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Two Results on Extremal Chemical Trees with Maximum General Randić Index R_α for $\alpha < 0$

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Abstract

A tree is called chemical if none of its vertices 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 $\alpha \neq 0$. This paper is contributed to the study of extremal chemical trees with maximum general Randić index R_α for $\alpha < 0$. It is proved that, among the chemical trees of order $n(n \geq 10)$, the path P_n is the extremal one with maximum $R_\alpha(\alpha < 0)$ if and only if $\alpha \in (\tilde{\alpha}(n), 0)$, where $-0.909 < \tilde{\alpha}(n) < -0.747$ and $\tilde{\alpha}(n)$ depends on n. Moreover, we characterize, among the chemical trees of order $n = 5k + d$, $(k \geq 3, k \in \mathbb{N}, d = 0, 2, 4)$, the asymptotic result for the extremal chemical trees with maximum R_α when $\alpha \to -\infty$.

1 Introduction

In 1975, in order to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons, the chemist M. Randić proposed the following chemical index, later named *Randić index* or *connectivity index*.

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.

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 [6, 7].

B. Bollobás and P. Erdös [2] later generalized the Randić index by replacing $-\frac{1}{2}$ with any real number $\alpha \neq 0$. It is called the *general Randić index* and denoted by $R_\alpha(G)$. That is,

$$R_\alpha(G) = \sum_{uv} (d(u)d(v))^\alpha. \tag{1}$$

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. A vertex with degree one is called a *pendent vertex*. As usual, we use P_n to denote the *path* with n vertices.

For terminology and notations not defined here, we refer the reader to [1].

The results in [3, 9, 11] are on the extremal unicyclic graphs and bicyclic graphs with minimum or maximum R_α. There are several papers on upper and lower bounds for R_{-1} of the extremal (chemical) trees [4, 12, 17]. The problem of finding the extremal trees with maximum R_α among all trees of order n is discussed in [5]. It was proved that when $\alpha \in [-\frac{1}{2}, 0)$, the path P_n is the extremal one with maximum R_α. However, when $\alpha \in (-2, -\frac{1}{2})$, the problem is still open. In [13], the authors successfully characterized the extremal chemical trees with maximum R_α for any $\alpha > 0$. For more results on R_α, please refer to [8, 10, 14, 15, 16].

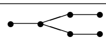
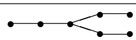
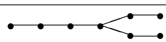
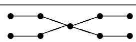
This paper focuses on the extremal chemical trees with maximum R_α for $\alpha < 0$. In the second section, it is proved that, for any integer $n (n \geq 10)$, there exists $\tilde{\alpha}(n)$, $-0.909 < \tilde{\alpha}(n) < -0.747$, such that among the chemical trees of order n, the path P_n is the extremal one with maximum $R_\alpha (\alpha < 0)$ if and only if $\alpha \in (\tilde{\alpha}(n), 0)$. In the third section, we obtain that for any $n = 5k + d$, where $k \geq 3, k \in \mathbb{N}, d = 0, 2, 4$, there exists $\hat{\alpha}(n) < 0$ such that when $\alpha \in (-\infty, \hat{\alpha}(n))$, each tree in $\mathcal{T}(n, d)$ (Definition 3.1) is extremal with maximum R_α among the chemical trees of order n. The discussions in the last section show that, for **any** $n \geq 10$ and **any** $\alpha < 0$, to completely determine the extremal chemical trees with maximum R_α is much more difficult.

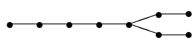
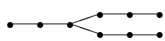
Some data will be mentioned in the following discussion.

Symbol	Explanation: the root of the equation	Value
α_0	$3 \times 4^x - 3^x - 2 \times 6^x = 0$	$-3.082 < \alpha_0 < -3.081$
α_1	$3 \times 4^x + 8^x - 2^x - 2 \times 6^x - 12^x = 0$	$-0.748 < \alpha_1 < -0.747$
α_2	$9^x + 4 \times 6^x + 2 \times 2^x - 7 \times 4^x = 0$	$-0.909 < \alpha_2 < -0.908$
α_3	$4 \times 12^x + 8 \times 6^x + 6 \times 2^x - 18 \times 4^x = 0$	$-0.834 < \alpha_3 < -0.833$

2 P_n as extremal chemical tree

We obtain the extremal chemical trees of order n ($4 \leq n \leq 9$) with maximum R_α when $\alpha < 0$ as the following tabular.

n	α	Extremal chemical tree	Maximum value of R_α
$n = 4$	$\alpha < 0$		$2 \times 2^\alpha + 4^\alpha$
$n = 5$	$\alpha < 0$		$2 \times 2^\alpha + 2 \times 4^\alpha$
$n = 6$	$\alpha_0 \leq \alpha < 0$		$3 \times 4^\alpha + 2 \times 2^\alpha$
	$\alpha \leq \alpha_0$		$3^\alpha + 2 \times 6^\alpha + 2 \times 2^\alpha$
$n = 7$	$-1 \leq \alpha < 0$		$4 \times 4^\alpha + 2 \times 2^\alpha$
	$\alpha \leq -1$		$3 \times 6^\alpha + 3 \times 2^\alpha$
$n = 8$	$-1 \leq \alpha < 0$		$5 \times 4^\alpha + 2 \times 2^\alpha$
	$\alpha \leq -1$		$3 \times 6^\alpha + 3 \times 2^\alpha + 4^\alpha$
$n = 9$	$-1 \leq \alpha < 0$		$6 \times 4^\alpha + 2 \times 2^\alpha$
	$\alpha \leq -1$		$4 \times 8^\alpha + 4 \times 2^\alpha$

Moreover, when $n = 9$ and $\alpha = -1$,  and  are also the extremal chemical trees with maximum R_α.

The results in the above tabular suggest a conjecture that, for $\forall\ \alpha \in [-1, 0)$, the path P_n is extremal with maximum R_α among the chemical trees of order n.

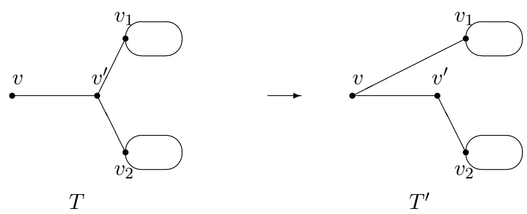
Unfortunately, this conjecture is false. (See Theorem 2.2.)

Theorem 4.3 in [5] implies that for any $\alpha \in [-\frac{1}{2}, 0)$, P_n is extremal with maximum R_α among the chemical trees of order n. We will show that the result can be improved by replacing $-\frac{1}{2}$ by $\tilde{\alpha}(n)$, where $-0.909 < \tilde{\alpha}(n) < -0.747$.

Lemma 2.1 *Among the chemical trees of order $n (n \geq 4)$, if T is the extremal one with maximum $R_\alpha (-1 < \alpha < 0)$, then the adjacent vertices of the pendent vertices in T are of degree two.*

Proof. Let v be a pendent vertex of a chemical tree T and v' be the adjacent vertex of v.

1. If $d(v') = 3$ and v_1, v_2 are adjacent vertices of v', do the following operation to change T to T'.



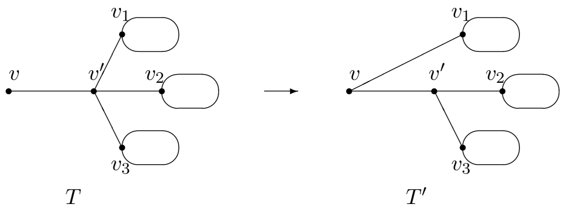
Suppose $d(v_1) = a, d(v_2) = b$ and $a \leq b$. Then

$$R_\alpha(T') - R_\alpha(T) = [4^\alpha + (2a)^\alpha + (2b)^\alpha] - [3^\alpha + (3a)^\alpha + (3b)^\alpha]. \tag{2}$$

For any integers a, b, $1 \leq a \leq b \leq 4$, the result for (2) is positive when $-1 < \alpha < 0$. That is,

$$R_\alpha(T') > R_\alpha(T).$$

2. If $d(v') = 4$ and v_1, v_2, v_3 are adjacent vertices of v', do the following operation to change T to T'.



Suppose $d(v_1) = a, d(v_2) = b, d(v_3) = c$ and $a \leq b \leq c$. Then

$$R_\alpha(T') - R_\alpha(T) = [6^\alpha + (2a)^\alpha + (3b)^\alpha + (3c)^\alpha] - [4^\alpha + (4a)^\alpha + (4b)^\alpha + (4c)^\alpha]. \quad (3)$$

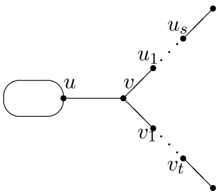
For any integers a, b, c, $1 \leq a \leq b \leq c \leq 4$, the result for (3) is positive when $-1 < \alpha < 0$. That is,

$$R_\alpha(T') > R_\alpha(T).$$

Two cases are both contradictory to the condition that T is the extremal one with maximum $R_\alpha(-1 < \alpha < 0)$. So the lemma is proved. ∎

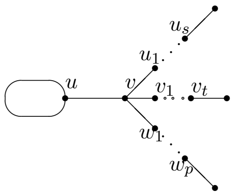
Theorem 2.2 *Among the chemical trees of order $n(n \geq 10)$, the path P_n is the extremal one with maximum $R_\alpha(\alpha < 0)$ if and only if $\alpha \in (\tilde{\alpha}(n), 0)$, where $-0.909 < \tilde{\alpha}(n) < -0.747$ and $\tilde{\alpha}(n)$ depends on n.*

Proof. Let T be an extremal chemical tree with maximum $R_\alpha(-1 < \alpha < 0)$. By Lemma 2.1, the adjacent vertices of the pendent vertices in T are of degree two. If T is not P_n, there exists a vertex v in T and T has one of the following structures.



$d(u_i) = d(v_j) = 2$
$1 \leq i \leq s, 1 \leq j \leq t$

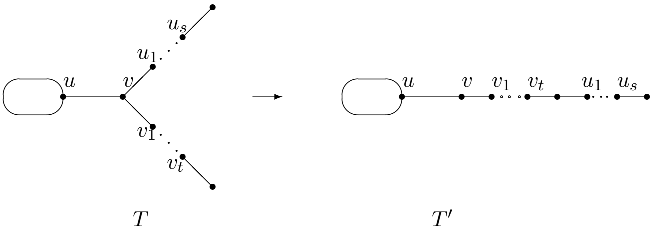
Structure A



$d(u_i) = d(v_j) = d(w_k) = 2$
$1 \leq i \leq s, 1 \leq j \leq t, 1 \leq k \leq p$

Structure B

1. If T is of Structure A, change T to T' as follows:

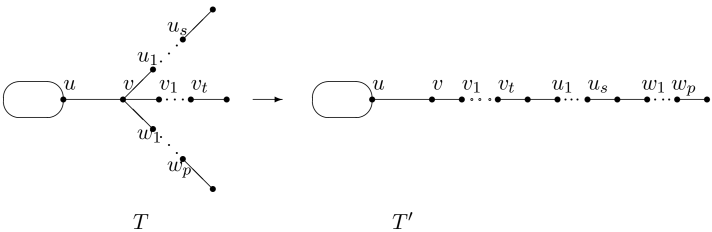


Assume $d(u) = a$ and $2 \leq a \leq 4$. (Lemma 2.1 implies $a \neq 1$.) Then

$$R_\alpha(T') - R_\alpha(T) = 3 \times 4^\alpha + (2a)^\alpha - 2^\alpha - 2 \times 6^\alpha - (3a)^\alpha \tag{4}$$

For any $\alpha \in (\alpha_1, 0)$, the result for (4) is positive. It means if T is an extremal chemical tree with maximum R_α when $\alpha \in (\alpha_1, 0)$, T can not be Structure A.

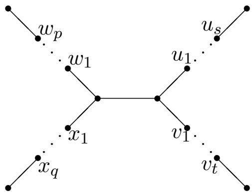
2. If T is of Structure B, change T to T' as follows:



By similar discussion as case 1, we can obtain that if T is an extremal chemical tree with maximum R_α when $\alpha \in (\alpha_1, 0)$, T can not be Structure B.

Thus we prove that when $\alpha \in (\alpha_1, 0)$, the path P_n is the extremal one with maximum R_α among all chemical trees of order n.

For any $n \geq 10$ and $\alpha < \alpha_2$, each chemical tree with the following structure has a greater R_α than that of P_n. So the path P_n is not the extremal chemical with maximum R_α when $\alpha \in (-\infty, \alpha_2)$.



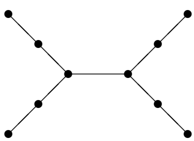
$s, t, p, q \geq 1$

$s + t + p + q = n - 6$

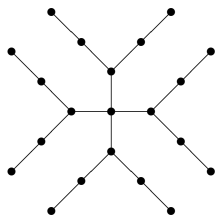
Since $-0.909 < \alpha_2 < \alpha_1 < -0.747$, we get that when $\alpha \in [-0.747, 0)$, P_n is the extremal one with maximum R_α among the chemical trees of order n and when $\alpha \in (-\infty, -0.909]$, P_n is not the extremal one with maximum R_α.

For any $n \geq 10$, suppose T' is the chemical tree of order n with maximum $R_\alpha(\alpha < 0)$ satisfying the following two conditions: (1) T' is not P_n and (2) As an extremal chemical tree with maximum R_α, the α of T' is nearest to 0. The function $R_\alpha(T') - R_\alpha(P_n)$ is obviously a continue function on the variable α. Moreover, $R_\alpha(T') - R_\alpha(P_n) < 0$ when $-0.747 \leq \alpha < 0$ and $R_\alpha(T') - R_\alpha(P_n) > 0$ when α is equal to some value smaller than -0.747. So by the Intermediate Value Theorem and the above discussion, there exists some $\tilde{\alpha}(n)$, $-0.909 < \tilde{\alpha}(n) < -0.747$, such that P_n is the extremal one with maximum $R_\alpha(\alpha < 0)$ if and only if $\alpha \in (\tilde{\alpha}(n), 0)$.

The following example shows that $\tilde{\alpha}(n)$ depends heavily on n. When $n = 10$, P_{10} is the extremal chemical tree with maximum $R_\alpha(\alpha < 0)$ if and only if $\alpha \in (\alpha_2, 0)$ and when $\alpha \in U^-(\alpha_2, \delta)$, where $\delta > 0$ and δ is small enough, the following chemical tree T_1 is the extremal one with maximum R_α. So $\tilde{\alpha}(10) = \alpha_2$. When $n = 21$, P_{21} is the extremal chemical tree with maximum $R_\alpha(\alpha < 0)$ if and only if $\alpha \in (\alpha_3, 0)$ and when $\alpha \in U^-(\alpha_3, \delta)$, where $\delta > 0$ and δ is small enough, the following chemical tree T_2 is the extremal one with maximum R_α. So $\tilde{\alpha}(21) = \alpha_3$.



T_1



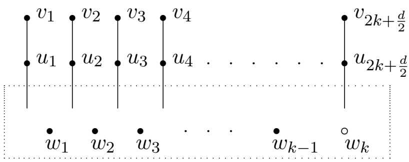
T_2

■

Corollary 2.3 *Among the chemical trees of order n, the path P_n is the extremal one with maximum Randić index and the maximum value is equal to $2 \times 2^\alpha + (n-3) \times 4^\alpha$.*

3 Asymptotic result when $\alpha \to -\infty$

Definition 3.1 *For any $n = 5k + d$ $(k > 1, k \in \mathbb{N}, d = 0, 2, 4)$, let $\mathcal{T}(n, d)$ be the set of trees that have the following structure*



$$d(v_1) = d(v_2) = \cdots = d(v_{2k+\frac{d}{2}}) = 1$$
$$d(u_1) = d(u_2) = \cdots = d(u_{2k+\frac{d}{2}}) = 2$$
$$d(w_1) = d(w_2) = \cdots = d(w_{k-1}) = 4$$
$$d(w_k) = 2 + \tfrac{d}{2}$$

Furthermore, w_k is a pendent vertex in the subtree induced by the vertices $w_1, w_2, \cdots, w_k$.

Theorem 3.2 *Among the chemical trees of order $n = 5k + d$ $(k \geq 3, k \in \mathbb{N}, d = 0, 2, 4)$, there exists $\hat{\alpha}(n) < 0$ such that when $\alpha \in (-\infty, \hat{\alpha}(n))$, each tree in $\mathcal{T}(n, d)$ is extremal with maximum R_α and the maximum value is equal to*

$$(2k + \frac{d}{2}) \times 2^\alpha + (2k + \frac{d}{2} - 1) \times 8^\alpha + (k-2) \times 16^\alpha + (1 + 2^\alpha) \times (4 + d)^\alpha.$$

Proof. Here we only prove the theorem when $d = 0$, the other two cases are completely similar.

Firstly, if a chemical tree T with $n = 5k$ vertices has $2k + p$ $(p > 0)$ edges (u, v) satisfying $d(u) = 2$ and $d(v) = 1$, then the average degree of the other vertices is

$$\bar{d} = \frac{2(5k-1) - (2k+p) - 2(2k+p)}{5k - 2(2k+p)} = \frac{4k - 2 - 3p}{k - 2p} > 4.$$

It is a contradiction to that T is a chemical tree. So a chemical tree with $n = 5k$ vertices has at most $2k$ edges (u, v) satisfying $d(u) = 2$ and $d(v) = 1$.

Secondly, if T' is a chemical tree with $n = 5k$ vertices and less than $2k$ edges (u, v) satisfying $d(u) = 2$ and $d(v) = 1$, then T' can not be the asymptotic extremal chemical tree with maximum R_α when $\alpha \to -\infty$. Choose an element T from the set $\mathcal{T}(5k, 0)$, then

$$\frac{R_\alpha(T')}{R_\alpha(T)} \leq \frac{(2k-1)(1 \times 2)^\alpha + (3k)(1 \times 3)^\alpha}{(2k)(1 \times 2)^\alpha + (3k-1)(4 \times 4)^\alpha} \to \frac{2k-1}{2k} < 1 \qquad (\alpha \to -\infty)$$

So T' can not be the asymptotic extremal chemical tree with maximum R_α.

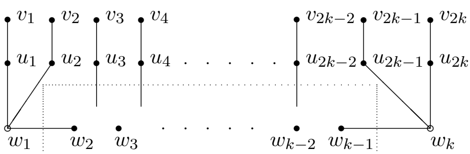
Thirdly, let T be a chemical tree with $n = 5k$ vertices and $2k$ edges (u, v) satisfying $d(u) = 2$ and $d(v) = 1$. Suppose there are still p_i vertices of degree i among the other $5k - 2 \times 2k = k$ vertices, $i = 1, 2, 3, 4$. Then we have the following two equations

$$\begin{cases} p_1 + p_2 + p_3 + p_4 = k \\ p_1 + p_2 + p_3 + p_4 = 2(5k-1) - 2k - 2(2k) \end{cases} \tag{5}$$

and (5) has the following two solutions,

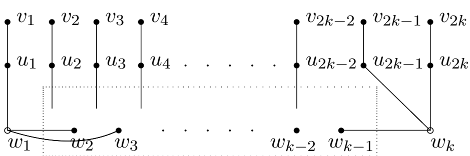
$$\begin{cases} p_1 = 0 \\ p_2 = 0 \\ p_3 = 2 \\ p_4 = k-2 \end{cases} \qquad\qquad \begin{cases} p_1 = 0 \\ p_2 = 1 \\ p_3 = 0 \\ p_4 = k-1. \end{cases}$$

There are four classes of chemical trees corresponding to the first solution and we can compute their R_α, respectively.

1. 

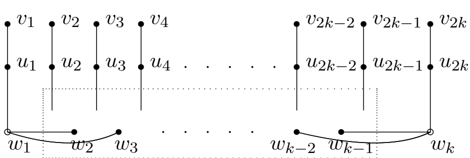
$d(w_2) = d(w_3) = \cdots = d(w_{k-1}) = 4$

$$R_\alpha = (2k) \times 2^\alpha + 4 \times 6^\alpha + 2 \times 12^\alpha + (2k-4) \times 8^\alpha + (k-3) \times 16^\alpha.$$

2. 

$d(w_2) = d(w_3) = \cdots = d(w_{k-1}) = 4$

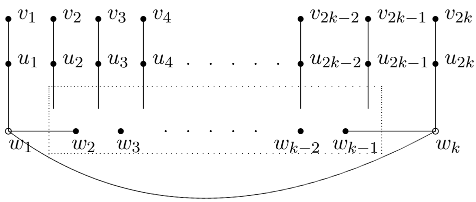
$$R_\alpha = (2k) \times 2^\alpha + 3 \times 6^\alpha + 3 \times 12^\alpha + (2k-3) \times 8^\alpha + (k-4) \times 16^\alpha.$$

3. 

$d(w_2) = d(w_3) = \cdots = d(w_{k-1}) = 4$

$$R_\alpha = (2k) \times 2^\alpha + 2 \times 6^\alpha + 4 \times 12^\alpha + (2k-2) \times 8^\alpha + (k-5) \times 16^\alpha.$$

4.

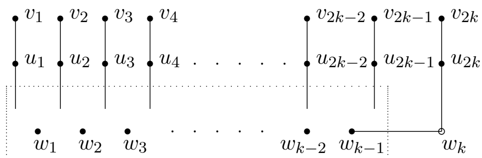


$d(w_2) = d(w_3) = \cdots = d(w_{k-1}) = 4$

$$R_\alpha = (2k) \times 2^\alpha + 2 \times 6^\alpha + 2 \times 12^\alpha + 9^\alpha + (2k-2) \times 8^\alpha + (k-4) \times 16^\alpha.$$

The following two classes of chemical trees correspond to the second solution and we can compute their R_α, respectively.

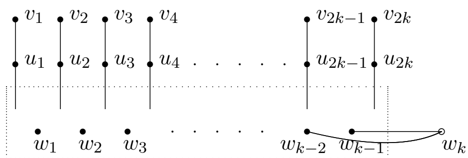
5



$d(w_1) = d(w_2) = \cdots = d(w_{k-1}) = 4$

$$R_\alpha = (2k) \times 2^\alpha + 4^\alpha + (2k) \times 8^\alpha + (k-2) \times 16^\alpha.$$

6



$d(w_1) = d(w_2) = \cdots = d(w_{k-1}) = 4$

$$R_\alpha = (2k) \times 2^\alpha + (2k+2) \times 8^\alpha + (k-3) \times 16^\alpha.$$

Compare the Randić indices R_α of the above six classes of chemical trees when $\alpha \to -\infty$. We obtain that there must exists $\hat{\alpha}(n) < 0$ such that when $\alpha \in (-\infty, \hat{\alpha}(n))$, the fifth class of chemical trees are extremal with maximum R_α. In fact, they are exactly the trees in $\mathcal{T}(5k, 0)$. Thus we finish the proof. ∎

4 Further discussions

During the study of extremal chemical trees with maximum general Randić index R_α for $\alpha < 0$, we meet much more difficulty than that for $\alpha > 0$. The reason is for any $\alpha < 0$, the values of $(1\times 2)^\alpha$, $(1\times 3)^\alpha$, $(1\times 4)^\alpha$, $(2\times 2)^\alpha$, $(2\times 3)^\alpha$, $(2\times 4)^\alpha$, $(3\times 3)^\alpha$, $(3\times 4)^\alpha$, $(4\times 4)^\alpha$ have small minus. So for **any** $\alpha < 0$ and **any** $n \in \mathbb{N}$, (for example, $\hat{\alpha}(n) < \alpha < \tilde{\alpha}(n)$,) to determine the extremal chemical tree with maximum R_α is of much more difficulty.

In fact, $\tilde{\alpha}(n)$ is an increasing function of n. That is $\tilde{\alpha}(n_1) \leq \tilde{\alpha}(n_2)$ if $n_1 \leq n_2$. There is a conjecture that $\tilde{\alpha}(n) \rightarrow \alpha_1$ when $n \rightarrow \infty$.

References

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