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A Survey on the Randić Index [*]

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Abstract

The general Randić index $R_\alpha(G)$ of a (chemical) graph G, is defined as the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α an arbitrary real number, which is called the Randić index or connectivity index (or branching index) for $\alpha = -1/2$ proposed by Milan Randić in 1975. The paper outlines the results known for the (general) Randić index of (chemical) graphs. Some very new results are released. We classify the results into the following categories: extremal values and extremal graphs of Randić index, general Randić index, zeroth-order general Randić index, higher-order Randić index. A few conjectures and open problems are mentioned.

1 Introduction

For a (chemical) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d(u)d(v))^\alpha$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u of G, i.e.,

$$R_\alpha(G) = \sum_{uv \in E} (d(u)d(v))^\alpha$$

where α is an arbitrary real number.

In 1975, the chemist Milan Randić [80] proposed a topological index R (R_{-1} and $R_{-\frac{1}{2}}$) under the name "*branching index*", suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Later, in 1998 Bollobás and Erdös [11] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the general Randić index.

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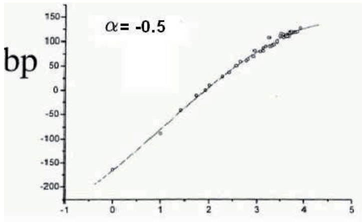

Figure 1.1 Correlation of the Randić index with the boiling point of a selected set of alkanes.

Already Randić noticed that there is a good correlation between the Randić index R and several physico–chemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc (see Figure 1.1). In subsequent years countless applications of R were reported, most of them concerned with medicinal and pharmacological issues. A turning point in the mathematical examination of the Randić and general Randić index happened in the second half of the 1990s, when a significant and ever growing research on this matter started, resulting in numerous publications. Here especially the work [11, 12] of the highly respected Paul Erdős should be mentioned (the preprints of which were available several years before their actual publication), because these stimulated many other colleagues to study R and R_α. For a comprehensive survey of its mathematical properties, see the book of Li and Gutman "*Mathematical Aspects of Randić-Type Molecular Structure Descriptors*" [48].

Let $d(u)$ and $N(u)$ denote the degree and neighborhood of vertex u, respectively. A vertex of degree i is also addressed as an i-*degree vertex.* The minimum and maximum degree of G is denoted by $\delta(G)$ and $\Delta(G)$, respectively. If G has a_i vertices of degree d_i $(i = 1, 2, \ldots, t)$, where $\Delta(G) = d_1 > d_2 > \cdots > d_t = \delta(G)$ and $\sum\limits_{i=1}^{t} a_i = n$. We define the degree sequence $D(G) = [d_1^{a_1}, d_2^{a_2}, \ldots, d_t^{a_t}]$. If $a_i = 1$, we use d_i instead of $d_i^{a_i}$ for convenience. Vertices of degrees 0 and 1 are said to be *isolated* and *pendent vertices*, respectively. A pendent vertex is also referred to as a *leaf* of the underlying graph. A connected graph without any cycle is a *tree*. The *path* P_n is a tree of order n with exactly two pendent vertices. The *star* of order n, denoted by S_n, is the tree with $n-1$ pendent vertices. The *double star* $S_{p,q}$ is the tree with $p+q-2$ pendent vertices, one p-degree vertex and one q-degree vertex. If $|p-q| \leq 1$, then the double star is said to be *balanced*. A simple connected graph is called *unicyclic* if it has exactly one cycle. We use S_n^+ to denote the unicyclic graph obtained from the star S_n by adding to it an edge between two pendent vertices of S_n. A *bicyclic graph* is a graph of order n with $n+1$ edges. A *comet* is a tree composed of a star and an pendent path. For any numbers n and $2 \leq n_1 \leq n-1$, we denote by $CS(n, n_1)$ the comet of order n with n_1 pendent vertices, i.e., a tree formed by a path P_{n-n_1} of which one end vertex coincides with a pendent vertex of a star S_{n_1+1} of order $n_1 + 1$.

A *chemical graph* is a graph in which no vertex has degree greater than four. Analogously, a *chemical tree* is a tree T for which $\Delta(T) \leq 4$. A graph of order n is addressed as an *n-vertex graph*, and a graph of order n and size m is addressed as an *(n, m)-graph*.

For terminology and notations not defined here, we refer the readers to [13].

From a mathematical point of view, the first question to be asked is which are the minimum and maximum R-values in (pertinently chosen) classes of graphs, and which are the graphs from these classes with extremal (minimum and maximum) R. Finding answers to such questions is often far from elementary, and the extremal graphs have sometimes quite unusual and interesting structures. This paper outlines the results known for the (general) Randić index of (chemical) graphs. In Sections 2 and 3, we survey the results of the Randić index and the general Randić index. In Section 4, we focus on the zeroth-order (general) Randić index. In Section 5, we give some results to the higher-order Randić index. In the last section, a few conjectures and open problems are mentioned.

2 The Randić index

In this section we survey some results of the Randić index. We will discuss the extremal value of Randić indices of general graphs and chemical graphs.

Caporossi et al [17] gave another description of the Randić index by using linear programming.

Theorem 2.1 *([17]) Let G be a graph with n vertices. Then*

$$R(G) = \frac{n - n_0}{2} - \sum_{e \in E(G)} \omega^*(e),$$

where n_0 be the number of isolated vertices and $\omega^*(e) = \frac{1}{2}\left(\frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}}\right)^2$ for $e = uv$. Especially, if G is connected (without isolated vertices), i.e., $n_0 = 0$, the expression is

$$R(G) = \frac{n}{2} - \sum_{e \in E(G)} \omega^*(e).$$

2.1 Graphs with Extremal Randić index

Theorem 2.2 *Among trees with n vertices, the star S_n has the minimum Randić index.*

Theorem 2.3 *([87], [17]) Among trees with n vertices, the path P_n attains the maximum Randić index.*

Yu [87] was the first to prove that among trees with n vertices, the path P_n has the maximum Randić index. Caporossi et al [17] put forward an alternative proof. In the same paper also the trees with second-maximum index was determined.

Theorem 2.4 *([17]) Among trees with $n \geq 7$ vertices, the trees with degree sequence $[3, 2^{n-4}, 1^3]$ have the second-maximum Randić index.*

Theorem 2.5 *([36]) Among trees of order $n \geq 3$ with n_1 pendent vertices, if $n_1 < n-1$, the comet $CS(n, n_1)$ attains the minimum Randić index.*

In the above theorem, Hansen and Mélot [36] considered trees with a given number of pendent vertices, which is an important class of trees. Li and Zhao [57], Wu and Zhang [85] determined the second-minimum, the third-minimum values of this class of trees, respectively, while recently Zhang, Lu and Tian [89] determined the maximum values of this class of trees.

Theorem 2.6 *([57]) Let T be a tree of order $n \geq 3$ with n_1 pendent vertices. If $n_1 < n-2$ and $T \ncong CS(n, n_1)$, then*

$$R(T) \geq \sqrt{n_1} + (\sqrt{2}-2)\frac{1}{\sqrt{n_1}} + \frac{n-n_1-3}{2} + \sqrt{2}$$

and the equality holds if and only if $T \in \{T_{n-n_1+2, v_i, n_1-2} |\ 3 \leq i \leq n-n_1\}$ shown in Figure 2.1.

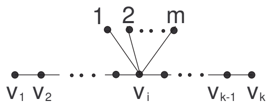

Figure 2.1 The structure of the tree $T_{k,v_i,m}$.

Theorem 2.7 *([85]) Among all trees of order n with n_1 pendent vertices, the trees obtained from a path of length $n-n_1-1$ by adding 2 pendent edges and n_1-2 pendent edges to the two ends of the path, attains the third-minimum Randić index.*

Denote a tree by $T(3,2)$ if each pendent vertex of the tree is on a pendent path with length at least 2, all the vertices but the vertices of degrees 1 and 2 are of degree 3 and the induced subgraph of the vertices with degree 3 is also a tree.

Theorem 2.8 *([89]) The tree $T(3,2)$ attains the maximum Randić index among all trees of order n with n_1 pendent vertices, where $n_1 \geq 3$ and $n \geq 3n_1 - 2$.*

Li and Zhao [57] considered the relation between the Randić index and the diameter of trees.

Theorem 2.9 *([57]) Among all trees of order n with diameter r,*
(i) for $r \geq 3$,

$$R(T) \geq \frac{n-r}{\sqrt{n-r+1}} + \frac{1}{\sqrt{2(n-r+1)}} + \frac{r-3}{2} + \frac{1}{\sqrt{2}} \ ,$$

and the equality holds if and only if $T \cong CS(n, n-r+1)$;
(ii) for $r \geq 4$ and $T \ncong CS(n, n-r+1)$,

$$R(T) \geq \frac{n-r-1}{\sqrt{n-r+1}} + \frac{\sqrt{2}}{\sqrt{2(n-r+1)}} + \frac{r-4}{2} + \frac{1}{\sqrt{2}} \ ,$$

and the equality holds if and only if $T \in \{T_{r+1,v_i,n-r-1} |\ 3 \leq i \leq r-1\}$.

Theorem 2.10 *([57]) Let T be a tree of order n and let $T \notin \{S_{n-3,3}, S_{n-2,2}, S_n\}$. Then*
(i) $R(T) \geq R(S_{n-4,4}) > R(S_{n-3,3}) > R(S_{n-2,2}) > R(S_n)$ for $n = 8, 9$ and the equality holds if and only if $T \cong S_{n-4,4}$;
(ii) $R(T) \geq R(CS(n, n-3)) > R(S_{n-3,3}) > R(S_{n-2,2}) > R(S_n)$ for $n = 6, 7$ or $n \geq 10$ and the equality holds if and only if $T \cong CS(n, n-3)$.

Gao and Lu [31] considered the unicyclic graphs with minimum Randić index.

Theorem 2.11 *([31]) The graph S_n^+ has the minimum Randić index among all unicyclic graphs of order $n \geq 3$.*

Caporossi et al [17] considered the maximum Randić values among all unicyclic, bicyclic and tricyclic graphs.

Theorem 2.12 *([17]) Among all unicyclic graphs of order n, the cycle C_n attains the maximum value, the unicyclic graphs obtained by attaching a pendent path to a vertex of a cycle, attain the second-maximum Randić index for $n \geq 5$.*

By using different methods, Bollobás et al [11] and Pavlović et al [73] independently gave the following result.

Theorem 2.13 *([11], [73]) Among all graphs of order n without isolated vertices, the star S_n attains the minimum Randić index.*

Caporossi et al [17] and Pavlović et al [73] showed

Theorem 2.14 *([17], [73]) Among all graphs of order n, regular graphs attain the maximum Randić index.*

Following Chung [20], associate with a connected graph G, a square matrix $\mathbf{C} = (c_{ij})_{n\times n}$ is defined

$$c_{i,j} = \begin{cases} 1 & \text{if } u = v \text{ and } d(u) \neq 0 \\ -\dfrac{1}{\sqrt{d(u)\,d(v)}} & \text{if the vertices } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

Denote the eigenvalues of $\mathbf{C}$ by $0 = \mu_0 \leq \mu_1 \leq \cdots \leq \mu_{n-1}$. Araujo and de la Peña [5] demonstrated the following result.

Theorem 2.15 *([5]) Let G be a simple connected graph of order n. Then*

$$\frac{1}{2}[n - \mu_{n-1}(n-\kappa)] \leq R(G) \leq \frac{1}{2}[n - \mu_1(n-\kappa)],$$

where κ is defined as

$$\kappa = \left(\sum_{i=1}^{n} \sqrt{d_i}\right)^2 \left(\sum_{i=1}^{n} d_i\right)^{-1}.$$

Moreover, $\kappa \leq n$ and $R(G) = n/2$ (and $\kappa = n$) if and only if G is regular.

There are some other results relating the Randić index to other graph parameters. For example, in [29] and [4], the authors gave the relations between the Randić index R and the maximum eigenvalue λ_1 of a graph.

Theorem 2.16 *([29]) For any connected graph G of size m,*

$$\lambda_1 \geq \frac{m}{R}.$$

Theorem 2.17 *([4]) For any connected graph G on $n \geq 3$ vertices,*

$$R + \lambda_1 \geq 2\sqrt{n-1} \quad \textit{and} \quad R \cdot \lambda_1 \geq n-1,$$

with equality for both the formulae if and only if G is the star S_n.

Theorem 2.18 *([4]) For any connected graph G on $n \geq 3$ vertices,*

$$\frac{2-n}{2} \leq R - \lambda_1 \leq \begin{cases} \dfrac{n-3+2\sqrt{2}}{2} - 2\cos(\dfrac{\pi}{n+1}) & \textit{if} \quad n \leq 9 \\ \dfrac{n-4}{2} & \textit{if} \quad n \geq 10 \end{cases}$$

The lower bound is attained if and only if G is K_n, and the upper bound is attained if and only if G is P_n for $n \leq 9$ or G is C_n for $n \geq 10$. Moreover

$$\frac{n}{2n-2} \leq \frac{R}{\lambda_1} \leq \begin{cases} \dfrac{n-3+2\sqrt{2}}{\cos(\frac{\pi}{n+1})} & \textit{if} \quad n \leq 26 \\ \dfrac{n}{4} & \textit{if} \quad n \geq 27 \end{cases}$$

The lower bound is attained if and only if G is K_n, and the upper bound is attained if and only if G is P_n for $n \leq 26$ or G is C_n for $n \geq 27$.

2.2 Chemical graphs with extremal Randić index

Gutman et al [35] characterized the chemical trees with minimum, second-minimum, third-minimum and maximum, second-maximum, third-maximum Randić indices.

Theorem 2.19 *([35]) (i) If $n = 3h + 2$ and $h \geq 1$, then among the n-vertex chemical trees, the trees without vertices of degrees 2 and 3 (that is, the trees possessing only vertices of degrees 1 and 4) have the minimum R-value, equal to $(5n - 1)/12$.*

(ii) If $n = 3h + 1$ and $h \geq 4$, then among the n-vertex chemical trees, the trees without vertices of degree 2 and with a single vertex of degree 3, adjacent to three vertices of degree 4, have the minimum R-value, equal to $(5n - 1)/12 + (3\sqrt{3} - 5)/6$.

(iii) If $n = 3h$ and $h \geq 3$, then among the n-vertex chemical trees, the trees without vertices of degree 3 and with a single vertex of degree 2, adjacent to two vertices of degree 4, have the minimum R-value, equal to $(5n - 1)/12 + (3\sqrt{3} - 4)/6$.

Theorem 2.20 *([35]) (i) If $n = 3h$ and $h \geq 7$, then among the n-vertex chemical trees, the trees without vertices of degree 2 and with two vertices of degree 3, each adjacent to three vertices of degree 4, have the second-minimum R-value, equal to $(5n - 1)/12 + (3\sqrt{3} - 5)/3$.*

(ii) If $n = 3h + 1$ and $h \geq 4$, then among the n-vertex chemical trees, the trees without vertices of degree 2 and with a single vertex of degree 3, adjacent to two vertices of degree 4 and a vertex of degree 1, have the second-minimum R-value, equal to $(5n - 1)/12 + (8\sqrt{3} - 13)/12$.

(iii) If $n = 3h + 2$ and $h \geq 5$, then among the n-vertex chemical trees, the trees with a single vertex of degree 2, adjacent to two vertices of degree 4, and a single vertex of degree 3, adjacent to three vertices of degree 4, have the second-minimum R-value, equal to $(5n - 1)/12 + (\sqrt{2} + \sqrt{3} - 3)/2$.

Theorem 2.21 *([35]) (i) If $n = 3h$ and $h \geq 7$, then among the n-vertex chemical trees, the trees without vertices of degree 2 and with two adjacent vertices of degree 3, each adjacent to two vertices of degree 4, have the third-minimum R-value, equal to $(5n - 1)/12 + (8\sqrt{3} - 13)/12$.*

(ii) If $n = 3h + 1$ and $h \geq 4$, then among the n-vertex chemical trees, the trees without vertices of degree 3 and with two vertices of degree 2, each adjacent to two vertices of degree 4, have the third-minimum R-value, equal to $(5n - 1)/12 + (3\sqrt{2} - 4)/3$.

(iii) If $n = 3h + 2$ and $h \geq 4$, then among the n-vertex chemical trees, the trees with a single vertex of degree 2, adjacent to a vertex of degree 4 and the vertex of degree 3, and a single vertex of degree 3, adjacent to two vertices of degree 4 and the vertex of degree 2, have the third-minimum R-value, equal to $(5n - 1)/12 + (3\sqrt{2} + 4\sqrt{3} + 2\sqrt{6} - 15)/12$.

Theorem 2.22 *([35]) (i) Among the n-vertex chemical trees, $n \geq 5$, the tree without vertices of degrees*

3 *and* 4 *(that is, the path) has the maximum Randić index. This maximum value is equal to* $(n-3)/2+\sqrt{2}$.

(ii) Among the n-vertex chemical trees, $n \geq 7$ *, the tree with a single vertex of degree* 3*, adjacent to three vertices of degree* 2*, and without vertices of degree* 4 *has the second-maximum Randić index. This second-maximum value is equal to* $(n-3)/2+\sqrt{2}-(4-\sqrt{2}-\sqrt{6})/2$.

(iii) Among the n-vertex chemical trees, $n \geq 7$ *, the tree with a single vertex of degree* 3*, adjacent to two vertices of degree* 2 *and one vertex of degree* 1*, and without vertices of degree* 4 *has the third-maximum Randić index. This third-maximum value is equal to* $(n-3)/2+\sqrt{2}-(9-2\sqrt{3}-2\sqrt{6})/6$.

Hansen and Mélot [36] considered the chemical trees with a given number of pendent vertices. The structure of $L_e(n, n_1)$ (n_1 is even): these trees are composed of subgraphs that are stars S_5 , and these stars are connected by paths, whose lengths can be 0.

Theorem 2.23 *([36]) Let* T *be a chemical tree of order* n *with* $n_1 \geq 3$ *pendent vertices. Then*

$$R(T) \geq \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}$$

with equality if and only if n_1 *is even and* $T \cong L_e(n, n_1)$.

Theorem 2.24 *([36]) Let* T *be a chemical tree of order* n *with* $n_1 \geq 3$ *pendent vertices. Then*

$$R(T) \leq \frac{n}{2} + n_1\left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} - \frac{7}{6}\right)$$

with equality if and only if T *is isomorphic to* $T(3,2)$.

Gutman and Miljković [34] characterized the unicyclic chemical graphs with maximum, second-maximum, third-maximum Randić indices.

Theorem 2.25 *([34]) Among unicyclic n-vertex chemical graphs,* $n \geq 3$ *, the cycle* C_n *has maximum Randić index, equal to* $n/2$.

Theorem 2.26 *([34]) Among unicyclic n-vertex chemical graphs,* $n \geq 5$ *, the graphs without vertices of degree* 4*, with a single vertex of degree* 3 *and a single vertex of degree* 1*, that are not mutually adjacent, have the second-maximum Randić index, equal to* $n/2-(4-\sqrt{2}-\sqrt{6})/2$.

Theorem 2.27 *([34]) Among unicyclic n-vertex chemical graphs,* $n \geq 5$ *, the graphs without vertices of degree* 4*, with a single vertex of degree* 3 *and a single vertex of degree* 1*, that are mutually adjacent, have the third-maximum Randić index, equal to* $n/2-(9-2\sqrt{3}-2\sqrt{6})/6$.

Gutman and Miljković [34] also characterized the (n, m)-chemical graphs with minimum, second-minimum, third-minimum Randić indices.

Theorem 2.28 *([34]) If* n *is sufficiently large, then for any value of* m , $n-1 \leq m \leq 2n$, *the following is true.*

(1) If $n+m \equiv 0 \pmod 3$, *then among* (n,m)*-chemical graphs, the graphs without vertices of degrees* 2 *and* 3 *(that is, the graphs possessing only vertices of degrees* 1 *and* 4*) have the minimum* R , *equal to* $(4n+m)/12$.

(2) If $n+m \equiv 1 \pmod 3$, *then among* (n,m)*-chemical graphs, the graphs without vertices of degree* 2 *and with a single vertex of degree* 3*, adjacent to three vertices of degree* 4*, have the minimum* R , *equal to* $(4n+m)/12 + (3\sqrt{3}-5)/6$.

(3) If $n+m \equiv 2 \pmod 3$, *then among* (n,m)*-chemical graphs, the graphs without vertices of degree* 3 *and with a single vertex of degree* 2*, adjacent to two vertices of degree* 4*, have the minimum* R , *equal to* $(4n+m)/12 + (3\sqrt{2}-4)/6$.

Theorem 2.29 *([34]) If* n *is sufficiently large, then for any value of* m , $n-1 \leq m \leq 2n$, *the following is true.*

(1) If $n+m \equiv 0 \pmod 3$, *then among* (n,m)*-chemical graphs, the graphs with a single vertex of degree* 2*, adjacent to two vertices of degree* 4*, and a single vertex of degree* 3*, adjacent to three vertices of degree* 4*, have the second-minimum* R , *equal to* $(4n+m)/12 + (\sqrt{2}+\sqrt{3}-3)/2$.

(2) If $n+m \equiv 1 \pmod 3$, *then among the* (n,m)*-chemical graphs, the graphs without vertices of degree* 2 *and with a single vertex of degree* 3*, adjacent to two vertices of degree* 4 *and a vertex of degree* 1*, have the second-minimum* R , *equal to* $(4n+m)/12 + (8\sqrt{3}-13)/12$.

(3) If $n+m \equiv 2 \pmod 3$, *then among the* (n,m)*-chemical graphs, the graphs without vertices of degree* 2 *and with two vertices of degree* 3*, each adjacent to three vertices of degree* 4*, have the second-minimum* R , *equal to* $(4n+m)/12 + (3\sqrt{3}-5)/3$.

Theorem 2.30 *([34]) If* n *is sufficiently large, then for any value of* m , $n-1 \leq m \leq 2n$, *the following is true.*

(1) If $n+m \equiv 0 \pmod 3$, *then among the* (n,m)*-chemical graphs, the graphs with a single vertex of degree* 2*, adjacent to a vertex of degree* 4 *and the vertex of degree* 3*, and a single vertex of degree* 3*, adjacent to two vertices of degree* 4 *and the vertex of degree* 2*, have the third-minimum* R , *equal to* $(4n+m)/12 + (3\sqrt{2}+4\sqrt{3}+2\sqrt{6}-15)/12$.

(2) If $n+m \equiv 1 \pmod 3$, *then among the* (n,m)*-chemical graphs, the graphs without vertices of degree* 3 *and with two vertices of degree* 2*, each adjacent to two vertices of degree* 4*, have the third-minimum* R , *equal to* $(4n+m)/12 + (3\sqrt{2}-4)/3$.

(3) If $n+m \equiv 2 \pmod 3$, *then among the* (n,m)*-chemical graphs, the graphs without vertices of*

degree 2 and with two adjacent vertices of degree 3, each adjacent to two vertices of degree 4, have the third-minimum R, equal to $(4n+m)/12+(8\sqrt{3}-13)/12$.

Gutman et al [33] determined the (n,m)-chemical graph with extremal Randić index.

Theorem 2.31 *([33]) For (n,m)-chemical graphs,*

$$L(n,m) \leq R(G) \leq U(n,m)$$

where

$$\begin{aligned} L = L(n,m) &= (4n+m)/12 && \text{if } n+m \equiv 0 (mod\ 3) \\ &= (4n+m)/12 + (3\sqrt{3}-5)/6 && \text{if } n+m \equiv 1 (mod\ 3) \\ &= (4n+m)/12 + (3\sqrt{2}-4)/6 && \text{if } n+m \equiv 2 (mod\ 3) \end{aligned}$$

$$\begin{aligned} U = U(n,m) &= (n-3)/2+\sqrt{2} && \text{if } m = n-1 \\ &= n/2 && \text{if } m = n \\ &= 1/3+(n-4)/2+4/\sqrt{6} && \text{if } m = n+1 \\ &= (3n-5)/6+2/\sqrt{6} && \text{if } m = n+k \\ &= n/2 && \text{if } m = 3n/2 \\ &= (3n-7)/6+2/\sqrt{3} && \text{if } m = (3n+1)/2\,. \end{aligned} \tag{2.1}$$

In Eq. (2.1) the parameter k assumes the values $2,3,\ldots,(n-2)/2$ if n is even, and $2,3,\ldots,(n-1)/2$ if n is odd. Note that the right–hand side expression in Eq. (2.1) is independent of k.

3 The general Randić index

In 1998, Bollobás and Erdös [11] generalized the Randić index by replacing $-\frac{1}{2}$ with any real number α,

$$R_\alpha(G) = \sum_{uv \in E} (d(u)d(v))^\alpha$$

which is called *the general Randić index*. Further, R_α for $\alpha = +1$ has been studied under the name "second Zagreb index" [7, 67].

3.1 Graphs with extremal general Randić index

Hu, Li and Yuan considered the extremal general Randić indices of trees, and characterized the extremal graphs.

Theorem 3.1 *([40]) Among all n-vertex trees, the path attains the minimum general Randić index for $\alpha > 0$, while the star attains the minimum general Randić index for $\alpha < 0$.*

A *Max (Min) tree* is a tree with the maximum (minimum) general Randić index among all trees of order n.

Theorem 3.2 *([41]) Among all n-vertex trees, the following table gives the max tree for α in different intervals.*

α	*Max Tree*
$(-\infty,-2]$	*subdivided star for $n \geq 7$, path for $n \leq 6$*
$(-2,-\frac{1}{2})$	
$[-\frac{1}{2},0)$	*path*
$(0,1]$	*star*
$(1,2)$	*star or balanced double star*
$[2,+\infty)^*$	*balanced double star for $n \geq 8$*

There is a natural task for further study along this table. As one can see, for $\alpha \in (-2,-1/2)$ the above table has one blank place. Completing this place is a challenge for the future. Clark and Gutman got some results about this [22]. Recently, Balister, Bollobás and Gerke [8] gave upper bounds of the general Randić index of trees for $\alpha < 0$. Let $\beta, \gamma > 0$ and d be a positive integer, define $c_d = c_d(\alpha,\beta,\gamma)$ inductively by

$$c_1 = -\gamma\beta,$$

and for $d \geq 2$,

$$c_d = (d-1)\max_{1\leq k<d}\{c_k + (kd)^\alpha\} - \beta. \tag{3.2}$$

Theorem 3.3 *([8]) For any $\alpha < 0$ and $\gamma > 0$, let T be a tree of order $n \geq 3$ with n_1 pendent vertices. Then,*

$$R_\alpha(T) \leq \beta_c((n-n_1) + \gamma n_1 + 1),$$

where β_c is the minimum of β satisfying (3.2) *for all $d \geq 2$.*

Theorem 3.4 *([8]) For any $\alpha < 0$ and $\gamma > 0$, let T be a tree of order n with maximum degree $\Delta > 1$. Then,*

$$R_\alpha(T) \leq \beta_\Delta((n-n_1) + \gamma n_1) + \frac{1}{\Delta-1}(\beta_\Delta + \Delta c_\Delta(\alpha,\beta_\Delta,\gamma)),$$

where β_Δ is the minimum of β satisfying (3.2) *for all $2 \leq d \leq \Delta$.*

Theorem 3.5 *([8]) For $0 < \gamma \leq 2^{-\alpha}$, there are infinitely many trees T with $R_\alpha(T) \geq \beta_c((n-n_1) + \gamma n_1 - 1)$.*

Theorem 3.6 *([8]) For $0 < \gamma \leq 2^{-\alpha}$, there are infinitely many trees T with maximum degree at most $\Delta > 1$ such that*

$$R_\alpha(T) \geq \beta_\Delta((n-n_1) + \gamma n_1 - 1),$$

where β_Δ is the minimum of β satisfying (3.2) *for all* $2 \leq d \leq \Delta$.

For $\alpha = -1$, the maximum value of R_α for trees has been completely determined, recently. At first, in 2000 Clark and Moon [24] gave the following result.

Theorem 3.7 *([24]) For a tree T of order n,* $1 \leq R_{-1}(T) \leq \frac{5n+8}{18}$.

We know that this lower bound is sharp, and the equality holds if and only if T is the star. But in [24] it was not established whether or not the upper bound is the best possible. In connection with the upper bound, Clark and Moon [24] proposed two open problems.

Problem 1: Find $K = \lim_{n\to\infty} f(n)/n$, where $f(n)$ is the maximum value of R_{-1} among all trees of order n. From above we know that $15/56 \leq K \leq 5/18$, and Clark and Moon conjectured that K is closer to the lower bound than to the upper bound.

Problem 2: Refine the upper bound for $R_{-1}(T)$ so that it becomes sharp for infinitely many values of n.

In 2002, Clark et al. [23] determined all trees with the maximum value of R_{-1} for $n \leq 20$. Hu et al [37] then determined the trees with the maximum value of R_{-1} for $21 \leq n \leq 102$. Hu, Li and Yuan [42] gave a first solution to the above two problems, however, there are gaps in their proof, found by Pavlovic and Stojanovic in [74]. Then, Pavlović, Stojanvoić and Li gave a sound proof in [75]. Recently, Pavlović, Stojanvoić and Li [76] determined the sharp upper bound for the Randić index R_{-1} among all trees of order n for every $n \geq 720$.

Theorem 3.8 *([42], [75]) For a tree of order $n \geq 103$,*

$$R_{-1}(T) \leq \frac{15n-1}{56},$$

which implies that $K = \lim_{n\to\infty} f(n)/n = 15/56$.

Theorem 3.9 *([76]) Let T_n^t be a tree of order $n \geq 720$ and $n-1 \equiv t$ (mod 7). Denote by R_{-1}^* the maximum value of the Randić index among all trees T_n^t. Then,*

$$R_{-1}^* = \begin{cases} \frac{15n-1}{56} & t=0 \\ \frac{15n-1}{56} - \frac{1}{56} + \frac{7}{4(n+5)} & t=1 \\ \frac{15n-1}{56} - \frac{3}{5}\cdot\frac{1}{56} - \frac{7}{20(n-3)} & t=2 \\ \frac{15n-1}{56} - \frac{2}{3}\cdot\frac{1}{56} + \frac{7}{6(n+3)} & t=3 \\ \frac{15n-1}{56} - \frac{6}{5}\cdot\frac{1}{56} - \frac{7}{20(n-12)} & t=4 \\ \frac{15n-1}{56} - \frac{1}{3}\cdot\frac{1}{56} + \frac{7}{12(n+1)} & t=5 \\ \frac{15n-1}{56} - \frac{29}{27}\cdot\frac{1}{56} - \frac{35}{36(n-3)} & t=6 \end{cases}$$

Liu et al [61] established a sharp lower bound of R_α, and an upper bound of R_α for $\alpha = 1$ and $-1 \le \alpha < 0$, among all trees of order n with n_1 pendent vertices, while Lu and Zhou [63] also gave a sharp lower bound for R_{-1} of trees with a given order and number of pendent vertices.

Theorem 3.10 *([61]) Let T be a tree with n vertices and n_1 pendent vertices, $3 \le n_1 \le n-2$, then*
(i) If $\alpha = 1$,

$$R_1(T) \le \begin{cases} 4n + 2n_1^2 - 6n_1 - 4 & \text{if } n \ge 2n_1 + 1 \\ (n_1+2)n - (3n_1+2) & \text{if } n \le 2n_1 \end{cases}$$

and

$$R_1(T) \ge \begin{cases} 4n - 6 & \text{if } n_1 = 3 \text{ and } n \ge 5 \\ 4n + 3n_1 - 16 & \text{if } 4 \le n_1 \le n-2 \end{cases}$$

(ii) For $-1 \le \alpha < 0$,

$$(n-n_1)4^\alpha + (n_1 + 2^\alpha - 1)n_1^\alpha + (1 - 2^{\alpha+1})2^\alpha \le R_\alpha(T) \le (n-1)4^\alpha + (1 + 3^\alpha - 2^{\alpha+1})2^\alpha \cdot n_1.$$

Lu and Zhou [63] gave the minimum, second-minimum, third-minimum and fourth-minimum value of R_{-1} among all trees of order n with n_1 pendent vertices.

Theorem 3.11 *([63]) Let T be a tree of order $n \ge 4$. If T is not the star S_n, then*

$$R_{-1}(T) \ge \frac{3}{2} - \frac{1}{2(n-2)}$$

with equality if and only if T is the comet $CS(n, n-2)$.

Theorem 3.12 *([63]) Let T be a tree of order n with $n \ge 6$. Suppose that T is neither the star S_n nor the comet $CS(n, n-2)$. Then*

$$R_{-1}(T) \ge 1 + \frac{2(n-4)}{3(n-3)}$$

with equality if and only if $T \cong S_{n-3,3}$.

Theorem 3.13 *([63]) Let T be a tree of order n, $n \ge 6$. Suppose that T is not the star S_n, the comet $CS(n, n-2)$, or $S_{n-3,3}$. Then*

$$R_{-1}(T) \ge 1 + \frac{3(n-5)}{4(n-4)}$$

with equality if and only if T is $S_{n-4,4}$, $n \ge 8$, and

$$R_{-1}(T) \ge \frac{7}{4} - \frac{1}{2(n-3)}$$

with equality if and only if T is the comet $CS(n, n-3)$, $n = 6, 7$.

Wu and Zhang [84], and Li, Wang and Zhang [52] determined the unicyclic graphs with minimum general Randić index, while Li, Shi and Xu [50] determined the unicyclic graphs with maximum general Randić index for $\alpha > 0$. In [60, 86], the authors considered the bicyclic graphs with minimum general Randić index.

Theorem 3.14 *([84], [52]) Among all unicyclic graphs with n vertices, the graphs with the minimum general Randić index are shown in the following table:*

α	*extremal unicyclic graph*
$(-\infty, -2]$	$t^{\star}_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}$ *for* $n \geq 42$
$(-2, -1)$	$t^{\star}_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}$ *or* S_n^+ *for* $n \geq 9$; S_n^+ *for* $5 \leq n \leq 8$
$[-1, 0)$	S_n^+
$(0, +\infty)$	C_n

where $t^{\star}_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}$ *is the triangle with two balanced leaf branches, i.e., a graph with a triangle as its unique cycle and the vertices not on the cycle are leaves that are adjacent to two vertices of the triangle such that the numbers of leaf vertices on the two branches are almost equal.*

Theorem 3.15 *([50]) Among all unicyclic graphs with n vertices, the graphs with the maximum general Randić index for $\alpha > 0$ are shown in the following table:*

α	$0 < \alpha < 1$	$1 < \alpha \leq 2$	$\alpha > 2$
extremal graph	S_n^+	*in* $\mathcal{G}$	*for* $n \geq 7$, $t^{\star}_{\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor}$

where $\mathcal{G}$ is a class of graphs defined as follows: $\mathcal{G}$ consists of the unicyclic graphs each of which has a triangle as its unique cycle, and the vertices not on the cycle are leaves.

Bollobás and Erdős [11] gave a sharp upper bound of R_α with $\alpha \in (0, 1]$, for graphs of size m, and a sharp lower bound of R_α with $\alpha \in [-1, 0)$, also for graphs of size m.

Theorem 3.16 *([11]) For $\alpha = 1$ and for G being a graph of size $m = |E(G)|$,*

$$R_1(G) \leq m \left(\frac{\sqrt{8m+1} - 1}{2} \right)^2 . \tag{3.3}$$

Equality holds if and only if m is of the form $m = \binom{n}{2}$ for some natural number n, and G is the union of K_n and isolated vertices.

Theorem 3.17 *([11]) For every graph G of size m,*

$$R_\alpha(G) \leq m \left(\frac{\sqrt{8m+1} - 1}{2} \right)^{2\alpha} \tag{3.4}$$

for $0 < \alpha \leq 1$ *, and*

$$R_\alpha(G) \geq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha} \tag{3.5}$$

for $-1 \leq \alpha < 0$ *. Furthermore, in Eq.*(3.4) *or Eq.*(3.5) *equality holds for a particular value of* α *if and only if* G *consists of a complete graph and some isolated vertices, in which case equality in Eq.*(3.4) *and Eq.*(3.5) *is satisfied for every* $\alpha, -1 \leq \alpha < 1, \alpha \neq 0$.

Eventually, Bollobás, Erdős and Sarkar [12] determined the maximum value for $\alpha > 0$, and the minimum value for $\alpha < 0$.

Theorem 3.18 *([12]) Let* k *and* r *be positive integers such that* $0 < r \leq k$ *. Then all graphs* G *of size* $m = \binom{k}{2} + r$ *and minimum degree at least 1, satisfy* $R_1(G) \leq R_1(G_m)$ *, where* G_m *is the graph consisting of the complete graph of order* k *together with an additional vertex joined to* r *vertices of the complete graph. In addition,*

$$R(m) = R_1(G_m) = \binom{r}{2}k^2 + \binom{k-r}{2}(k-1)^2 + rk(k-r)(k-1) + r^2k\ .$$

Theorem 3.19 *([12]) Let* G *be a graph of size* m *with no isolated vertices. Then*

$$R_\alpha(G) \leq m^{1-\alpha}\, R(m)^\alpha$$

for $0 \leq \alpha < 1$ *. For* $\alpha \neq 0$ *, equality holds if and only if* G *is the complete graph.*

Theorem 3.20 *([12]) For* $\alpha > 1$ *,*

$$R_\alpha(G) \leq \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}}\, m^{2\alpha} + O(m^{2\alpha-((\alpha-1)/(\alpha+1))})\ .$$

In particular,

$$R_\alpha(G) \sim \frac{(2\alpha-2)^{2\alpha-2}}{2(2\alpha-1)^{2\alpha-1}}\, m^{2\alpha}\ ,$$

provided $1/(2\alpha-2)$ *is an integer.*

Theorem 3.21 *([12]) For fixed* $\alpha \geq 2$ *and* $m \to \infty$ *,*

$$R_\alpha(G) = \left(\frac{m}{2}\right)^{2\alpha} + O\left(m^{2\alpha-((\alpha-1)/(\alpha+1))}\right)\ .$$

Theorem 3.22 *([12]) Let* G *be a graph of size* m *with no isolated vertices. Then for* $\alpha < 0$ *,*

$$R_\alpha(G) \geq m^{1-\alpha} R(m)^\alpha$$

with equality if and only if G *is complete.*

Li and Yang [55] obtained lower and upper bounds for the general Randić index of n-vertex graphs.

Theorem 3.23 *([55]) Let G be a graph of order n, containing no isolated vertices. Then the following results hold.*

α	*min*	*max*
$[0,\infty)$	$\frac{n}{2}$ *(n even) and* $\frac{n-3}{2}+2^{1+\alpha}$ *(n odd)*	$\frac{n(n-1)^{1+2\alpha}}{2}$
$(-\frac{1}{2},0)$	$\min\{(n-1)^{1+\alpha}$, $\frac{n}{2}$ *(n even) and* $\frac{n-3}{2}+2^{1+\alpha}$ *(n odd)*$\}$	$\frac{n(n-1)^{1+2\alpha}}{2}$
$-\frac{1}{2}$	$\sqrt{n-1}$	$\frac{n}{2}$
$(-1,-\frac{1}{2})$		$\frac{n}{2}$ *(n even)*
-1	$\frac{n}{2(n-1)}$	$\lfloor\frac{n}{2}\rfloor$
$(-\infty,-1)$	$\frac{n(n-1)^{1+2\alpha}}{2}$	$\frac{n}{2}$ *(n even) and* $\frac{n-3}{2}+2^{1+\alpha}$ *(n odd)*

Actually, the authors of [55] did not realize that their Lemma 4.8 holds for $\alpha \leq -\frac{1}{2}$, instead of -1. Therefore, the maximum value of R_α is totally determined: when $-\infty < \alpha \leq -\frac{1}{2}$, $maxR_\alpha = \frac{n}{2}$ (n even) and $\frac{n-3}{2}+2^{1+\alpha}$ (n odd); when $-\frac{1}{2} < \alpha < +\infty$, $maxR_\alpha = \frac{n(n-1)^{1+2\alpha}}{2}$. But, the unsolved cases for the minimum value are still open.

3.2 Chemical graphs with extremal general Randić index

Li and Yang [54] gave the sharp lower and upper bounds for R_{-1} among all chemical trees.

Theorem 3.24 *([54]) Let T be a chemical tree of order n. Then*

$$R_{-1}(T) \geq \begin{cases} 1 & \text{if } n \leq 5 \\ 11/8 & \text{if } n = 6 \\ 3/2 & \text{if } n = 7 \\ 2 & \text{if } n = 10 \\ (3n+1)/16 & \text{for other values of } n\ . \end{cases}$$

Theorem 3.25 *([54]) Let T be a chemical tree of order n, $n > 6$. Then*

$$R_{-1}(T) \leq \max\{F_1(n)\,,\, F_2(n)\,,\, F_3(n)\}$$

where

$$F_1(n) = \begin{cases} \dfrac{3n+1}{16} + \dfrac{1}{144}\dfrac{31n+53}{3} & if\ n = 1\ mod\ 3 \\[2ex] \dfrac{3n+1}{16} + \dfrac{1}{144}\left(\dfrac{31n+22}{3}+9\right) & if\ n = 2\ mod\ 3 \\[2ex] \dfrac{3n+1}{16} + \dfrac{1}{144}\left(\dfrac{31n-9}{3}+18\right) & if\ n = 0\ mod\ 3 \end{cases}$$

$$F_2(n) = \frac{3n+1}{16} + \frac{1}{144} \max\{11n - N_4 - 2k + 10\ ,\ k = 0, 1, 2\}$$

with N_4 *being the minimum integer solution of* n_4 *of the following system:*

$$\begin{cases} n_3 + 2n_4 + 2 = n_1 \\ 2n_1 + n_3 + n_4 = n - k \\ n_3 \leq 2n_4 + 2 \end{cases}$$

and

$$F_3(n) = \frac{3n+1}{16} + \frac{1}{144} \max\{4n + 19N_1 + 5k + 4\ ,\ k = 0, 1, 2\}$$

with N_1 *being the maximum integer solution for* n_1 *of the following system:*

$$\begin{cases} n_3 + 2n_4 + 2 = n_1 \\ 2n_1 + n_3 + n_4 = n - k \\ n_3 \geq 2n_4 + 2 \\ n_4 \geq 1\ . \end{cases}$$

Rautenbach [82], and Li and Yang [54] independently determined the best possible upper bound for R_{-1} of trees with maximum degree 3.

Theorem 3.26 *([82], [54]) Let* T *be a tree of order* n *and maximum degree* 3. *Then*

$$R_{-1}(T) \leq \begin{cases} 0 & if\ n = 1 \\ 1 & if\ n = 2 \\ (n+1)/4 & if\ 3 \leq n \leq 9 \\ 7n/27 + 5/27 & if\ n \geq 10\ and\ n \equiv\ 1\ mod\ 3 \\ 7n/27 + 19/108 & if\ n \geq 11\ and\ n \equiv\ 2\ mod\ 3 \\ 7n/27 + 1/6 & if\ n \geq 12\ and\ n \equiv\ 0\ mod\ 3\ . \end{cases}$$

Li and Zheng [59] determined the chemical trees with minimum and maximum R_α-value for $\alpha > 0$. For any integer $n \geq 2$, define an integer sequence $d(n)$ of length n as follows: Let $n - 2 = 3p + q$, where $p \geq 0$ and $0 \leq q < 3$ are both integers, then

$$d(n) = \underbrace{4, 4, \ldots, 4}_{p}, q+1, \underbrace{1, 1, \ldots, 1}_{n-p-1}.$$

Denote the subgraph of a tree T, induced by the non-leaf vertices by $C(T)$. Evidently, $C(T)$ is also a tree. Let $\mathcal{D}(n)$ be the set of such trees T satisfying the conditions that the degree sequence of T is $d(n)$, and if $q \neq 0$ then the vertex of degree $q+1$ in T is a leaf of $C(T)$.

Theorem 3.27 *([59]) Among all chemical trees with* $n \geq 5$ *vertices,* P_n *is the unique one with minimum general Randić index* R_α *for* $\alpha > 0$ *and the extremal value is* $(n-3)4^\alpha + 2^{\alpha+1}$.

Theorem 3.28 *([59]) Among all chemical trees with n vertices, the extremal chemical trees with maximum general Randić index R_α are given in the following table:*

n	α	*Extremal chemical trees*	*Maximum value of* R_α
$n=4$	$0<\alpha<\alpha_0$	S_4	$3\times 3^\alpha$
	$\alpha=\alpha_0$	S_4 *and* P_4	$3\times 3^\alpha$
	$\alpha>\alpha_0$	P_4	$4^\alpha+2\times 2^\alpha$
$n=5$	$0<\alpha<\alpha_0'$	S_5	$4\times 4^\alpha$
	$\alpha=\alpha_0'$	S_5 *and* $S_{2,3}$	$4\times 4^\alpha$
	$\alpha>\alpha_0'$	$S_{2,3}$	$6^\alpha+2\times 3^\alpha+2^\alpha$
$n=6$	$0<\alpha<\alpha_0''$	$S_{2,4}$	$8^\alpha+3\times 4^\alpha+2^\alpha$
	$\alpha=\alpha_0''$	$S_{2,4}$ *and* $S_{3,3}$	$9^\alpha+4\times 3^\alpha$
	$\alpha>\alpha_0''$	$S_{3,3}$	$9^\alpha+4\times 3^\alpha$
$7\le n\le 11$	$\alpha>0$	$P^{d(n)}$ *is the unique extremal chemical tree*	$(p-1)16^\alpha+4^\alpha(q+1)^\alpha+q(q+1)^\alpha+(n-p-q-1)4^\alpha$
$n>11$	$\alpha>0$	*There are several extremal chemical trees; all elements of* $\mathcal{D}(n)$ *are extremal*	$(p-1)16^\alpha+4^\alpha(q+1)^\alpha+q(q+1)^\alpha+(n-p-q-1)4^\alpha$

p and q are defined above via the integer sequence $d(n)$. α_0, α_0', and α_0'' are, respectively, the unique positive roots of the equations $4^x-3\cdot3^x+2\cdot2^x=0$, $6^x-4\cdot4^x+2\cdot3^x+2^x=0$, and $9^x-8^x-3\cdot4^x+4\cdot3^x-2^x=0$.

Li, Shi and Zhong [51] considered the chemical trees with a given order and number of pendent vertices and determined the extremal graph with the minimum general Randić index for arbitrary α among these kind of trees.

Theorem 3.29 *([51]) For $\alpha\le -1$ and $3\le n_1\le n-2$, let T be a chemical tree of order n with n_1 pendent vertices. Then*

$$R_\alpha(T)\ge n\cdot 4^\alpha+\frac{1}{3}(8^\alpha+3\cdot 6^\alpha-4^{\alpha+1})n_1+5\cdot 4^\alpha-6^{\alpha+1}.$$

Theorem 3.30 *([51]) Let $3\le n_1\le n-2$ and $\alpha\ge 1$. If T is a chemical tree of order n with n_1 pendent vertices, then*

$$R_\alpha(T)\ge\begin{cases} n\cdot 4^\alpha+6^\alpha-5\cdot 4^\alpha+2\cdot 3^\alpha+2^\alpha & if\ n_1=3\\ \varphi(n,n_1) & if\ 4\le n_1\le n-2\end{cases}$$

Theorem 3.31 *([51]) Let T be a chemical tree of order n with $n_1\ge 5$ pendent vertices. Then for $-1<\alpha<0$,*

$$R_\alpha(T)\ge n\cdot 4^\alpha+(8^\alpha-4^\alpha)n_1+3\cdot 4^\alpha$$

with equality if and only if n_1 is even and $T\cong L_e(n,n_1)$.

Theorem 3.32 *([51]) Let T be a chemical tree of order n with $n_1 \geq 5$ pendent vertices. Then for $0 < \alpha < 1$,*

$$R_\alpha(T) \geq n \cdot 4^\alpha + (3^\alpha + 2 \cdot 6^\alpha - 3 \cdot 4^\alpha)n_1 + 5 \cdot 4^\alpha - 6^{\alpha+1}.$$

Li, Wang and Wei [53] gave the lower and upper bounds for R_α among all (n,m)-chemical graphs.

Theorem 3.33 *([53]) The general Randić index $R_\alpha(G)$ of (n,m)-chemical graphs has the following lower and upper bounds:*

1. *For $-\infty < \alpha \leq \alpha_1$ and $\alpha_2 < \alpha < \infty$,*
$$R(G) \leq (2^\alpha - 16^\alpha)n + \left(\frac{3}{2} \cdot 16^\alpha - 2^{\alpha-1}\right) m;$$
2. *For $\alpha_1 < \alpha \leq 0$,*
$$R(G) \leq (2^{\alpha+1} - 2 \cdot 4^\alpha)n + (3 \cdot 4^\alpha - 2^{\alpha+1})m;$$
3. *For $0 < \alpha \leq \alpha_2$,*
$$R(G) \leq (2^{\alpha+2} - 4^{\alpha+1})n + (6 \cdot 4^\alpha - 5 \cdot 2^\alpha)m;$$
4. *For $-\infty < \alpha < \alpha_3$ and $0 \leq \alpha < \infty$,*
$$R(G) \geq (12^{\alpha+1} - 12 \cdot 16^\alpha)n + (7 \cdot 16^\alpha - 6 \cdot 12^\alpha)m;$$
5. *For $\alpha_3 \leq \alpha < 0$,*
$$R(G) \geq \frac{1}{3}\left[(4^{\alpha+1} - 4 \cdot 16^\alpha)n + (5 \cdot 16^\alpha - 2 \cdot 4^\alpha)m\right],$$

where α_1, α_2 and α_3 are the non-zero roots of the equations $2^\alpha + 16^\alpha - 2 \cdot 4^\alpha = 0$, $3 \cdot 2^\alpha + 16^\alpha - 4 \cdot 4^\alpha = 0$ and $9 \cdot 12^\alpha - 8 \cdot 16^\alpha - 4^\alpha = 0$, respectively.

4 The (general) zeroth-order Randić index

The zeroth-order Randić index, defined by Kier and Hall [46], is ${}^0R = \sum_{u \in V(G)} d(u)^{-\frac{1}{2}}$. Later Li and Zheng in [58] defined the zeroth-order general Randić index ${}^0R_\alpha(G)$ of a graph G as

$${}^0R_\alpha(G) = \sum_{v \in V(G)} d(u)^\alpha$$

for general real number α. It should be noted that the same quantity is sometimes referred to as the "general first Zagreb index" [44, 45], in view of the fact that $\sum_u (d_u)^2$ is sometimes called "the first Zagreb index" [7, 67]. In fact, there are many researches on this index, which has many useful applications in

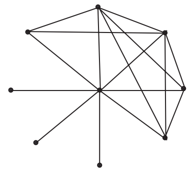

Figure 4.1 The structure of graph L^*.

information theory and network reliability, and received considerable attentions also in graph theory (see [1, 10, 65, 77, 43, 21, 9, 25, 14, 30, 66]).

Pavlović [69] determined the (n, m)-graph with the maximum zeroth-order Randić index. We first specify the structure of the graph L^* with n vertices and m edges. For $m = n - 1$, it is the star S_n. For $m \geq n$ it is constructed as follows: Add a new edge between two vertices of degree 1 and get a clique of 3 vertices. Choose a pendent vertex and connect it to the vertices of the clique, until a clique of 4 vertices is obtained. Choose another pendent vertex and connect it to the vertices of the clique, until a clique of 5 vertices is obtained, etc. Continue the addition of edges until the total number of edges becomes m. An illustrative example is shown in Figure 4.

Theorem 4.1 *([69]) Let $G(n, m)$ be a connected graph without loops and multiple edges with n vertices and m edges. If $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$, then*

$$^0R(G(n,m)) \leq {}^0R(L^*) = \frac{n-k-1}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} + \frac{1}{\sqrt{n-1}}\ .$$

Li and Zhao [56] determined the trees with the first three minimum and maximum zeroth-order general Randić index.

Theorem 4.2 *([56]) Among all trees with n vertices, the trees with extremal zeroth-order general Randić index are listed in the following table:*

	$\alpha < 0$ *or* $\alpha > 1$	$0 < \alpha < 1$
minimum	*the path* P_n	*the star* S_n
second minimum	*trees with* $[3, 2^{n-4}, 1^3]$	*the double star* $S_{n-2,2}$
third minimum	*trees with* $[3^2, 2^{n-6}, 1^4]$	*the double star* $S_{n-3,3}$
maximum	*the star* S_n	*the path* P_n
second maximum	*the double star* $S_{n-2,2}$	*trees with* $[3, 2^{n-4}, 1^3]$
third maximum	*the double star* $S_{n-3,3}$	*trees with* $[3^2, 2^{n-6}, 1^4]$

Zhang and Zhang [91] determined the unicyclic graphs with the first three minimum and maximum zeroth-order general Randić index. Zhang, Wang, Cheng [90] determined the bicyclic graphs with the first three minimum and maximum zeroth-order general Randić index. Guo, Zhang and Cheng [32] determined the minimum and maximum zeroth-order general Randić index values of bipartite graphs with a given number of vertices and edges for $\alpha = 2$.

Theorem 4.3 *([91]) Among all unicyclic graphs with n vertices, the trees with extremal zeroth-order general Randić index are listed in the following table:*

	$\alpha < 0$ *or* $\alpha > 1$	$0 < \alpha < 1$
minimum	*the cycle* C_n	*the graph* S_n^+
second minimum	*graphs with* $[3, 2^{n-2}, 1]$	*graphs with* $[n-2, 3, 2, 1^{n-3}]$
third minimum	*graphs with* $[3^2, 2^{n-4}, 1^2]$	**
maximum	*the star* S_n^+	*the cycle* C_n
second maximum	*graphs with* $[n-2, 3, 2, 1^{n-3}]$	*graphs with* $[3, 2^{n-2}, 1]$
third maximum	**	*graphs with* $[3^2, 2^{n-4}, 1^2]$

*where "**" denotes unicyclic graphs with degree sequence $[n-3, 3, 2, 1^{n-3}]$ or $[n-2, 2^3, 1^{n-4}]$.*

Hu, Li, Shi and Xu [38] obtained some bounds on connected (n, m)-graphs with the minimum and maximum zeroth-order general Randić index. A graph G is *nearly regular* if $|\Delta(G) - \delta(G)| \leq 1$. Note that, for given order n and size m, the nearly regular graphs, denoted by $C^*(n, m)$, may not be unique, which form a class of graphs. However, they have the same ${}^0R_\alpha$-value. For convenience, we introduce a family of graphs, denoted by $\mathcal{F}$, as described in [12]. Let $N < n$ be a positive integer, and $d_1, d_2, \ldots, d_N$ be a sequence of positive integers. The graph $G(d_1, d_2, \ldots, d_N)$ has vertex set defined as the disjoint union

$$\bigcup_{0 \leq j \leq N} I_j,$$

where $I_0 = \{v_1, v_2, \ldots, v_N\}$, $|I_j| = d_j - d_{j+1}$ for $1 \leq j \leq N-1$ and $|I_N| = d_N - (N-1)$. For $1 \leq j \leq N$ we arrange that

$$N(v_j) = (I_0 - \{v_j\}) \cup \left(\bigcup_{j \leq k \leq N} I_k \right) \qquad \text{and} \qquad E\left(G\left[\bigcup_{0 \leq j \leq N} I_j \right] \right) = \emptyset,$$

so that $d(v_j) = d_j$ for all j and $e((d_1, d_2, \ldots, d_N)) = \sum_{i=1}^{N} d_i - \binom{N}{2}$. We will, of course, always have $d_1 \geq d_2 \geq \cdots \geq d_N \geq N-1$. Each of these graphs of order n, say, is the unique realization of a sequence corresponding to a vertex of the polytope K^n of degree sequences in E^n. Let $\mathcal{F}$ denote the family of graphs of the form $G(d_1, d_2, \ldots, d_N)$ for $d_1 \geq d_2 \geq \cdots \geq d_N \geq N-1$. From the definition of $\mathcal{F}$, we have $L^* \in \mathcal{F}$.

Theorem 4.4 *([38]) For $\alpha < 0$ or $\alpha > 1$, a minimum (n, m)-graph G is a nearly regular graph C^*; whereas for $0 < \alpha < 1$, a maximum (n, m)-graph G is a nearly regular graph C^*. The extremal value is ${}^0R_\alpha(C^*) = (2m - ns)(s+1)^\alpha + [n(s+1) - 2m]s^\alpha$, where s denotes the minimum degree of C^*.*

Theorem 4.5 *([38]) For $0 < \alpha < 1$, if G be a minimum (n,m)-graph, then $G \in \mathcal{F}$; whereas for $\alpha < 0$ and $\alpha > 1$, if G be a maximum (n,m)-graph, then $G \in \mathcal{F}$.*

Theorem 4.6 *([38]) Let $G(n,m)$ be a simple connected graph with n vertices and m edges. If $m = n + k(k-3)/2 + p$, where $2 \le k \le n-1$ and $0 \le p \le k-2$, then for $\alpha \le -1$,*

$$\begin{aligned}&{}^0R_\alpha(G(n,m)) \le {}^0R_\alpha(L^*)\\ &= (n-k-1)\cdot 1^\alpha + (p+1)^\alpha + (k-p-1)(k-1)^\alpha + p \cdot k^\alpha + (n-1)^\alpha.\end{aligned}$$

Li and Zhao [56] determined the chemical trees with the minimum, second-minimum and maximum, second-maximum zeroth-order general Randić index.

Theorem 4.7 *([56]) Let T be an n-vertex chemical tree. Then, for $\alpha < 0$ or $\alpha > 1$, and $n-2 = 3a+i$, $i = 0,1,2$,*

(i) ${}^0R_\alpha(T)$ attains the maximum value if and only if $D(T) = [4^a, i+1, 1^{n-a-1}]$;

(ii) ${}^0R_\alpha(T)$ attains the second-maximum value if and only if $D(T) = [4^{a-1}, 3, 2, 1^{n-a-1}]$ for $i = 0$, $D(T) = [4^{a-1}, 3^2, 1^{n-a-1}]$ for $i = 1$, and $D(T) = [4^a, 2^2, 1^{n-a-2}]$ for $i = 2$.

Theorem 4.8 *([56]) Let T be an n-vertex chemical tree. Then, for $0 < \alpha < 1$, and $n-2 = 3a+i$, $i = 0,1,2$,*

(i) ${}^0R_\alpha(T)$ is minimum if and only if $D(T) = [4^a, i+1, 1^{n-a-1}]$;

(ii) ${}^0R_\alpha(T)$ is second-minimum if and only if $D(T) = [4^{a-1}, 3, 2, 1^{n-a-1}]$ for $i = 1$, $D(T) = [4^{a-1}, 3^2, 1^{n-a-1}]$ for $i = 2$ and $D(T) = [4^a, 2^2, 1^{n-a-2}]$ for $i = 3$.

Hu, Li, Shi, Xu and Gutman [39] determined the (n,m)-chemical graphs with the minimum and maximum zeroth-order general Randić index.

Theorem 4.9 *([39]) For $\alpha < 0$ or $\alpha > 1$, the nearly regular graph C^* has the minimum zeroth-order general Randić index among all chemical (n,m)-graphs, whereas for $0 < \alpha < 1$, C^* has the maximum zeroth-order general Randić index among all chemical (n,m)-graphs. Moreover,*

$${}^0R_\alpha(C^*) = \begin{cases} 2 + 2^\alpha(n-2) & \text{if} \quad m = n-1 \\ 2^\alpha(3n-2m) + 3^\alpha(2m-2n) & \text{if} \quad n \le m \le \lfloor 3n/2 \rfloor \\ 3^\alpha(4n-2m) + 4^\alpha(2m-3n) & \text{if} \quad \lfloor 3n/2 \rfloor < m \le 2n\ . \end{cases}$$

Theorem 4.10 *([39]) Let G^* be a chemical (n,m)-graph with at most one vertex of degree 2 or 3. If one of the following conditions holds:*

(I) $m = n-1$;

(II) $m \geq n \geq 6$, *for* $n = 6$, $m \geq 10$, *and for* $n = 7$, $m \neq 8$,

then for $\alpha < 0$ *or* $\alpha > 1$, G^* *has the maximum zeroth-order general Randić index among all chemical* (n, m)*-graphs, whereas for* $0 < \alpha < 1$, *the same graph has the minimum zeroth-order general Randić index among all chemical* (n, m)*-graphs. Moreover,*

$$^0R_\alpha(G^*) = \begin{cases} (4n-2m)/3 + 4^\alpha(2m-n)/3 & \text{if } \ 2m-n \equiv 0 \ (mod\ 3) \\ (4n-2m-2)/3 + 2^\alpha + 4^\alpha(2m-n-1)/3 & \text{if } \ 2m-n \equiv 1 \ (mod\ 3) \\ (4n-2m-1)/3 + 3^\alpha + 4^\alpha(2m-n-2)/3 & \text{if } \ 2m-n \equiv 2 \ (mod\ 3). \end{cases}$$

5 The Higher-order Randić index

For $m \geq 1$, one defines the m-Randić index (or m-th order Randić index) [45] as

$$^mR(G) = \sum_{i_1 i_2 \dots i_{m+1}} \frac{1}{\sqrt{d_{i_1} d_{i_2} \cdots d_{i_{m+1}}}}$$

where the summation runs over all trails $i_1 i_2 \dots i_{m+1}$ of length m, contained in G. Note that in a trail an edge appear exactly once, but a vertex can appear more than once. Some people also defines this index on "paths", instead of "trails". But then the meaning is different.

So far very few results have been obtained on this graph invariant, see [5, 47, 78, 79, 83, 88]. We list the following two results as examples. Araujo and de la Peña [5] found an upper bound for $^mR(G)$, where they said that the definition of $^mR(G)$ is in terms of paths, but actually their result holds only for trails.

Theorem 5.1 *([5]) Let* G *be a simple graph of order* n, Δ *the maximum degree of* G, *and* $\Xi = (\Delta - 1)/\sqrt{\Delta}$. *Then*

$$^mR(G) \leq \frac{1}{2}\left[n^{(m)}(G) + c^{(m)}(G)\right] \Xi^{m-1}$$

where $n^{(m)}(G)$ *is the number of vertices* i *in* G *such that there is at least one trail of length* m *starting at* i, *and* $c^{(m)}(G)$ *counts those vertices* i *which accept a trail of length* m *from* i *to* i.

We define the *weighted adjacency matrix* of a graph G of order n as the $n \times n$ matrix $\mathcal{A}$ whose (i, j)-entry is

$$a_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i d_j}} & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

Denote the eigenvalues of $\mathcal{A}$ by $1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. In [83], the authors gave the following result.

Theorem 5.2 *([83]) Let* G *be a simple, connected, and non-regular graph of order* n *and size* m. *Then*

$$^2R(G) \geq \left(\frac{(^1R(G) - \phi)^2}{n - \phi} + \phi - \tau\right)\frac{\sqrt{\delta}}{2},$$

where $\phi = \left(\sum\limits_{i=1}^n \sqrt{d_i}\right)^2 /(2m)$ *and* $\tau = \sum\limits_{i=1}^n \lambda_i^2$.

6 Some conjectures and open problems

Bollobás and Erdös [11] proved that among all graphs of order n with $\delta(G) \geq 1$, the star S_n attains the minimum Randić index $\sqrt{n-1}$. Fajtlowicz [28] mentioned that Bollobás and Erdös asked for the minimum value of the Randić index for graphs G with given minimum degree $\delta(G)$. Delorme, Favaron and Rautenbach [26] gave an answer of $k = 2$ and proposed the following conjecture.

Conjecture 6.1 *([26]) Let $G = (V, E)$ be a graph of order n with $\delta(G) \geq k$. Then*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1} ,$$

with equality if and only if $G = K^*_{k,n-k}$, where $K^*_{k,n-k}$ is a graph obtained from a complete bipartite graph $G = K_{k,n-k}$ by joining each pair of vertices in the part with k vertices by a new edge.

In [3] Aouchiche and Hansen found examples showing that the conjecture is not true, and gave a modified form. In [72] Pavlović and Divnićthe introduced a new approach based on quadratic programming and showed that the conjecture is true for $n_k \geq n-k$ $(k \leq n/2)$, and also true for $1 \leq n_k \leq n-k-1$ and $n_{n-1} = k$, where n_i denotes the number of the vertices of degree i. Li and Shi [49] showed that

Theorem 6.2 *([49]) (i) for $k = 3$, the conjecture is true;*
(ii) for $k \geq 4$, if $n \geq \frac{3}{2}k^3$ or $k \leq \sqrt[3]{\frac{2n}{3}}$, the conjecture is true.
(iii) the conjecture is true for all chemical graphs.

Delorme et al [26] claimed a weaker result: if $G = (V, E)$ is a triangle-free graph of order n with $\delta(G) \geq k \geq 1$, then

$$R(G) \geq \sqrt{k(n-k)}$$

with equality if and only if $G = K_{k,n-k}$. However, Liu et al [62] found a mistake in their proof, and only proved the case for $k = 2$. We refer [71] for more results along this line.

Conjecture 6.3 *([27]) For all connected graphs G, $r(G) \leq 1 + R(G)$, where $r(G)$ denotes the radius of G.*

Caporossi and Hansen [18] proposed a stronger conjecture.

Conjecture 6.4 *([18]) For all connected graphs G except even paths, $r(G) \leq R(G)$. They also proved that for all trees T , $R(T) - r(T) \geq \sqrt{2} - 3/2$, with equality if and only if $T \cong P_n$, where n is even.*

Conjecture 6.5 *([27]) For all connected graphs G , $R(G) \geq \bar{l}(G)$, i.e., $\bar{l}(G)$ is the average distance between the vertices of G.*

The following conjecture was given by Caporossi and Hansen [18], which generalizes Conjecture 6.5.

Conjecture 6.6 *([18]) For all connected graphs G of order n,*

$$R(G) - \bar{l}(G) \geq \sqrt{n-1} + \frac{2}{n} - 2$$

and the bound is sharp for all $n \geq 1$.

Conjecture 6.7 *([18]) For any connected graph of order $n \geq 2$ with chromatic number $\chi(G)$ and Randić index $R(G)$,*

$$R(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}\left(\sqrt{\chi(G)-1} + n - \chi(G)\right).$$

Moreover, the bound is sharp for all n and $2 \leq \chi(G) \leq n$.

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