{2l} + 2^{m+k}M^{k+2l}(\Gamma_2)(2\Delta_{\Gamma_1})^k \right] + \sum_{i=0}^{\alpha} \left( \begin{array}{c} a \\ i \end{array} \right) \left[ 2M^r(\Gamma_2)\chi_\alpha(\Gamma_1)(\Delta_{\Gamma_1})^{a-i} \right] + n_2\chi_\alpha(\Gamma_1)(2\Delta_{\Gamma_1})^a, \]

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

\[ 4630 \leq R_2(P_5+QP_4) = 8682 \leq 10502. \]

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

Theorem 5. Let $\Gamma_1$ and $\Gamma_2$ be two simple, finite, and connected graphs. For $\alpha \in \mathcal{N}$, the general Randić index of $T$-sum graph is $LB_T \leq R_\alpha(\Gamma_1+\Gamma_2) \leq UB_T$, where
and $P_{m,k,l} = (m+k+l)!/m!k!l!$. Equality holds if and only if $\Gamma_1$ and $\Gamma_2$ are regular graphs with same regularity.

**Proof.** In total graph, we know $d_{\Gamma_1 + \Gamma_2}(v,w) = d_{\Gamma_1}(v,w)$ for $v \in V(\Gamma_1)$ and $w \in V(\Gamma_2)$ and $d_{\Gamma_1 + \Gamma_2}(v,w) = d_{\Gamma_1}(v) + d_{\Gamma_2}(w)$ for $v \in V(\Gamma_1) - V(\Gamma_1)$ 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.

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

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

### 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 $C_a + Q C_b$, $C_a + Q C_b$, $C_a + Q C_b$, and $C_a + Q C_b$, are given as follows:

\[
\begin{align*}
LB_S &= UB_S = \sum_{m,k,l=0}^\alpha P_{m,k,l} \left[ ab2^{2m+3k+2l} \right] + \sum_{i=0}^\alpha \binom{\alpha}{i} k^2 2^{2i+1}, \\
LB_R &= UB_R = \sum_{i=0}^\alpha \binom{\alpha}{i} ab2^{2i+1} + \sum_{m,k,l=0}^\alpha P_{m,k,l} \left[ ab2^{2m+3k+2l} + b2^{m+4k+2l}(1 + (a - 2)2^{m-1}) \right], \\
LB_Q &= UB_Q = \sum_{m,k,l=0}^\alpha P_{m,k,l} \left[ ab2^{2m+3k+2l} \right] + \sum_{i=0}^\alpha \binom{\alpha}{i} ab2^{2i+1} + ab2^4a, \\
LB_T &= UB_T = \sum_{m,k,l=0}^\alpha P_{m,k,l} \left( ab2^{2m+4k} \right) \left[ 2^k + 2^{2m+2l} \right] + \sum_{i=0}^\alpha \binom{\alpha}{i} ab2^{2i+1} + ab2^4a.
\end{align*}
\]

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 $P_{a+\bar{S}}P_b$, $P_{a+R}P_b$, $P_{a+Q}P_b$, and $P_{a+T}P_b$, are given as

\[ LB_S = \sum_{m,k,l} P_{m,k,l} \left[ 2^{1(2 + (a - 2)2^{2m+2k})} \left( 2 + (b - 2)2^{i+1} \right) \right] + \left( \sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b - 2)2^{i+1}) \right) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ UB_S = \sum_{m,k,l} P_{m,k,l} \left[ 2^{1(2 + (a - 2)2^{2m+2k})} \left( 2 + (b - 2)2^{i+1} \right) \right] + \left( \sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{a-1} (2 + (b - 2)2^{i+1}) \right) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ LB_R = \left[ \sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b - 2)2^{i+1}) \right] + 2^{3m+2k} (2 + (a - 2)2^{2m+2k}) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ UB_R = \sum_{m,k,l} P_{m,k,l} \left[ 2^{1(2 + (a - 2)2^{2m+2k})} \left( 2 + (b - 2)2^{i+1} \right) \right] + \left( \sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{a-1} (2 + (b - 2)2^{i+1}) \right) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ LB_Q = \left[ \sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b - 2)2^{i+1}) \right] + 2^{3m+2k} (2 + (a - 2)2^{2m+2k}) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ UB_Q = \sum_{m,k,l} P_{m,k,l} \left[ 2^{1(2 + (a - 2)2^{2m+2k})} \left( 2 + (b - 2)2^{i+1} \right) \right] + \left( \sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{a-1} (2 + (b - 2)2^{i+1}) \right) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ LB_T = \left[ \sum_{i=0}^{\alpha} \binom{\alpha}{i} (4 + (b - 2)2^{i+1}) \right] + 2^{3m+2k} (2 + (a - 2)2^{2m+2k}) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right), \]

\[ UB_T = \sum_{m,k,l} P_{m,k,l} \left[ 2^{1(2 + (a - 2)2^{2m+2k})} \left( 2 + (b - 2)2^{i+1} \right) \right] + \left( \sum_{i=0}^{\alpha} \binom{\alpha}{i} 2^{a-1} (2 + (b - 2)2^{i+1}) \right) + b2^a \left( 2(3)^a + (a - 2)2^{2a} \right). \]

(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 $\Gamma_1+\bar{S}\Gamma_2$, $\Gamma_1+R\Gamma_2$, $\Gamma_1+Q\Gamma_2$, 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 $\Gamma_1$ and $\Gamma_2$ along with different parameter $\alpha$ 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**

Tl: 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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