Which generalized Randić indices are suitable measures of molecular branching?

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ABSTRACT

Molecular branching is a very important notion, because it influences many physicochemical properties of chemical compounds. However, there is no consensus on how to measure branching. Nevertheless two requirements seem to be obvious: star is the most branched graph and path is the least branched graph. Every measure of branching should have these two graphs as extremal graphs. In this paper we restrict our attention to chemical trees (i.e. simple connected graphs with maximal degree at most 4), hence we have only one requirement that the path be an extremal graph. Here, we show that the generalized Randić index \( R_p(G) = \sum_{u,v \in E(G)} (d_u d_v)^p \) is a suitable measure for branching if and only if \( p \in [\lambda, 0) \cup (0, \lambda') \) where \( \lambda \) is the solution of the equation \( 2^x + 6^x + \frac{1}{2} \cdot 12^x + \frac{1}{4} \cdot 16^x - \frac{11}{4} \cdot 4^x = 0 \) in the interval \((-0.793, -0.792)\) and \( \lambda' \) is the positive solution of the equation \( 3^x \cdot 3^x - 2 \cdot 2^x - 4^x = 0 \). These results include the solution of the problem proposed by Clark and Gutman.

1. Introduction

Randić index [12] is one of the most famous molecular descriptors whose chemical and mathematical properties have been extensively studied [5,10,13]. It is defined as

\[
R(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u \cdot d_v}}.
\]

where \( E(G) \) is the set of edges of graph \( G \) and \( d_u \) and \( d_v \) are degrees of vertices \( u \) and \( v \), respectively. This index is generalized to

\[
R_p(G) = \sum_{u,v \in E(G)} (d_u d_v)^p.
\]

Note that this can be rewritten as

\[
R_p(G) = \sum_{1 \leq i \leq j \leq \Delta} (i \cdot j)^p \cdot m_{ij},
\]

where \( \Delta \) is the maximal degree of graph \( G \) and \( m_{ij} \) is the number of the edges connecting vertices of degrees \( i \) and \( j \). Numbers \( m_{ij} \) have been extensively studied [1,2,4,11,14,15,17,19,20,22,23].

Branching [6] of molecules is very important, but there is no unique measure of this property. However every molecular descriptor used as a branching descriptor should have a path and a star graph as two opposing extremal graphs (it is readily
seen that star $S_N = K_{1,N-1}$ is the most branched graph and path $P_N$ is the least branched graph among all trees with $N \geq 4$ vertices. More precisely we are interested in descriptors $\chi$ such that one of the following holds:

1. $\chi(K_{1,3}) < \chi(P_4)$ and $\chi(K_{1,N-1}) < \chi(P_N)$ for every tree $T_N \neq P_N$, $K_{1,N-1}$ with $N \geq 5$ vertices;
2. $\chi(P_4) < \chi(K_{1,3})$ and $\chi(P_N) < \chi(K_{1,N-1})$ for every tree $T_N \neq P_N$, $K_{1,N-1}$ with $N \geq 5$ vertices.

Sometimes authors require some more restrictive conditions [7,24,25], but here, similarly as is done in paper [3], we restrict ourselves to the above requirements. Moreover, since we restrict our attention to chemical graphs our requirements are even less restrictive. Namely, we just require that

1. $\chi(T_N) < \chi(P_N)$ for every tree $T_N \neq P_N$ with $N \geq 4$ vertices;
2. $\chi(P_N) < \chi(T_N)$ for every tree $T_N \neq P_N$ with $N \geq 4$ vertices.

In papers [8,9], it has been shown that requirement (1) for $p < 0$ implies that it is sufficient to take $p \in [-0.5, 0)$ and necessary to take $p \in (-2, 0)$. These results have been furthered in [3], where it is shown that $R_p(T_N) < R_p(P_N)$ for $p < 0$ implies that it is necessary to take $p \in (-0.826077, 0)$. Moreover, it is shown that there is a value such that it is necessary and sufficient to take $p \in [\mu, 0)$ and it is conjectured that $\mu \approx -0.8$.

Here, we further these results by finding $\mu$. Namely, by showing that $\mu$ is the solution of the equation

$$2^4 + 6^4 + \frac{1}{2} \cdot 12^4 + \frac{1}{4} \cdot 16^4 - \frac{11}{4} \cdot 4^4 = 0,$$

in the interval $(-0.793, -0.792)$. Hence, $\mu = \lambda \approx -0.79263$. Moreover, we show that for $p \in (0, \lambda^{'})$ it holds that

$$R_p(T_N) > R_p(P_N)$$

for every $N \in \mathbb{N}$ and every tree $T_N \neq P_N$ with $N \geq 4$ vertices

where $\lambda^{'}$ is the positive solution of the equation

$$3 \cdot 3^4 - 2 \cdot 2^4 - 4^4 = 0.$$

Hence, $\lambda^{'} \approx 3.08164$.

2. Analysis of $R_p$ for $p < 0$

First, let us note that there is no $p < 0$ such that requirement (2') holds. It is sufficient to note that

$$R_p(P_5) = 2 \cdot 2^p + 2 \cdot 4^p > 4 \cdot 4^p = R_p(K_{1,4}).$$

Hence, we just need to analyze requirement (1'). In these analyses, we shall need the concept of push-to-leaves function defined in paper [16] and used in papers [18,21]. The definition is repeated here for the sake of the completeness of the results.

Let $T$ be any tree with at least three vertices and $f : E(T) \rightarrow \mathbb{R}$ be any function, where $\mathbb{R}$ is the set of real numbers. Let $r$ be any vertex of degree greater than 1 in $T$. Denote by $L(T)$ the set of leaves (or pendant vertices) in $T$. The function $f^{ptl}(r) = f^{ptl} : L(T) \rightarrow \mathbb{R}$ is called $r$-pushed to leaves $f$ and it is defined by

$$f^{ptl}(l) = f(lv_1) + \frac{f(v_1v_2)}{d(v_1) - 1} + \frac{f(v_2v_3)}{(d(v_1) - 1) \cdot (d(v_2) - 1)} + \cdots + \frac{f(v_kv_{k-1})}{(d(v_1) - 1) \cdot (d(v_2) - 1) \cdots (d(v_{k-1}) - 1)} \cdot \frac{f(v_kr)}{d(v_k) - 1} \cdot \cdots \cdot (d(v_{k-1}) - 1),$$

where $lv_1v_2 \cdots v_kr$ is a path from $r$ to $l$ (specially, if $rl \in E(T)$, then $f^{ptl}(l) = f(rl)$). In the following figure “pushing to the leaves” (Fig. 1) of just one single value $f(vw)$ is presented.
It can be easily seen that
\[ \sum_{e \in E(T)} f(e) = \sum_{l \in L(T)} f^{ptl}(l), \]
because all the values \( f(e) \) are “pushed to the leaves”. Let us denote by \( G(d_1, d_2, \ldots, d_n) \) the tree such that
(1) there is a distinguished vertex \( r \) of degree \( d \), such that all pendant vertices are at distance \( n \) from \( r \);
(2) for every leaf \( l \) and every path \( l v_1 v_2 \cdots v_k \) (\( v_n = r \)) it holds that \( d_i = d_i \).

Let \( T_{p} \neq P_{n} \) be a chemical tree with \( N \) vertices and let \( r \) be any vertex of degree greater than 2. Let us define the function \( F_p \) by:
\[ F_p(uv) = (d_i d_j)^p - 4^p \text{ for } u, v \neq r \text{ and by } F_p(rv) = (d_i d_j)^p - 4^p - \frac{1}{2^p}(2^p - 4^p). \]
Also, denote \( F_p(G) = \sum_{e \in E(T)} F_p(e) \).

It can be easily seen that
\[ R_p(T_N) - R_p(P_N) = \sum_{e \in E(T)} f^{ptl}(l). \]
Hence,
\[ R_p(T_N) - R_p(P_N) = \sum_{l \in L(T)} f^{ptl}(l). \]

Let \( x_1, \ldots, x_n \in \{1, 2, 3\} \) such that \( x_n > 1 \). Let us define
\[ \Phi_p(x_1, \ldots, x_n) = [(x_1 + 1)^p - 4^p] + \frac{1}{x_1} [(x_1 + 1)^p (x_2 + 1)^p - 4^p] + \frac{1}{x_1 x_2} [(x_2 + 1)^p (x_3 + 1)^p - 4^p] + \cdots \]
\[ + \frac{1}{x_1 x_2 \cdots x_{n-2}} [(x_{n-2} + 1)^p (x_{n-1} + 1)^p - 4^p] \]
\[ + \frac{1}{x_1 x_2 \cdots x_{n-2} x_{n-1}} [(x_{n-1} + 1)^p (x_n + 1)^p - 4^p] - \frac{2}{x_n - 1} (2^p - 4^p) \cdot \]

Let \( l v_1 v_2 \cdots v_k, v_k = r \) be a path from any leaf \( l \) to \( r \). Then,
\[ f^{ptl}(l) = \Phi_p(d_l - 1, d_{l-1} - 1, \ldots, d_{l-1} - 1). \]
Hence, in order to prove that \( R_p(T_N) < R_p(P_N) \) for every chemical tree \( T_N \neq P_N \), it is sufficient to prove that
\[ \Phi_p(x_1, \ldots, x_n) < 0 \quad \text{for every } n \in \mathbb{N} \text{ and every } x_1, x_2, \ldots, x_n \in \{1, 2, 3\} \text{ such that } x_n > 1. \]

On the other hand, suppose that there is some \( \Phi_p(x_1, \ldots, x_n) \geq 0 \), then the function \( \Phi_p \) has greater value on the graph \( G(x_1 + 1, x_2 + 1, \ldots, x_n + 1) \) than on the path with the same number of vertices.

This implies the following theorem.

**Theorem 1.** Let \( p \in \mathbb{R} \). Then, \( R_p(T_N) < R_p(P_N) \) for every \( N \in \mathbb{N} \) and for every chemical tree \( T_N \neq P_N \) if and only if \( \Phi_p(x_1, \ldots, x_n) < 0 \) for every \( n \in \mathbb{N} \) and every \( x_1, \ldots, x_n \in \{1, 2, 3\} \) such that \( x_n > 1 \). \( \square \)

Denote \( g(x) = 2^x + 6^x + \frac{1}{2} \cdot 12^x + \frac{1}{4} \cdot 16^x - \frac{11}{4} \cdot 4^x. \) Let us prove:

**Lemma 1.** The function \( g(x) \) is a decreasing function on the interval \((-0.83, -0.79)\).

**Proof.** It is sufficient to show that
\[ 2^x \cdot \ln 2 + 6^x \cdot \ln 6 + \frac{1}{2} \cdot 12^x \cdot \ln 12 + \frac{1}{4} \cdot 16^x \cdot \ln 16 < \frac{11}{4} \cdot 4^x \cdot \ln 4 \]
for every \( x \in (-830, -790) \) and this holds, because, both sides of the inequality are increasing and
\[ 2^{-0.79} \cdot \ln 2 + 6^{-0.79} \cdot \ln 6 + \frac{1}{2} \cdot 12^{-0.79} \cdot \ln 12 + \frac{1}{4} \cdot 16^{-0.79} \cdot \ln 16 < \frac{11}{4} \cdot 4^{-0.83} \cdot \ln 4 \]
holds. \( \square \)

Since \( g(-0.83) > 0 \) and \( g(-0.79) < 0 \), it follows that function \( g \) has exactly one zero point in this interval. Let us denote this zero point by \( \lambda \). It holds:

**Corollary 1.** \( g(p) > 0 \) for every \( p \in (-0.83, \lambda) \) and \( g(p) < 0 \) for every \( p \in (\lambda, -0.79) \). \( \square \)

**Lemma 2.** For every \( p \in (-0.83, \lambda) \), there is \( k \in \mathbb{N} \) such that \( F_p(G(2, 3, k \times 4)) > 0 \).

**Proof.** Just note that \( F^{ptl}_p(l) \), for each leaf \( l \) of graph \( G(2, 3, k \times 4) \), tends to \( g(p) \) as \( k \) tends to infinity. \( \square \)

Combining this lemma with the results of [1], we get:

**Corollary 2.** For every \( p < \lambda \), there is \( N \in \mathbb{N} \) and tree \( T_N \neq P_N \) such that \( R_p(T_N) > R_p(P_N) \). \( \square \)
Let us prove:

**Lemma 3.** Let \( p \in (\lambda, -0.79125) \). If there is a graph \( G \) such that \( F_p(G) > 0 \). Then, there is a graph \( G' \) such that \( F_p(G') > 0 \) that has no vertices of degree 2 that satisfy one of the following conditions:

1. both neighbors have degree greater than 2.
2. at least one neighbor has degree 2.

**Proof.** Let us call vertices of degree 2 that satisfy (1) or (2) bad vertices. Let \( \Phi \) be a class of graphs \( G \) such that \( F_p(G) > 0 \) and let \( G' \in \Phi \) be a graph with the smallest number of bad vertices. Suppose to the contrary that \( G' \) has at least one bad vertex \( v \). Let us distinguish two cases:

**CASE 1:** \( v \) has a neighbor of degree 2.

Let \( u \) be a neighbor of \( v \) of degree 2 and let \( w \) be its other neighbor. Note that \( F_p(G - u + vw) = F_p(G) \), but graph \( G - u + vw \) has less bad vertices.

**CASE 2:** \( v \) has both neighbors of degree greater than 2.

In order to obtain a contradiction, it is sufficient to show that \( F_p(G - u + vw) - F_p(G) > 0 \), because \( G - u + vw \) has less bad vertices. It holds that

\[
F_p(G - u + vw) - F_p(G) = (uv)^p + 4p^2 - 2u^p - 2v^p = (u^p - 2u^2) \cdot (v^p - 2v^2) > 0. \]

Let \( x_1, \ldots, x_n \in \{1, 2, 3\} \) such that \( x_n > 1 \). Let us define

\[
\varphi_p(x_1, x_2, \ldots, x_{n-1}) = \lim_{k \to \infty} \Phi_p(x_1, x_2, \ldots, x_{n-1}, k \times 3).
\]

Note that

\[
\varphi_p(x_1, \ldots, x_{n-1}) = \left[(x_1 + 1)^p - 4p^2\right] + \frac{1}{x_1} \left[(x_1 + 1)^p (x_2 + 1)^p - 4p^2\right] + \frac{1}{x_1 x_2} \left[(x_2 + 1)^p (x_3 + 1)^p - 4p^2\right] + \cdots
\]

Hence,

\[
\Phi_p(x_1, \ldots, x_n) = \varphi_p(x_1, \ldots, x_{n-1}) = \left[(x_1 + 1)^p - 4p^2\right] + \frac{1}{x_1} \left[(x_1 + 1)^p (x_2 + 1)^p - 4p^2\right] + \frac{1}{x_1 x_2} \left[(x_2 + 1)^p (x_3 + 1)^p - 4p^2\right] + \cdots
\]

**Lemma 4.** Let \( p \in (\lambda, -0.79125) \), \( 1 \leq i \leq n - 5, x_i = 3, x_{i+1} = 2, x_1, \ldots, x_{i-1} \in \{1, 2, 3\} \) and \( x_{i+2}, x_{i+3}, \ldots, x_n \in \{2, 3\} \). Then, it holds that \( \Phi_p(x_1, \ldots, x_n) \leq \varphi_p(x_1, \ldots, x_{i-1}) \).

**Proof.** Note that

\[
\Phi_p(x_1, \ldots, x_n) \leq \left[(x_1 + 1)^p - 4p^2\right] + \frac{1}{x_1} \left[(x_1 + 1)^p (x_2 + 1)^p - 4p^2\right] + \frac{1}{x_1 x_2} \left[(x_2 + 1)^p (x_3 + 1)^p - 4p^2\right] + \cdots
\]

Hence,

\[
\Phi_p(x_1, \ldots, x_n) = \varphi_p(x_1, \ldots, x_{i-1}) = \left[(x_1 + 1)^p - 4p^2\right] + \frac{1}{x_1} \left[(x_1 + 1)^p (x_2 + 1)^p - 4p^2\right] + \frac{1}{x_1 x_2} \left[(x_2 + 1)^p (x_3 + 1)^p - 4p^2\right] + \cdots
\]
We need to prove that
\[
\left( \frac{1}{6x_{i+2}} + \frac{1}{6x_{i+2}x_{i+3}} + \frac{1}{6x_{i+2}x_{i+3}x_{i+4}} \right) \cdot 4^p + \frac{1}{2} \cdot 16^p \geq \frac{1}{3} \cdot 12^p + \frac{1}{6} 3^p (x_{i+2} + 1)^p + \frac{1}{6x_{i+2}} (x_{i+2} + 1)^p (x_{i+3} + 1)^p \\
+ \frac{1}{6x_{i+2}x_{i+3}} (x_{i+3} + 1)^p (x_{i+4} + 1)^p + \frac{1}{6x_{i+2}x_{i+3}x_{i+4}} (x_{i+4} + 1)^p (x_{i+5} + 1)^p.
\]
Since $3^p > 4^p$, it is sufficient to prove that
\[
\left( \frac{1}{6x_{i+2}} + \frac{1}{6x_{i+2}x_{i+3}} + \frac{1}{6x_{i+2}x_{i+3}x_{i+4}} \right) \cdot 4^p + \frac{1}{2} \cdot 16^p \geq \frac{1}{3} \cdot 12^p + \frac{1}{6} 3^p (x_{i+2} + 1)^p + \frac{1}{6x_{i+2}} (x_{i+2} + 1)^p (x_{i+3} + 1)^p \\
+ \frac{1}{6x_{i+2}x_{i+3}} (x_{i+3} + 1)^p (x_{i+4} + 1)^p + \frac{1}{6x_{i+2}x_{i+3}x_{i+4}} (x_{i+4} + 1)^p 3^p.
\]
Moreover, it is sufficient to prove that
\[
\left( \frac{1}{6x_{i+2}} + \frac{1}{6x_{i+2}x_{i+3}} + \frac{1}{6x_{i+2}x_{i+3}x_{i+4}} \right) \cdot 4^p + \frac{1}{2} \cdot 16^p \\
\geq \frac{1}{3} \cdot 12^p + \frac{1}{6} 3^p (x_{i+2} + 1)^p + \frac{1}{6x_{i+2}} (x_{i+2} + 1)^p (x_{i+3} + 1)^p \\
+ \frac{1}{6x_{i+2}x_{i+3}} (x_{i+3} + 1)^p (x_{i+4} + 1)^p + \frac{1}{6x_{i+2}x_{i+3}x_{i+4}} (x_{i+4} + 1)^p 3^p
\]
for every $x_{i+2}, x_{i+3}, x_{i+4} \in \{2, 3\}$ and every $p \in \{-0.79265, -0.79255, -0.79245, \ldots, -0.79125\}$, where $p_1 = \frac{10000}{10000}$ and $p_2 = \frac{10000+1}{10000}$. This is verified by computer. □

**Lemma 5.** Let $p \in (\lambda, -0.79125)$, $x_1, \ldots, x_{n-1} \in \{1, 2, 3\}$. Then,
\[
\Phi_p(x_1, \ldots, x_{n-1}, 3) < \Phi_p(x_1, \ldots, x_{n-1}).
\]

**Proof.** It holds that
\[
\Phi_p(x_1, \ldots, x_{n-1}, 3) - \Phi_p(x_1, \ldots, x_{n-1}) = \frac{1}{x_1x_2 \cdots x_{n-2}x_{n-1}} [(x_{n-1} + 1)^p \cdot 4^p - 4^p - \frac{1}{2} (2^p - 4^p)] \\
- \frac{1}{x_1x_2 \cdots x_{n-2}x_{n-1}} [(x_{n-1} + 1)^p \cdot 4^p - 4^p] - \frac{1}{x_1x_2 \cdots x_{n-2}x_{n-1}} \cdot \frac{1}{2} [16^p - 4^p].
\]
Hence, we need to prove that
\[
\frac{1}{2} \left[ 16^p - 4^p \right] > \frac{1}{2} \left[ 4^p - 2^p \right] \\
16^p + 2^p > 2 \cdot 4^p.
\]
Since both sides of the inequality are increasing, it is sufficient to note that
\[
16^p - 0.79264 > 2^p - 0.79264 > 2 \cdot 4^p - 0.79125
\]
holds. □

**Lemma 6.** Let $p \in (\lambda, -0.79125)$, $n \in \mathbb{N}$ and $x_1, \ldots, x_n \in \{1, 2, 3\}$. Then, it holds that $\Phi_p(x_1, \ldots, x_n) \leq \Phi_p(x_1, \ldots, x_n, 3)$.

**Proof.** It holds that
\[
\Phi_p(x_1, \ldots, x_n) - \Phi_p(x_1, \ldots, x_n, 3) = \frac{1}{x_1x_2 \cdots x_{n-2}x_{n-1}} [(x_{n-1} + 1)^p \cdot (x_{n} + 1)^p - 4^p - \frac{2}{x_n} (2^p - 4^p)] \\
- \frac{1}{x_1x_2 \cdots x_{n-2}x_{n-1}} [(x_{n-1} + 1)^p \cdot (x_{n} + 1)^p - 4^p] - \frac{1}{x_1x_2 \cdots x_{n-2}x_{n-1}x_n} [(x_{n} + 1)^p \cdot 4^p - 4^p - \frac{1}{2} (2^p - 4^p)].
\]
Hence, it is sufficient to prove that
\[
-4^p - \frac{2}{x_n} (2^p - 4^p) \leq \frac{1}{x_n} [(x_{n} + 1)^p \cdot 4^p - 4^p - \frac{1}{2} (2^p - 4^p)]
\]
\[
(x_{n-1} \cdot 4^p + (x_{n} + 1)^p \cdot 4^p + \frac{3}{2} (2^p - 4^p)) \geq 0,
\]
which proves the claim. □
Combining Lemmas 3–6, it follows that:

**Lemma 7.** Let $p \in (\lambda, -0.79125)$. It holds that

$$\max_{\ell \in \mathbb{N}} \Phi_p(x_1, \ldots, x_9) < \max \left\{ \max_{\ell \in \mathbb{N}} \varphi_p(1, l \times 2), \max_{\ell \in \mathbb{N}} \varphi_p(l \times 2), \varphi_p(3) \right\}.$$

Let us prove:

**Lemma 8.** Let $p \in (\lambda, -0.79125)$. It holds that $\varphi_p(3) \leq 0$.

**Proof.** $\varphi_p(3) = (4^p - 4^p) + \frac{1}{2} (4^p \cdot 4^p - 4^p) + \frac{1}{6} (16^p - 4^p) < 0$. □

**Lemma 9.** Let $p \in (\lambda, -0.79125)$. It holds that $\max_{\ell \in \mathbb{N}} \varphi_p(l \times 2) \leq 0$.

**Proof.** If $l = 1$, then

$$\varphi_p(x_1, \ldots, x_{n-1}) = \left[ 3^p - 4^p \right] + \frac{1}{2} \left[ 3^p \cdot 4^p - 4^p \right] + \frac{1}{4} \left[ 16^p - 4^p \right] \leq \left[ 3^p - 4^p \right] + \frac{3}{4} \left[ 9^p - 4^p \right].$$

If $l > 1$, then

$$\varphi_p(x_1, \ldots, x_{n-1}) = \left[ 3^p - 4^p \right] + \frac{1}{2} \left[ 9^p - 4^p \right] + \frac{1}{4} \left[ 9^p - 4^p \right] + \cdots + \frac{1}{2^{l-2}} \left[ 9^p - 4^p \right] + \frac{1}{2^{l-2}} \left[ 12^p - 4^p \right] + \frac{1}{2^{l-2}} \left[ 16^p - 4^p \right].$$

Hence, in any case

$$\varphi_p(x_1, \ldots, x_{n-1}) \leq \left[ 3^p - 4^p \right] + \frac{3}{4} \left[ 9^p - 4^p \right].$$

It is sufficient to prove that

$$\frac{7}{4} \cdot 4^p \geq 3^p + \frac{3}{4} \cdot 9^p.$$

Since, both sides of the inequality are increasing, it is sufficient to note that

$$\frac{7}{4} \cdot 4^{-0.79264} \geq 3^{-0.79125} + \frac{3}{4} \cdot 9^{-0.79125}$$

holds. □

**Lemma 10.** Let $p \in (\lambda, -0.79125)$. It holds that $\max_{\ell \in \mathbb{N}} \varphi_p(1, l \times 2) \leq \max \{ 0, \varphi_p(1, 2) \}$.

**Proof.** Let us distinguish four cases:

**CASE 1:** $l = 0$.

It holds that $\varphi_p(1) = (2^p - 4^p) + (8^p - 4^p) + \frac{1}{2} (16^p - 4^p)$. It is sufficient to prove that

$$\frac{5}{2} \cdot 4^p \geq 2^p + 8^p + \frac{1}{2} \cdot 16^p.$$

Since, both sides of the inequality are increasing, it is sufficient to note that

$$\frac{5}{2} \cdot 4^{-0.79264} \geq 2^{-0.79125} + 8^{-0.79125} + \frac{1}{2} \cdot 16^{-0.79125}$$

holds. □

**CASE 2:** $l = 1$.

This case is trivial.

**CASE 3:** $2 \leq l \leq 5$. 

This case is trivial.
It is sufficient to prove that
\[
(2^p - 4^p) + (6^p - 4^p) + \sum_{i=1}^{1} \frac{1}{2i} (9^p - 4^p) + \frac{1}{4} (12^p - 4^p) + \frac{1}{8} (16^p - 4^p) < 0;
\]
\[
(2^p - 4^p) + (6^p - 4^p) + \sum_{i=1}^{2} \frac{1}{2i} (9^p - 4^p) + \frac{1}{8} (12^p - 4^p) + \frac{1}{16} (16^p - 4^p) < 0;
\]
\[
(2^p - 4^p) + (6^p - 4^p) + \sum_{i=1}^{3} \frac{1}{2i} (9^p - 4^p) + \frac{1}{16} (12^p - 4^p) + \frac{1}{32} (16^p - 4^p) < 0;
\]
\[
(2^p - 4^p) + (6^p - 4^p) + \sum_{i=1}^{4} \frac{1}{2i} (9^p - 4^p) + \frac{1}{32} (12^p - 4^p) + \frac{1}{64} (16^p - 4^p) < 0;
\]
i.e.
\[
2^p + 6^p + \sum_{i=1}^{1} \frac{1}{2i} \cdot 9^p + \frac{1}{4} \cdot 12^p + \frac{1}{8} \cdot 16^p < \left( 3 - \frac{1}{8} \right) \cdot 4^p;
\]
\[
2^p + 6^p + \sum_{i=1}^{2} \frac{1}{2i} \cdot 9^p + \frac{1}{8} \cdot 12^p + \frac{1}{16} \cdot 16^p < \left( 3 - \frac{1}{16} \right) \cdot 4^p;
\]
\[
2^p + 6^p + \sum_{i=1}^{3} \frac{1}{2i} \cdot 9^p + \frac{1}{16} \cdot 12^p + \frac{1}{32} \cdot 16^p < \left( 3 - \frac{1}{32} \right) \cdot 4^p;
\]
\[
2^p + 6^p + \sum_{i=1}^{4} \frac{1}{2i} \cdot 9^p + \frac{1}{32} \cdot 12^p + \frac{1}{64} \cdot 16^p < \left( 3 - \frac{1}{64} \right) \cdot 4^p.
\]
Since both sides of the inequality are increasing, it is sufficient to note (similarly as above) that all the inequalities hold when \( p \) is replaced by \(-0.79125\) on the left hand side and by \(-0.79264\) on the right hand side.

**CASE 4: \( I \geq 6 \).**

Note that
\[
\psi (1, I \times 2) < (2^p - 4^p) + (6^p - 4^p) + \sum_{i=1}^{5} \frac{1}{2i} (9^p - 4^p).
\]

Hence, it is sufficient to note that
\[
2^p + 6^p + \sum_{i=1}^{5} \frac{1}{2i} \cdot 9^p < \left( 3 - \frac{1}{32} \right) \cdot 4^p.
\]

Since both sides of the inequality are increasing, it is sufficient to note that
\[
2^{-0.7922} + 6^{-0.7922} + \sum_{i=1}^{5} \frac{1}{2i} \cdot 9^{-0.7922} < \left( 3 - \frac{1}{32} \right) \cdot 4^{-0.79264};
\]
\[
2^{-0.7917} + 6^{-0.7917} + \sum_{i=1}^{5} \frac{1}{2i} \cdot 9^{-0.7917} < \left( 3 - \frac{1}{32} \right) \cdot 4^{-0.7922};
\]
\[
2^{-0.79125} + 6^{-0.79125} + \sum_{i=1}^{5} \frac{1}{2i} \cdot 9^{-0.79125} < \left( 3 - \frac{1}{32} \right) \cdot 4^{-0.7917}.
\]

All the cases are exhausted and the lemma is proved. \( \Box \)

From **Corollary 1** and **Lemmas 7–10**, it follows that:

**Lemma 11.** Let \( p \in \mathbb{N} \setminus [-0.79125) \). It holds that
\[
\max_{\mathbf{x} \in [1,2,3]} \Phi_p (x_1, \ldots, x_n) < 0.
\]
Let
\[ \Phi^0_p (x_1, \ldots, x_n) = \left[ (x_1 + 1)^p - 4^p \right] + \frac{1}{x_1} \left[ (x_1 + 1)^p (x_2 + 1)^p - 4^p \right] + \frac{1}{x_1x_2} \left[ (x_2 + 1)^p (x_3 + 1)^p - 4^p \right] + \cdots \]
\[ + \frac{1}{x_1x_2 \cdots x_{n-2}} \left[ (x_{n-2} + 1)^p \cdot (x_{n-1} + 1)^p - 4^p \right] \]
\[ + \frac{1}{x_1x_2 \cdots x_{n-2}X_{n-1}} \left[ (x_{n-1} + 1)^p \cdot (x_n + 1)^p - 4^p \right] ; \]
\[ \Phi_{p,r} (x_1, \ldots, x_n) = \left[ (x_1 + 1)^{p+r} - 4^p \right] + \frac{1}{x_1} \left[ (x_1 + 1)^{p+r} (x_2 + 1)^{p+r} - 4^p \right] + \frac{1}{x_1x_2} \left[ (x_2 + 1)^{p+r} (x_3 + 1)^{p+r} - 4^p \right] \]
\[ + \cdots + \frac{1}{x_1x_2 \cdots x_{n-2}} \left[ (x_{n-2} + 1)^{p+r} \cdot (x_{n-1} + 1)^{p+r} - 4^p \right] \]
\[ + \frac{1}{x_1x_2 \cdots x_{n-2}X_{n-1}} \left[ (x_{n-1} + 1)^{p+r} \cdot (x_n + 1)^{p+r} - 4^p \right] - \frac{2}{x_n} (2^p - 4^p) \]
\[ \Phi^0_{p,r} (x_1, \ldots, x_n) = \left[ (x_1 + 1)^{p+r} - 4^p \right] + \frac{1}{x_1} \left[ (x_1 + 1)^{p+r} (x_2 + 1)^{p+r} - 4^p \right] \]
\[ + \frac{1}{x_1x_2} \left[ (x_2 + 1)^{p+r} (x_3 + 1)^{p+r} - 4^p \right] + \cdots \]
\[ + \frac{1}{x_1x_2 \cdots x_{n-2}} \left[ (x_{n-2} + 1)^{p+r} \cdot (x_{n-1} + 1)^{p+r} - 4^p \right] \]
\[ + \frac{1}{x_1x_2 \cdots x_{n-2}X_{n-1}} \left[ (x_{n-1} + 1)^{p+r} \cdot (x_n + 1)^{p+r} - 4^p \right] . \]

It can be easily seen that:

**Lemma 12.** Let \( p < 0 \), then \( \Phi^0_p (x_1, \ldots, x_n) > \Phi_p (x_1, \ldots, x_n, y_1, y_2, \ldots, y_k) \).

Let \( X_{10} \) be the set of all 10-tuples of elements from the set \( \{1, 2, 3\} \) that do not contain two consecutive ones; and let \( X_{<10} \) be the set of all sequences of elements from the set \( \{1, 2, 3\} \) of length at most 10 such that they do not contain two consecutive ones and such that the last entry is larger than 1.

It holds:

**Lemma 13.** Let \( p \in [-0.79125, -0.5] \). It holds that
\[ \max_{x_1,\ldots,x_n \in \{1,2,3\}} \Phi_p (x_1, \ldots, x_n) < 0. \]

**Proof.** It is sufficient to prove that
\[
\Phi_p (t) < 0, \quad \text{for every } t \in X_{\leq 10} \text{ and every } p \in [-0.79125, -0.5]
\]
\[
\Phi^0_p (t) < 0, \quad \text{for every } t \in X_{10} \text{ and every } p \in [-0.79125, -0.5].
\]

Let us distinguish two cases:

**CASE 1:** \( p \leq -0.785 \).

It is sufficient to show that
\[
\Phi_{p,0.00005} (t) < 0, \quad \text{for every } t \in X_{\leq 10} \text{ and every } p \in [-0.79125, -0.7912, \ldots, -0.785]
\]
\[
\Phi^0_{p,0.00005} (t) < 0, \quad \text{for every } t \in X_{10} \text{ and every } p \in [-0.79125, -0.7912, \ldots, -0.785].
\]

This is verified by computer.

**CASE 2:** \( p \geq -0.785 \).

It is sufficient to show that
\[
\Phi_{p,0.001} (t) < 0, \quad \text{for every } t \in X_{\leq 10} \text{ and every } p \in [-0.785, -0.784, \ldots, -0.5]
\]
\[
\Phi^0_{p,0.001} (t) < 0, \quad \text{for every } t \in X_{10} \text{ and every } p \in [-0.785, -0.784, \ldots, -0.5].
\]

This is also verified by computer.

All the cases are exhausted and the lemma is proved. □

Combining **Lemmas 11 and 13**, and **Theorem 1**, we get:

**Theorem 2.** Let \( p \in [\lambda, -0.5] \). Then, \( R_p (T_N) < R_p (P_N) \) for every chemical tree \( T_N \) with \( N \geq 4 \) vertices. □
Combining this with the results of papers [8,9], we get:

**Theorem 3.** Let \( p \in [\lambda, 0) \). Then, \( R_p(T_N) < R_p(P_N) \) for every chemical tree \( T_N \) with \( N \geq 4 \) vertices. \( \square \)

This completes our analyses of cases \( p < 0 \). Namely, it has been shown that \( R_p \) satisfies the necessary requirements and may be a suitable measure of branching for \( p \in [\lambda, 0) \). On the other hand \( R_p \), for \( p < \lambda \), does not satisfy the necessary requirements and is not a suitable measure of branching.

3. Analysis of \( R_p \) for \( p \geq 0 \)

First, note that \( R_0(T_N) = N - 1 \) for every tree \( T_N \) with \( N \) vertices, hence obviously, this is not a suitable measure for branching. Further, if \( p > 0 \), then

\[
R_p(p_3) = 2 \cdot 2^p + 2 \cdot 4^p < 4 \cdot 4^p = R_p(K_{1,4}).
\]

Hence requirement (1') cannot hold for any \( p > 0 \). It remains to check for which \( p \) requirement (2') holds. Note that

\[
R_p(K_{1,3}) - R_p(p_4) = 3 \cdot 3^p - 2 \cdot 2^p - 4^p.
\]

Let us analyze function \( h : (0, +\infty) \rightarrow \mathbb{R} \) defined by

\[
h(x) = 3 \cdot 3^x - 2 \cdot 2^x - 4^x.
\]

**Lemma 14.** Function \( h(x) \) has only one positive solution \( \lambda' \). Moreover \( h(x) \) is positive for \( x \in (0, \lambda') \), \( h(\lambda') = 0 \) and \( h(x) \) is negative for \( x > \lambda' \).

**Proof.** It is sufficient to prove that

1. \( h(x) > 0 \) for each \( x \in (0, 2) \);
2. \( h(x) > 0 \) for each \( x \in [2, 2.6) \);
3. \( h(x) < 0 \) for each \( x \geq 2.6 \).

Let us prove (1).

\[
3 \cdot 3^x - 2 \cdot 2^x - 4^x > 3 \cdot 2^{3x/2} - 2 \cdot 2^x - 2^{2x} = (-2^x) \cdot (2^x - 3 \cdot 2^{x/2} + 2) = (-2^x) \cdot (2^{x/2} - 1) \cdot (2^{x/2} - 2) > 0.
\]

Let us prove (2).

\[
3 \cdot 3^x - 2 \cdot 2^x - 4^x = 3 \cdot \left( \frac{3}{2^{3/2}} \right)^x \cdot 2^{3x/2} - 2 \cdot 2^x - 4^x \geq 3 \cdot \left( \frac{3}{2^{3/2}} \right)^2 \cdot 2^{3x/2} - 2 \cdot 2^x - 4^x
\]

\[
= -2^x \left( 2^x - \frac{27}{8} \cdot 2^{x/2} + 2 \right)
\]

\[
= -2^x \left( 2^{x/2} - 1 \right) \cdot \left( 2^{x/2} - \left( \frac{27}{8} - 2^{1.3} \right) \right) + 2 - 2^{1.3} \cdot \left( \frac{27}{8} - 2^{1.3} \right)
\]

Note that \( \frac{27}{8} - 2^{1.3} < 2 \), hence \( 2^{x/2} - \left( \frac{27}{8} - 2^{1.3} \right) > 0 \) and that \( 2 - 2^{1.3} \cdot \left( \frac{27}{8} - 2^{1.3} \right) < 0 \), hence

\[
-2^x \left( 2^{x/2} - 1 \right) \cdot \left( 2^{x/2} - \left( \frac{27}{8} - 2^{1.3} \right) \right) + 2 - 2^{1.3} \cdot \left( \frac{27}{8} - 2^{1.3} \right) > 0.
\]

It remains to prove (3), i.e.

\[
3 \cdot 3^x \cdot \ln 3 - 2 \cdot 2^x \cdot \ln 2 - 4^x \cdot \ln 4 < 0.
\]

It holds that

\[
3 \cdot 3^x \cdot \ln 3 - 2 \cdot 2^x \cdot \ln 2 - 4^x \cdot \ln 4 = 3 \cdot 3 \cdot 3^{2.6} \cdot \left( 3^{x-2.6} - \frac{2 \cdot 2^{2.6} \cdot \ln 2}{3 \cdot \ln 3} \cdot 3^{2.6} \cdot 2^{x-2.6} - \frac{4^{2.6} \cdot \ln 4}{3 \cdot \ln 3} \cdot 3^{2.6} \cdot 2^{x-2.6} \right) = (\ast).
\]

Note that \( \frac{2^{2.6} \ln 2}{3 \ln 3} \cdot 3^{2.6} > \frac{1}{7} \) and \( \frac{4^{2.6} \ln 4}{3 \ln 3} \cdot 3^{2.6} > \frac{6}{7} \). Hence,

\[
(\ast) < 3 \cdot \ln 3 \cdot 3^{2.6} \cdot \left( 3^{x-2.6} - \frac{2 \cdot 2^{2.6} \cdot \ln 2}{3 \cdot \ln 3} \cdot 3^{2.6} \cdot 2^{x-2.6} + \frac{6 \cdot 4^{x-2.6}}{3 \cdot \ln 3} \cdot 3^{2.6} \cdot 2^{x-2.6} \right)
\]

\[
< \{ \text{applying the inequality between arithmetic and geometric mean} \}
\]

\[
< 3 \cdot \ln 3 \cdot 3^{2.6} \cdot \left( 3^{x-2.6} - \left( \frac{2 \cdot 4^0}{1/7} \right)^{x-2.6} \right) < 0.
\]

This proves the lemma. \( \square \)
Hence, \( R_p(K_{1,3}) < R_p(P_4) \) for \( p > \lambda' \) and \( R_p(P_4) < R_p(K_{1,3}) \) for \( p < \lambda' \). In paper [9], it has been proved that
\[
R_p(T_N) < R_p(P_N) \quad \text{for every } p > 0, \text{ every } N \geq 5 \text{ and every tree } T_N \neq P_N \text{ with } N \text{ vertices.}
\]
Hence,

**Theorem 4.** It holds that
\[
R_p(T_N) > R_p(P_N) \quad \text{for every } N \in \mathbb{N}, \text{ every tree } T_N \neq P_n \text{ and every } p \in (0, \lambda');
R_{\lambda'}(K_{1,3}) = R_{\lambda'}(P_4);
R_p(K_{1,3}) < R_p(P_4) \quad \text{for every } p > \lambda'.
\]

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**References**