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Extremal Chemical Trees with Minimum or Maximum General Randić Index *

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Abstract

A tree is called chemical if no vertex of it has a degree greater than four. The general Randić index $R_\alpha(G)$ for a graph G is defined as $\sum_{(uv)}(d_u d_v)^\alpha$, where uv is an edge of G, $\alpha \in \mathbb{R}$ and $\alpha \neq 0$. In this paper, we completely characterize the structures of chemical trees with the minimum or maximum general Randić index R_α for $\alpha > 0$.

1 Introduction

One of the most active fields of research in contemporary chemical graph theory is the study of topological indices, or graph invariants, that can be used for describing and predicting physicochemical and pharmacologic properties of organic compounds. Since 1947, when H. Wiener [14] conceived the first molecular graph-based structure descriptor, eventually named the "Wiener index", hundreds topological indices have been considered in the mathematical and/or chemical literature [1, 5, 12, 13].

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The only topological index to which two books [8, 9] are devoted is the *connectivity index*, also called *Randić index.* It was designed in 1975 to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It was demonstrated that the Randić index is well correlated with a variety of physico-chemical properties of alkanes, such as boiling point, enthalpy of formation, surface area and solubility in water.

Definition 1.1 *Let uv be an edge connecting the vertices u and v. Then the connectivity index of a graph G, also called the Randić index, is defined as*

$$R(G) = \sum_{uv} \frac{1}{\sqrt{d_u d_v}},$$

where d_u and d_v stand for the degrees of the vertices u and v, respectively, and the summation goes over all edges uv of G.

B. Bollobás and P. Erdös [3] generalized the Randić index by replacing $-\frac{1}{2}$ with any real number $\alpha \neq 0$, called the *general Randić index.*

$$R_\alpha(G) = \sum_{uv} (d_u d_v)^\alpha. \qquad (1)$$

Trees are connected graphs that do not contain any cycle. The graphical representation of the carbon-atom skeleton of an alkane is usually called a chemical tree. Hence, a *chemical tree* is a tree in which no vertex has a degree greater than four.

In [6] and [7] the authors discussed the problem of finding the extremal trees with minimum or maximum general Randić index R_α among all trees with n vertices. However, to determine the extremal chemical trees with minimum or maximum general Randić index R_α are of much more difficulty.

In [10] the authors got upper and lower bounds for the Rnadić index of chemical (n, m)-graphs, but they could not give the extremal chemical such graphs. The structures of extremal chemical trees with minimum Randić index R (Definition 1.1) was completely characterized [4]. This paper focuses on the extremal chemical trees with minimum or maximum general Randić index R_α defined by (1).

2 Main results

In [6] the authors proved that for $\alpha > 0$, among all trees with n ($n \geq 5$) vertices, the path P_n is the unique tree with minimum general Randić index R_α. Since P_n is a chemical tree, the following theorem is immediate.

Theorem 2.1 *Among all chemical trees with n ($n \geq 5$) vertices, P_n is the unique one with minimum general Randić index R_α for $\alpha > 0$ and the extremal value is $(n-3)4^\alpha + 2^{\alpha+1}$.*

When dealing with the problem of determining the chemical trees with maximum general Randić index R_α for $\alpha > 0$, one can find that the situation becomes much more complicated. However, we completely solve the problem and the result is Theorem 2.4. For $\alpha < 0$, the extremal problem becomes extremally difficult. For α at some specific points, say $-\frac{1}{2}$ or -1, some results are known, see the Concluding remarks.

Let us introduce some definitions and notations first. For other terminology not defined here, please refer to [2].

Denote by S_n the star with n vertices, and by $S_{m,n}$ the double star which has only two non-leaf vertices whose degrees are m and n, respectively.

Definition 2.2 *For any integer $n \geq 2$, we can 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*

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

Denote the induced subgraph by the non-leaf vertices of a tree T by $C(T)$. Obviously, $C(T)$ is a tree, too.

Definition 2.3 *Let $\mathcal{D}(n)$ be the set of such trees T satisfying the following two conditions:*

1. *The degree sequence of T is $d(n)$.*

2. *If $q \neq 0$, then the vertex of degree $q+1$ in T is a leaf of $C(T)$.*

Let us denote by $P^{d(n)}$ the unique element T^* in $\mathcal{D}(n)$ such that $C(T^*)$ is a path.

We discuss the problem for $n \geq 4$ in the following. For $n = 1, 2$ or 3, each is a trivial case, since each case has only one (chemical) tree.

Theorem 2.4 *Among all chemical trees with n vertices, the extremal chemical trees with maximum general Randić index R_α are given in the following diagram.*

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* $S_{3,3}$	$9^\alpha + 4 \times 3^\alpha$
	$\alpha > \alpha_0''$	$S_{3,3}$	$9^\alpha + 4 \times 3^\alpha$
$7 \leq n \leq 11$	$\alpha > 0$	$P^{d(n)}$ *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 more than one extremal chemical trees. All the elements in $\mathcal{D}(n)$ are extremal ones.*	$(p-1)16^\alpha + 4^\alpha(q+1)^\alpha + q(q+1)^\alpha + (n-p-q-1)4^\alpha$

where p, q are defined by Definition 2.2 and α_0, α_0' and α_0'' are, respectively, the positive roots of the equations $4^x - 3 \times 3^x + 2 \times 2^x = 0$, $6^x - 4 \times 4^x + 2 \times 3^x + 2^x = 0$ and $9^x - 8^x - 3 \times 4^x + 4 \times 3^x - 2^x = 0$. It is not difficult to see that each of the three equations has a unique positive root.

To prove the theorem, we first need the following three lemmas.

Lemma 2.5 *Let T be a chemical tree with n ($n \geq 7$) vertices. If T has two vertices of degree 2, then T is not extremal with maximum general Randić index R_α ($\alpha > 0$).*

Proof. Suppose T is an extremal chemical tree with maximum general Randić index R_α, where $\alpha > 0$ and u and v are vertices of degree 2 in T. Let $P_{uv} = uu_i \cdots v_i v$ be the path connecting u and v. Assume another neighbor of u is u_o and another neighbor of v is v_o. We continue to discuss the problem in two cases:

Case 1. The length of P_{uv} is greater than 1. Without loss of generality, assume $d_{u_i} \geq d_{v_i}$. (u_i and v_i may be the same.) We make the following change to transform T into T': Delete the edge vv_o and connect v_o to u. Then in T', the degree of v is 1, the degree of u is 3 and other vertices' degrees do not change. Then

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T) \\ = \; & [(3d_{u_i})^\alpha + (3d_{u_o})^\alpha + (3d_{v_o})^\alpha + d_{v_i}^\alpha] - [(2d_{u_i})^\alpha + (2d_{u_o})^\alpha + (2d_{v_o})^\alpha + (2d_{v_i})^\alpha] \\ = \; & (3^\alpha - 2^\alpha)(d_{u_i}^\alpha + d_{u_o}^\alpha + d_{v_o}^\alpha) - (2^\alpha - 1)d_{v_i}^\alpha \\ \geq \; & (3^\alpha - 2 \times 2^\alpha + 1)d_{v_i}^\alpha + (3^\alpha - 2^\alpha)(d_{u_o}^\alpha + d_{v_o}^\alpha)(since\ d_{u_i} \geq d_{v_i}) \end{aligned} \tag{2}$$

If $\alpha \geq 1$, (2) is obviously positive. If $0 < \alpha < 1$, we can continue to estimate (2) as follows:

$$\begin{aligned} & (3^\alpha - 2 \times 2^\alpha + 1)d_{v_i}^\alpha + (3^\alpha - 2^\alpha)(d_{u_o}^\alpha + d_{v_o}^\alpha) \\ \geq \; & (3^\alpha - 2 \times 2^\alpha + 1)4^\alpha + (3^\alpha - 2^\alpha)(1 + 1) \\ > \; & 0. \end{aligned} \tag{3}$$

Case 2. The length of P_{uv} is 1. That is to say, uv is an edge of T. Delete the edge vv_o and connect v_o to u to change T into T'. Then in T', the degree of v is 1, the degree of u is 3 and other vertices' degrees do not change. Similarly,

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T) \\ = \; & [3^\alpha + (3d_{u_o})^\alpha + (3d_{v_o})^\alpha] - [4^\alpha + (2d_{u_o})^\alpha + (2d_{v_o})^\alpha] \\ = \; & (3^\alpha - 2^\alpha)(d_{u_o}^\alpha + d_{v_o}^\alpha) - (4^\alpha - 3^\alpha). \end{aligned} \tag{4}$$

As $n \geq 7$, at least one of d_{u_o} and d_{v_o} is greater than 1. Then for (4), we have the following estimate:

$$(3^\alpha - 2^\alpha)(d_{u_o}^\alpha + d_{v_o}^\alpha) - (4^\alpha - 3^\alpha) \geq (3^\alpha - 2^\alpha)(2^\alpha + 1) - (4^\alpha - 3^\alpha) > 0 \tag{5}$$

for any $\alpha > 0$. From (2), (3) and (5), we get $R_\alpha(T') > R_\alpha(T)$, a contradiction. ∎

Lemma 2.6 *Let T be a chemical tree with n $(n \geq 7)$ vertices. If T has two vertices of degree* 2 *and degree* 3*, respectively, then T is not extremal with maximum general Randić index* R_α $(\alpha > 0)$.

Proof. Assume T is an extremal chemical tree with maximum general Randić index R_α, where $\alpha > 0$ and u is a vertex of degree 2 in T and v is of degree 3. Let $P_{uv} = uu_i \cdots v_i v$ be the path connecting u and v. Suppose u has another neighbor u_o and v has the other two neighbors v_o and v'_o. Then there are two cases to consider:

Case1. The length of P_{uv} is greater than 1. Here u_i and v_i may be the same. We make the following change to transform T into T': Delete the edge uu_o and connect u_o to v. Then in T', the degree of u is 1, the degree of v is 4 and other vertices' degrees do not change. Then

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T) \\ = \; & [d_{u_i}^\alpha + (4d_{u_o})^\alpha + (4d_{v_i})^\alpha + (4d_{v_o})^\alpha + (4d_{v'_o})^\alpha] \\ & -[(2d_{u_i})^\alpha + (2d_{u_o})^\alpha + (3d_{v_i})^\alpha + (3d_{v_o})^\alpha + (3d_{v'_o})^\alpha] \\ = \; & (4^\alpha - 3^\alpha)(d_{v_i}^\alpha + d_{v_o}^\alpha + d_{v'_o}^\alpha) + (4^\alpha - 2^\alpha)d_{u_o}^\alpha - (2^\alpha - 1)d_{u_i}^\alpha \qquad (6) \end{aligned}$$

By Lemma 2.5, we can assume $d_{v_i} \geq 3$. Then (6) can be estimated as

$$\begin{aligned} & (4^\alpha - 3^\alpha)(d_{v_i}^\alpha + d_{v_o}^\alpha + d_{v'_o}^\alpha) + (4^\alpha - 2^\alpha)d_{u_o}^\alpha - (2^\alpha - 1)d_{u_i}^\alpha \\ \geq \; & (4^\alpha - 3^\alpha)(3^\alpha + 2) + (4^\alpha - 2^\alpha) - (2^\alpha - 1)4^\alpha > 0 \qquad (7) \end{aligned}$$

for any $\alpha > 0$.

Case 2. The length of P_{uv} is 1. That is to say, uv is an edge of T. Delete the edge uu_o and connect u_o to v to change T into T'. Then in T', the degree of u is 1, the degree of v is 4 and other vertices' degrees do not change. Then

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T) \\ = \; & [4^\alpha + (4d_{u_o})^\alpha + (4d_{v_o})^\alpha + (4d_{v'_o})^\alpha] - [6^\alpha + (2d_{u_o})^\alpha + (3d_{v_o})^\alpha + (3d_{v'_o})^\alpha] \\ = \; & (4^\alpha - 2^\alpha)d_{u_o}^\alpha + (4^\alpha - 3^\alpha)(d_{v_o}^\alpha + d_{v'_o}^\alpha) - (6^\alpha - 4^\alpha). \qquad (8) \end{aligned}$$

Since $n \geq 7$, at least one of d_{u_o}, d_{v_o} and $d_{v'_o}$ are greater than 1. Then for (8), we have

$$\begin{aligned} & (4^\alpha - 2^\alpha)d_{u_o}^\alpha + (4^\alpha - 3^\alpha)(d_{v_o}^\alpha + d_{v'_o}^\alpha) - (6^\alpha - 4^\alpha) \\ \geq \; & (4^\alpha - 2^\alpha) + (4^\alpha - 3^\alpha)(2^\alpha + 1) - (6^\alpha - 4^\alpha) > 0 \end{aligned} \quad (9)$$

for any $\alpha > 0$. From (7) and (9), we obtain $R_\alpha(T') > R_\alpha(T)$, a contradiction. ∎

Lemma 2.7 *Let T be a chemical tree with n ($n \geq 7$) vertices. If T has two vertices of degree 3, then T is not extremal with maximum general Randić index R_α ($\alpha > 0$).*

Proof. Assume T is an extremal chemical tree with maximum general Randić index R_α, where $\alpha > 0$ and u and v are both of degree 3 in T. Let $P_{uv} = uu_i \cdots v_i v$ be the path connecting u and v. Assume the other two neighbors of u are u_o, u'_o and the other two neighbors of v are v_o, v'_o, respectively. We still discuss the problem in two cases.

Case 1. The length of P_{uv} is greater than 1. Here u_i and v_i may be the same. Without loss of generality, assume $d_{v_i} \geq d_{u_i}$ and $d_{u'_o} \geq d_{u_o}$. We make the following change to transform T into T': Delete the edge uu'_o and connect u'_o to v. Then in T', the degree of u is 2, the degree of v is 4 and other vertices' degrees do not change. Then

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T) \\ = \; & [(2d_{u_i})^\alpha + (2d_{u_o})^\alpha + (4d_{u'_o})^\alpha + (4d_{v_i})^\alpha + (4d_{v_o})^\alpha + (4d_{v'_o})^\alpha] \\ & -[(3d_{u_i})^\alpha + (3d_{u_o})^\alpha + (3d_{u'_o})^\alpha + (3d_{v_i})^\alpha + (3d_{v_o})^\alpha + (3d_{v'_o})^\alpha] \\ = \; & [(4^\alpha - 3^\alpha)d_{u'_o}^\alpha - (3^\alpha - 2^\alpha)d_{u_o}^\alpha] + [(4^\alpha - 3^\alpha)d_{v_i}^\alpha - (3^\alpha - 2^\alpha)d_{u_i}^\alpha] + \\ & [(4^\alpha - 3^\alpha)(d_{v_o}^\alpha + d_{v'_o}^\alpha)]. \\ \geq \; & [(4^\alpha - 2 \times 3^\alpha + 2^\alpha)d_{u_o}^\alpha] + [(4^\alpha - 2 \times 3^\alpha + 2^\alpha)d_{u_i}^\alpha] + \\ & [(4^\alpha - 3^\alpha)(d_{v_o}^\alpha + d_{v'_o}^\alpha)]. \end{aligned} \quad (10)$$

If $\alpha \geq 1$, we can see easily that $R_\alpha(T') - R_\alpha(T) > 0$ from (10). If $0 < \alpha < 1$, we can continue to estimate (10) as follows:

$$\begin{aligned}
& [(4^\alpha - 2 \times 3^\alpha + 2^\alpha) d_{u_o}^\alpha] + [(4^\alpha - 2 \times 3^\alpha + 2^\alpha) d_{u_i}^\alpha] + \\
& [(4^\alpha - 3^\alpha)(d_{v_o}^\alpha + d_{v_o'}^\alpha)] \\
\geq\ & [(4^\alpha - 2 \times 3^\alpha + 2^\alpha) 4^\alpha] + [(4^\alpha - 2 \times 3^\alpha + 2^\alpha) 4^\alpha] + 2(4^\alpha - 3^\alpha) \\
>\ & 0. \qquad (11)
\end{aligned}$$

Case 2. The length of P_{uv} is 1. That is to say, uv is an edge of T. Without loss of generality, assume $d_{u_o'} \geq d_{u_o}$. Delete the edge uu_o' and connect u_o' to v to change T into T'. Then in T', the degree of u is 2, the degree of v is 4 and other vertices' degrees do not change. Then

$$\begin{aligned}
& R_\alpha(T') - R_\alpha(T) \\
=\ & [8^\alpha + (2d_{u_o})^\alpha + (4d_{u_o'})^\alpha + (4d_{v_o})^\alpha + (4d_{v_o'})^\alpha] \\
& -[9^\alpha + (3d_{u_o})^\alpha + (3d_{u_o'})^\alpha + (3d_{v_o})^\alpha + (3d_{v_o'})^\alpha] \\
=\ & (4^\alpha - 3^\alpha)(d_{u_o'}^\alpha + d_{v_o}^\alpha + d_{v_o'}^\alpha) - (3^\alpha - 2^\alpha) d_{u_o}^\alpha - (9^\alpha - 8^\alpha). \qquad (12)
\end{aligned}$$

By the assumption $n \geq 7$, $d_{u_o'} \geq d_{u_o}$ and Lemma 2.6, we only need to check (12) in the following several cases.

(a) $d_{v_o} = d_{v_o'} = 1$, $d_{u_o'} = 3$, $d_{u_o} = 3$;

(b) $d_{v_o} = d_{v_o'} = 1$, $d_{u_o'} = 3$, $d_{u_o} = 1$;

(c) $d_{v_o} = d_{v_o'} = 1$, $d_{u_o'} = 4$, $d_{u_o} = 4$;

(d) $d_{v_o} = d_{v_o'} = 1$, $d_{u_o'} = 4$, $d_{u_o} = 3$;

(e) $d_{v_o} = d_{v_o'} = 1$, $d_{u_o'} = 4$, $d_{u_o} = 1$;

(f) At least one of d_{v_o} and $d_{v_o'}$ is greater than 2, $d_{u_o'} = 1$, $d_{u_o} = 1$;

(g) At least one of d_{v_o} and $d_{v_o'}$ is greater than 2, $d_{u_o'} = 3$, $d_{u_o} = 3$;

(h) At least one of d_{v_o} and $d_{v_o'}$ is greater than 2, $d_{u_o'} = 3$, $d_{u_o} = 1$;

(i) At least one of d_{v_o} and $d_{v_o'}$ is greater than 2, $d_{u_o'} = 4$, $d_{u_o} = 4$;

(j) At least one of d_{v_o} and $d_{v_o'}$ is greater than 2, $d_{u_o'} = 4$, $d_{u_o} = 3$;

(k) At least one of d_{v_o} and $d_{v_o'}$ is greater than 2, $d_{u_o'} = 4$, $d_{u_o} = 1$;

Calculations show that in each case, (12) is positive for any $\alpha > 0$. From (10) (11) and (12), we have $R_\alpha(T') > R_\alpha(T)$, a contradiction. ∎

Next we turn to proving Theorem 2.4.

Proof of Theorem 2.4: For $n = 4, 5$ and 6, we can obtain the extremal chemical trees with n vertices by direct calculation. The results are shown in the diagram. For $n \geq 7$, by Lemmas 2.5, 2.6 and 2.7, $d(n)$ is the degree sequence of the extremal chemical tree. If $q = 0$, then all trees with degree sequence $d(n)$ have the same general Randić index

$$(p-1)16^\alpha + (n-p)4^\alpha.$$

If $q \neq 0$, then there is a unique vertex v of degree $q+1$. By checking all possible cases, (There are altogether $q+1$ cases.) we get that the chemical trees in $\mathcal{D}(n)$ (Definition 2.3) are all extremal ones with maximum general Randić index R_α $(\alpha > 0)$. Moreover, the extremal value is

$$(p-1)16^\alpha + 4^\alpha(q+1)^\alpha + q(q+1)^\alpha + (n-p-q-1)4^\alpha.$$

When $q = 0$, the above is exactly $(p-1)16^\alpha + (n-p)4^\alpha$. So we can say that the extremal value of R_α is

$$(p-1)16^\alpha + 4^\alpha(q+1)^\alpha + q(q+1)^\alpha + (n-p-q-1)4^\alpha.$$

Notice that when $7 \leq n \leq 11$, $\mathcal{D}(n) = \{P^{d(n)}\}$, which completes the prove. ∎

3 Concluding remarks

For R_α $(\alpha < 0)$, the problem of finding extremal chemical trees has not been completely solved. For some known results, please refer to [4, 11], which solved the problem for $\alpha = -1$ and $\alpha = -\frac{1}{2}$. It is necessary to point out that using the method in this paper, the extremal chemical tree for $R_{-\frac{1}{2}}$ can be found and the result is as same as that in [4].

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