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NOVEL EXTREMAL RESULTS ON THE RANDIĆ INDEX OF TREES WITH A SPECIFIED TOTAL DOMINATION NUMBER AND IMPLICATIONS IN QSPR MODELING OF ALKANES

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Abstract. The Randić index is a fundamental topological invariant in graph theory, extensively explored for its significance, especially within chemical graph theory. It plays a crucial role in characterizing molecular structures and serves as a key tool for analyzing their properties. It is defined as the sum of the reciprocals of the square root of the product of the degrees of the end vertices for each edge in a graph. Understanding extremal properties of this index has considerable significance. This study refines the existing upper bound on the Randić index of trees in terms of their order and total domination number and identifies the extremal tree structures corresponding to these parameters. To evaluate the effectiveness of the proposed bound in QSPR studies, an in-depth analysis was conducted to examine its correlation with the physicochemical characteristics of alkanes. Utilizing the QSPR approach, models were developed to predict these properties, producing promising and satisfactory outcomes.

Keywords: Randić index, extremal trees, total domination number, QSPR analysis.

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1. Introduction

Consider a connected, simple graph G with a vertex set $V(G)$ and an edge set $E(G)$. An edge connecting two vertices $\alpha_1, \alpha_2 \in V(G)$ is denoted by $\alpha_1\alpha_2$. The open neighborhood of a vertex α is defined as $N(\alpha) = \{\beta \in V(G) \mid \alpha\beta \in E(G)\}$, and its cardinality corresponds to the degree of α, denoted as d_α. A tree $\mathscr{T}$ is a connected acyclic graph, and a pendant vertex in $\mathscr{T}$ has degree one. The symbols S_n and P_n denote the star and path on n vertices, respectively. Additional graph-theoretic terminology can be found in [23].

Topological indices are widely used in chemical graph theory to quantify molecular structure and predict physicochemical properties. The Randić index, introduced in 1975

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[16], is particularly significant due to its strong correlations with properties such as molar volume, boiling point, and molecular stability [9, 21]. It is defined as

$$R(G) = \sum_{\alpha\beta \in E(G)} \frac{1}{\sqrt{d_\alpha d_\beta}}.$$

The R index has been extensively applied in quantitative structure-property relationship (QSPR) modeling, where it serves as a predictive tool for molecular behavior. Trees are especially relevant in this context, as they represent alkane structures, which serve as baseline compounds in physical chemistry. Various physicochemical properties exhibit smooth, incremental variations with increasing chain length, making unbranched alkanes particularly well-suited for the development and validation of QSPR models.

In graph theory, the domination number $\gamma(G)$ is the smallest set of vertices such that every vertex in G is either in the set or adjacent to it [11]. The total domination number (TDN), $\gamma_t(G)$, requires that every vertex be adjacent to at least one in the set [8]. Previous studies have linked the domination number to various topological indices [4, 6, 3, 19], while recent research has examined the TDN in relation to indices like Zagreb [6, 13], geometric-arithmetic [5], and Sombor [20]. Notably, the connection between the Randić index and TDN has been explored in [1, 10].

This paper establishes a new upper bound on the Randić index of trees in terms of their total domination number, extending the results in [10]. To demonstrate its practical significance, the bound is applied in a QSPR study of 15 alkanes, illustrating its correlation with physicochemical properties through regression models. These findings contribute to chemical graph theory and computational chemistry, offering potential applications in molecular property prediction.

2. Upper bound for the Randić index on $\mathscr{T}_{n,\gamma_t}$

Denote by $\mathscr{T}_{n,\gamma_t}$ the set of trees on n vertices and total domination number γ_t. Let $\phi(a,b) = \frac{1}{\sqrt{ab}}$. The subsequent results follow directly.

Lemma 2.1. *Let $\mathscr{T}$ be a tree of order $n \geq 3$. Then*

$$\sqrt{n-1} = R(S_n) \leq R(\mathscr{T}) \leq R(P_n) = \frac{(n-3)}{2} + \sqrt{2}.$$

Lemma 2.2. *The function $\zeta(y) = \frac{1}{\sqrt{y(b+1)}} - \frac{1}{\sqrt{yb}}$ with $y, b \geq 1$ is negative and increasing.*

Consider the construction of a family of trees $\mathscr{H}$ [5]: The path on $4l$ vertices belongs to the class $\mathscr{H}$ for all $l \geq 1$. Suppose $\mathscr{T} \in \mathscr{H}$ and there are vertices $\tau_1, \tau_2 \in V(\mathscr{T})$ such that $N(\tau_1) = \{\theta_1, \tau_2\}$, $N(\tau_2) = \{\tau_1, \theta_2\}$, with both θ_1 and θ_2 having degree 2. Further assume that τ_1, τ_2 are in a minimum total dominating set (TDS) $\mathscr{D}$ in $\mathscr{T}$. Consider two paths P_{4m_1+1} and P_{4m_2+1} of orders $4m_1+1$ and $4m_2+1$, respectively. Construct a new tree $\mathscr{T}'$ by adjoining P_{4m_1+1} and P_{4m_2+1} to $\mathscr{T}$ via edges $\tau_1\eta_1$ and $\tau_2\eta_2$, where η_1 and η_2 are pendant vertices in P_{4m_1+1} and P_{4m_2+1}, respectively. Then $\mathscr{T}' \in \mathscr{H}$ (refer Fig. 1).

Define $\mathscr{H}_{n,\gamma_t} = \{\mathscr{T} \in \mathscr{H} : \ |V(\mathscr{T})| = n, \ |\mathscr{D}(\mathscr{T})| = \gamma_t\}$.

Denote

$$\Phi_{n,\gamma_t} = (n - 2\gamma_t)\Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) + \gamma_t + \sqrt{2} - \frac{3}{2}.$$

Lemma 2.3. *$R(\mathscr{T}) = \Phi_{n,\gamma_t}$ for each $\mathscr{T} \in \mathscr{H}_{n,\gamma_t}$.*

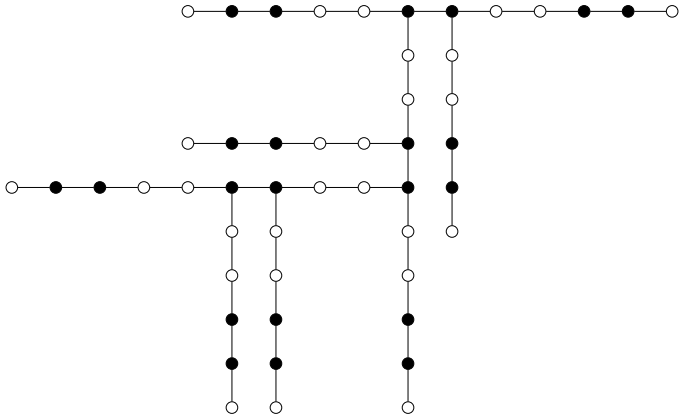


FIGURE 1. A tree from the family $\mathscr{H}$ with $n = 50$ and $\gamma_t = 22$

Proof. Let m_p represent the number of vertices of degree p in a tree. For $\mathscr{T} \in \mathscr{H}_{n,\gamma_t}$,

$$\begin{aligned} n &= m_1 + m_2 + m_3, \\ 2(n-1) &= m_1 + 2m_2 + 3m_3, \\ \gamma_t &= m_3 + \frac{n - 3m_3}{2}. \end{aligned}$$

Hence, $m_1 = n - 2\gamma_t + 2$, $m_2 = 4\gamma_t - n - 2$, and $m_3 = n - 2\gamma_t$. Applying these equations to the definitions of $\mathscr{H}_{n,\gamma_t}$ and the R index,

$$\begin{aligned} R(\mathscr{T}) &= m_1\phi(1,2) + 2m_3\phi(2,3) + \frac{m_3}{2}\phi(3,3) + (n - 1 - m_1 - \frac{5}{2}m_3)\phi(2,2) \\ &= (\frac{1}{\sqrt{2}})(n - 2\gamma_t + 2) + (\frac{2}{\sqrt{6}})(n - 2\gamma_t) + \frac{n - 2\gamma_t}{6} + (\frac{1}{2})\Big(- \frac{5}{2}n + 7\gamma_t - 3\Big) \\ &= (n - 2\gamma_t)\Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) + \gamma_t + \sqrt{2} - \frac{3}{2} \\ &= \Phi_{n,\gamma_t}. \end{aligned}$$

□

Lemma 2.4. *Let* $g(x) = \sqrt{x-1} - (x-4)\Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - \sqrt{2} - \frac{1}{2}$. *Then,* $g(x) < 0$ *whenever* $x \geq 3$.

Proof.

$$g'(x) = \frac{1}{2\sqrt{x-1}} - 0.4403 < 0;\ \forall\ x \geq 3.$$

Thus, $g(x) \leq g(3) = \sqrt{2} + \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - \sqrt{2} - \frac{1}{2} = -0.0597 < 0.$ □

Theorem 2.1 establishes Φ_{n,γ_t} as an upper bound for $R(\mathscr{T})$ and characterizes the extremal trees.

Theorem 2.1. *For* $\mathscr{T} \in \mathscr{T}_{n,\gamma_t}$, *it holds that* $R(\mathscr{T}) \leq \Phi_{n,\gamma_t}$, *with equality occurring if and only if* $\mathscr{T} \in \mathscr{H}_{n,\gamma_t}$.

Proof. When $n = 3$, $R(P_3) = \sqrt{2} < \Phi_{3,2}$. If $n = 4$, $R(S_4) = \sqrt{3} < \Phi_{4,2}$, $R(P_4) = \frac{1}{2} + \sqrt{2} = \Phi_{4,2}$. A tree $\mathscr{T}$ in $\mathscr{T}_{n,\gamma_t}$; $n \geq 5$ is considered under the inductive hypothesis that all trees of order $n - 1$ satisfy the inequality. For a diameter $\tau_1, \tau_2, \ldots, \tau_{d+1}$ of $\mathscr{T}$,

$\mathscr{T} \cong S_n$ whenever $d = 2$, and $R(S_n) - \Phi_{n,2} = \sqrt{n-1} - (n-4)\Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - \sqrt{2} - \frac{1}{2} < 0$ by Lemma 2.4. Assume $d \geq 3$. Denote, $d_{\tau_2} = k,\ N(\tau_2) = \{\tau_1, \tau_3, \omega_1, \ldots, \omega_{k-2}\},\ d_{\tau_3} = q,\ N(\tau_3) = \{\tau_2, \tau_4, \beta_1, \ldots, \beta_{q-2}\},\ d_{\tau_4} = r,\ N(\tau_4) = \{\tau_3, \tau_5, \eta_1, \ldots, \eta_{r-2}\},\ d_{\tau_5} = s,\ N(\tau_5) = \{\tau_4, \tau_6, \theta_1, \ldots, \theta_{s-2}\}$, and $d_{\tau_6} = p,\ N(\tau_6) = \{\tau_5, \tau_7, z_1, \ldots, z_{p-2}\}$. Subsequently, the following claims are established, which facilitate a case-wise analysis. Lemma 2.2 is employed for simplifications.

Claim 1. Consider $d_{\tau_1} = d_{\omega_1} = \cdots = d_{\omega_{k-2}} = 1$ and $d_{\tau_3} \geq 2$. If $k \geq 3$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 1. Let $\mathscr{T}_1 = \mathscr{T} - \{\tau_1\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_1) - (k-2)\phi(k-1,1) + (k-1)\phi(k,1) + \phi(d_{\tau_3},k) - \phi(d_{\tau_3},k-1) \\ &\leq \Phi_{n-1,\gamma_t} + \frac{1}{\sqrt{k}} + (k-2)\Big(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{k-1}}\Big) + \Big(\frac{1}{\sqrt{kd_{\tau_3}}} - \frac{1}{\sqrt{(k-1)d_{\tau_3}}}\Big) \\ &\leq \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) + \frac{1}{\sqrt{3}} + \Big(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\Big) + \Big(\frac{1}{\sqrt{6}} - \frac{1}{2}\Big) \\ &\approx \Phi_{n,\gamma_t} - 0.0844 < \Phi_{n,\gamma_t}. \end{aligned}$$

Claim 2. Consider $d_{\tau_1} = 1,\ d_{\tau_2} = 2,\ d_{\beta_m} \leq 2;\ m \in \{1, 2, \ldots, q-2\}$. If $|\mathscr{D} \cap N(\tau_3)| \geq 2$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 2. Take $\mathscr{T}_2 = \mathscr{T} - \{\tau_1\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_2) - \phi(q,1) + \phi(q,2) + \phi(2,1) \\ &\leq \Phi_{n-1,\gamma_t - 1} + \frac{1}{\sqrt{2q}} - \frac{1}{\sqrt{q}} + \frac{1}{\sqrt{2}} \\ &= \Phi_{n,\gamma_t} + \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 1 + \frac{1}{2} - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \\ &\approx \Phi_{n,\gamma_t} - 0.0597 < \Phi_{n,\gamma_t}. \end{aligned}$$

Claim 3. Consider $d_{\tau_1} = 1,\ d_{\tau_2} = 2,\ d_{\tau_3} \geq 4$. If $d_{\beta_1} = \cdots = d_{\beta_{q-2}} = 1$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 3. Let $\mathscr{T}_3 = \mathscr{T} - \{\beta_{q-2}\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_3) - \phi(q-1,2) - (q-3)\phi(q-1,1) - \phi(d_{\tau_4},q-1) \\ &\quad + \phi(q,2) + (q-2)\phi(q,1) + \phi(d_{\tau_4},q) \\ &< \Phi_{n-1,\gamma_t} + \phi(4,1) + \phi(4,2) - \phi(3,2) + \phi(4,1) - \phi(3,1) \\ &< \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) + \frac{1}{\sqrt{4}} + \Big(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}}\Big) \\ &\approx \Phi_{n,\gamma_t} - 0.0176 < \Phi_{n,\gamma_t}. \end{aligned}$$

Claim 4. Consider $d_{\tau_1} = 1, d_{\tau_2} = 2, d_{\tau_3} = 3, d_{\tau_4} \leq 3$ and $d_{\beta_1} = 1$. Then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 4. Take $\mathscr{T}_4 = \mathscr{T} - \{\beta_1\}$ and as in Claim 3,

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_4) - \phi(2,2) + \phi(3,2) + \phi(3,1) + \phi(d_{\tau_4},3) - \phi(d_{\tau_4},2) \\ &\leq \Phi_{n-1,\gamma_t} - \phi(2,2) + \phi(3,2) + \phi(3,1) + \phi(3,3) - \phi(3,2) \\ &= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - \frac{1}{2} + \frac{1}{\sqrt{3}} + \frac{1}{3} \\ &\approx \Phi_{n,\gamma_t} - 0.0296 < \Phi_{n,\gamma_t}. \end{aligned}$$

Claim 5. Consider $d_{\tau_1} = 1, d_{\tau_2} = 2, d_{\tau_3} = 3, d_{\tau_4} \geq 4$ and $d_{\beta_1} = 1$. If $|N(\tau_4) \cap \mathscr{D}| \geq 2$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 5. Let $\mathscr{T}_5 = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \beta_1\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_5) - \phi(d_{\tau_5}, r-1) + \phi(d_{\tau_5}, r) + \phi(r,3) + \phi(3,2) + \phi(3,1) \\
&\quad + \phi(2,1) + \sum_{m=1}^{r-2} [\phi(d_{\eta_m}, r) - \phi(d_{\eta_m}, r-1)] \\
&< \Phi_{n-4,\gamma_t-2} + \phi(4,3) + \phi(3,2) + \phi(3,1) + \phi(2,1) \\
&= \Phi_{n,\gamma_t} - 2 + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} \\
&\approx \Phi_{n,\gamma_t} - 0.0186 < \Phi_{n,\gamma_t}.
\end{aligned}$$

Claim 6. Consider $d_{\tau_1} = 1, d_{\tau_2} = d_{\tau_3} = 2, d_{\tau_4} \geq 3$. If $|N(\tau_4) \cap \mathscr{D}| \geq 2$ with $d_{\eta_m} \leq 4;\ m \in \{1, \ldots, r-2\}$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 6. Take $\mathscr{T}_6 = \mathscr{T} - \{\tau_1, \tau_2, \tau_3\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_6) - \phi(d_{\tau_5}, r-1) + \phi(d_{\tau_5}, r) + \phi(r,2) + \phi(2,2) + \phi(2,1) \\
&\quad + \sum_{m=1}^{r-2} [\phi(d_{\eta_m}, r) - \phi(d_{\eta_m}, r-1)] \\
&< \Phi_{n-3,\gamma_t-2} + \phi(3,2) + \phi(2,2) + \phi(2,1) + \phi(4,3) - \phi(4,2) \\
&= \Phi_{n,\gamma_t} + \frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12} - 2 + \frac{1}{\sqrt{6}} + \frac{1}{2} + \frac{1}{\sqrt{2}} + \frac{1}{12} - \frac{1}{8} \\
&\approx \Phi_{n,\gamma_t} - 0.0092 < \Phi_{n,\gamma_t}.
\end{aligned}$$

Claim 7. Consider $d_{\tau_1} = 1, d_{\tau_2} = d_{\tau_3} = d_{\tau_4} = 2, d_{\tau_5} \geq 4$ with $d_{\theta_m} \leq 4;\ m \in \{1, \ldots, s-2\}$. Then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 7. Suppose that $\tau_4 \notin \mathscr{D}$. Let $\mathscr{T}_7 = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_7) - \phi(d_{\tau_6}, s-1) + \phi(d_{\tau_6}, s) + \phi(s,2) + 2\phi(2,2) + \phi(2,1) \\
&\quad + \sum_{m=1}^{s-2} [\phi(d_{\theta_m}, s) - \phi(d_{\theta_m}, s-1)] \\
&\leq \Phi_{n-4,\gamma_t-2} + \phi(4,2) + 2\phi(2,2) + \phi(2,1) + 2[\phi(4,4) - \phi(4,3)] \\
&= \Phi_{n,\gamma_t} - 2 + \frac{1}{\sqrt{8}} + 1 + \frac{1}{\sqrt{2}} + 2\Big(\frac{1}{4} - \frac{1}{\sqrt{12}}\Big) \\
&\approx \Phi_{n,\gamma_t} - 0.0167 < \Phi_{n,\gamma_t}.
\end{aligned}$$

Claim 8. Consider $d_{\tau_1} = 1, d_{\tau_2} = d_{\tau_3} = d_{\tau_4} = 2, d_{\tau_5} = 3$, where $\tau_5 \in \mathscr{D}$. Then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 8. Let $\mathscr{T}_8 = \mathscr{T} - \{\tau_1, \tau_2, \tau_3\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_8) - \phi(3,1) + \phi(3,2) + 2\phi(2,2) + \phi(2,1) \\
&\leq \Phi_{n-3,\gamma_t-2} + \phi(3,2) - \phi(3,1) + 2\phi(2,2) + \phi(2,1) \\
&= \Phi_{n,\gamma_t} + \frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12} - 2 + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}} + 1 + \frac{1}{\sqrt{2}} \\
&\approx \Phi_{n,\gamma_t} - 0.0217 < \Phi_{n,\gamma_t}.
\end{aligned}$$

Claim 9. Consider $u_2u_1\theta_1\tau_5$ as a path attached to τ_5 such that $d_{u_2} = 1, d_{u_1} = d_{\theta_1} = 2, d_{\tau_5} = 3$. If $d_{\tau_1} = 1, d_{\tau_2} = d_{\tau_3} = d_{\tau_4} = 2$, along with $d_{\tau_6} \geq 2$ and $d_{\tau_7} \geq 2$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 9. Assume $\tau_4, \tau_5 \notin \mathscr{D}$. Let $\mathscr{T}_9 = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4, \tau_5, \theta_1, u_1, u_2\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_9) - \phi(d_{\tau_7}, p-1) + \phi(d_{\tau_7}, p) + \phi(p,3) + 2\phi(3,2) + 3\phi(2,2) \\ &\quad + 2\phi(2,1) + \sum_{m=1}^{p-2} [\phi(d_{z_m}, p) - \phi(d_{z_m}, p-1)] \\ &< \Phi_{n-8,\gamma_t-4} + \phi(2,2) - \phi(2,1) + \phi(3,2) + 2\phi(3,2) + 3\phi(2,2) + 2\phi(2,1) \\ &= \Phi_{n,\gamma_t} - 4 + \frac{1}{2} - \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} + \frac{3}{2} + \sqrt{2} \\ &\approx \Phi_{n,\gamma_t} - 0.0681 < \Phi_{n,\gamma_t}. \end{aligned}$$

Claim 10. Consider $u_3u_2u_1\theta_1\tau_5$ as a path attached to τ_5 such that $d_{u_3} = 1, d_{u_2} = d_{u_1} = d_{\theta_1} = 2, d_{\tau_5} = 3$. Further, if $d_{\tau_1} = 1$ and $d_{\tau_2} = d_{\tau_3} = d_{\tau_4} = 2$, then $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Proof of Claim 10. Let $\tau_5 \notin \mathscr{D}, \tau_6 \in \mathscr{D}$. If $p \geq 2$, take $\mathscr{T}_{10} = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4, \theta_1, u_1, u_2, u_3\}$.

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_{10}) - \phi(p,1) + \phi(p,3) + 2\phi(3,2) + 4\phi(2,2) + 2\phi(2,1) \\ &\leq \Phi_{n-8,\gamma_t-4} + \phi(3,2) - \phi(2,1) + 2\phi(3,2) + 4\phi(2,2) + 2\phi(2,1) \\ &= \Phi_{n,\gamma_t} - 4 + \frac{3}{\sqrt{6}} + 2 + \frac{1}{\sqrt{2}} \\ &\approx \Phi_{n,\gamma_t} - 0.0681 < \Phi_{n,\gamma_t}. \end{aligned}$$

Let $d_{\tau_7} = i,\ N(\tau_7) = \{\tau_6, \tau_8, y_1, \ldots, y_{i-2}\}$ and $d_{\tau_8} = l,\ N(\tau_8) = \{\tau_7, \tau_9, x_1, \ldots, x_{l-2}\}$. It follows from Claims 1-10 that $d \geq 7$ with $d_{\tau_2} = d_{\tau_3} = d_{\tau_4} = d_{\tau_5} = 2$, where $\tau_2, \tau_3, \tau_6 \in \mathscr{D}$ and $\tau_4, \tau_5 \notin \mathscr{D}$, as $R(P_5) < \Phi_{5,3}$, $R(P_6) < \Phi_{6,4}$, and $R(P_7) < \Phi_{7,4}$. Furthermore, it can be supposed that every vertex $z \in N(\tau_6) \setminus \{\tau_5, \tau_7\}$ satisfies $d_z \leq 2$.

Case 1. Let $d_{\tau_6} = 2$. Take $\mathscr{T}_{11} = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_{11}) - \phi(2,1) + \phi(2,2) + 3\phi(2,2) + \phi(2,1) \\ &\leq \Phi_{n-4,\gamma_t-2} + 2 \\ &= \Phi_{n,\gamma_t} - 2 + 2 = \Phi_{n,\gamma_t}, \end{aligned}$$

with equality holding precisely when $\mathscr{T}_{11} \in \mathscr{T}_{n-4,\gamma_t-2}$. i.e., $\mathscr{T} \in \mathscr{H}_{n,\gamma_t}$ (see Fig. 2).

Case 2. Let $d_{\tau_6} = 3$.

Case 2.1. Consider $d_{z_1} = 1$.

Case 2.1.1. For $d_{\tau_7} \leq 3$, take $\mathscr{T}_{12} = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4, \tau_5\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_{12}) - \phi(d_{\tau_7}, 2) + \phi(d_{\tau_7}, 3) - \phi(2,1) + \phi(3,1) + \phi(3,2) \\ &\quad + 3\phi(2,2) + \phi(2,1) \\ &\leq \Phi_{n-5,\gamma_t-2} - \phi(3,2) + \phi(3,3) + \phi(3,2) + 3\phi(2,2) + \phi(3,1) \\ &= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 2 + \frac{1}{3} + \frac{1}{\sqrt{3}} + \frac{3}{2} \\ &\approx \Phi_{n,\gamma_t} - 0.0296 < \Phi_{n,\gamma_t}. \end{aligned}$$

Case 2.1.2. Consider $d_{\tau_7} \geq 4$.

Case 2.1.2.1. Let $|N(\tau_7) \cap \mathscr{D}| \geq 2$ and $d_{y_m} \leq 3$; $m \in \{1, \ldots, i-2\}$. Take $\mathscr{T}_{13} = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4, \tau_5, \tau_6, z_1\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_{13}) - \phi(d_{\tau_8}, i-1) + \phi(d_{\tau_8}, i) + \phi(i,3) + \phi(3,2) + \phi(3,1) \\
&\quad + 3\phi(2,2) + \phi(2,1) + \sum_{m=1}^{i-2} [\phi(d_{y_m}, i) - \phi(d_{y_m}, i-1)] \\
&< \Phi_{n-7,\gamma_t-3} + \phi(4,3) + \phi(3,2) + \phi(3,1) + 3\phi(2,2) + \phi(2,1) + 2[\phi(4,3) - \phi(3,3)] \\
&= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 3 + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{3}{2} + \frac{1}{\sqrt{2}} + 2\Big(\frac{1}{\sqrt{12}} - \frac{1}{3}\Big) \\
&\approx \Phi_{n,\gamma_t} - 0.0482 < \Phi_{n,\gamma_t}.
\end{aligned}$$

Case 2.1.2.2. Let $N(\tau_7) \cap \mathscr{D} = \{\tau_6\}$.
Case 2.1.2.2.1. Assume that $d_{y_1} \geq 2$. Then, by the previously established claims, there exists a pendant path $\tau_7 y_1 b_1 b_2 b_3 b_4$ attached at τ_7, where $d_{y_1} = d_{b_1} = d_{b_2} = d_{b_3} = 2$ and $d_{b_4} = 1$. Given that $d_{\tau_7} \geq 4$, it follows from the preceding cases that $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.
Case 2.1.2.2.2. When $d_{y_m} = 1$; $m \in \{1, 2, \ldots, i-2\}$, take $\mathscr{T}_{14} = \mathscr{T} - \{y_1\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_{14}) - \phi(d_{\tau_8}, i-1) + \phi(d_{\tau_8}, i) - \phi(i-1,3) + \phi(i,3) \\
&\quad + \phi(i,1) + (i-3)[\phi(i,1) - \phi(i-1,1)] \\
&< \Phi_{n-1,\gamma_t} + \phi(4,3) - \phi(3,3) + \phi(4,1) + \phi(4,1) - \phi(3,1) \\
&= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) + \frac{1}{\sqrt{12}} - \frac{1}{3} + 1 - \frac{1}{\sqrt{3}} \\
&\approx \Phi_{n,\gamma_t} - 0.0623 < \Phi_{n,\gamma_t}.
\end{aligned}$$

Case 2.2. Let $d_{z_1} = 2$. Then there is a pendant path $\tau_6 z_1 v_1 v_2 v_3 v_4$ attached to τ_6 with $d_{v_1} = d_{v_2} = d_{v_3} = 2$ and $d_{v_4} = 1$, based on the claims proved above.
Case 2.2.1. For $d_{\tau_7} = 2$, take $\mathscr{T}_{15} = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4, \tau_5\}$. Then

$$\begin{aligned}
R(\mathscr{T}) &= R(\mathscr{T}_{15}) - \phi(d_{\tau_7}, 2) + \phi(d_{\tau_7}, 3) - \phi(2,2) + \phi(3,2) + \phi(3,2) \\
&\quad + 3\phi(2,2) + \phi(2,1) \\
&\leq \Phi_{n-5,\gamma_t-2} + 3\phi(3,2) + \phi(2,2) + \phi(2,1) \\
&= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 2 + \frac{3}{\sqrt{6}} + \frac{1}{2} + \frac{1}{\sqrt{2}} \\
&\approx \Phi_{n,\gamma_t} - 0.0084 < \Phi_{n,\gamma_t}.
\end{aligned}$$

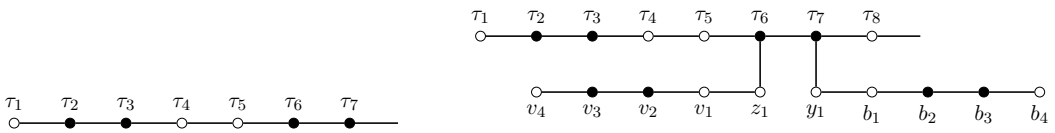


FIGURE 2. Trees with equality conditions in Cases 1 and 2.2.2.2.2.1, respectively

Case 2.2.2. Consider $d_{\tau_7} \geq 3$.

Case 2.2.2.1. While $|N(\tau_7)\cap\mathscr{D}|\geq 2$, consider $d_{y_m}\leq 3;\ m\in\{1,2,\ldots,i-2\}$. If $d_{\tau_8}\geq 2$, take $\mathscr{T}_{16}=\mathscr{T}-\{\tau_1,\tau_2,\tau_3,\tau_4,\tau_5,\tau_6,z_1,v_1,v_2,v_3,v_4\}$. Then

$$\begin{aligned}R(\mathscr{T}) &= R(\mathscr{T}_{16})-\phi(d_{\tau_8},i-1)+\phi(d_{\tau_8},i)+\phi(i,3)+2\phi(3,2)+6\phi(2,2)\\ &\quad+2\phi(2,1)+\sum_{m=1}^{i-2}[\phi(d_{y_m},i)-\phi(d_{y_m},i-1)]\\ &\leq \Phi_{n-11,\gamma_t-5}+\phi(3,2)-\phi(2,2)+\phi(3,3)+2\phi(3,2)+6\phi(2,2)+2\phi(2,1)\\ &\quad+\phi(3,3)-\phi(3,2)\\ &= \Phi_{n,\gamma_t}-\Big(\frac{2+\sqrt{3}}{\sqrt{6}}-\frac{13}{12}\Big)-5+\frac{2}{3}+\frac{2}{\sqrt{6}}+3+\sqrt{2}-\frac{1}{2}\\ &\approx \Phi_{n,\gamma_t}-0.0429<\Phi_{n,\gamma_t}.\end{aligned}$$

Case 2.2.2.2. Let $N(\tau_7)\cap\mathscr{D}=\{\tau_6\}$, and suppose $d_{y_m}\leq 2;\ m\in\{1,2,\ldots,i-2\}$.
Case 2.2.2.2.1. Consider $d_{y_1}=1$.
Case 2.2.2.2.1.1. While $d_{\tau_7}\geq 4$, take $\mathscr{T}_{17}=\mathscr{T}-\{y_1\}$. Then

$$\begin{aligned}R(\mathscr{T}) &= R(\mathscr{T}_{17})-\phi(d_{\tau_8},i-1)+\phi(d_{\tau_8},i)-\phi(i-1,3)+\phi(i,3)+\phi(i,1)\\ &\quad+\sum_{m=1}^{i-2}[\phi(d_{y_m},i)-\phi(d_{y_m},i-1)]\\ &< \Phi_{n-1,\gamma_t}+\phi(4,3)-\phi(3,3)+\phi(4,1)+2[\phi(4,2)-\phi(3,2)]\\ &= \Phi_{n,\gamma_t}-\Big(\frac{2+\sqrt{3}}{\sqrt{6}}-\frac{13}{12}\Big)+\frac{1}{\sqrt{12}}-\frac{1}{3}+\frac{1}{2}+2\Big(\frac{1}{\sqrt{8}}-\frac{1}{\sqrt{6}}\Big)\\ &\approx \Phi_{n,\gamma_t}-0.0943<\Phi_{n,\gamma_t}.\end{aligned}$$

Case 2.2.2.2.1.2. Let $d_{\tau_7}=3$.
Case 2.2.2.2.1.2.1. While $d_{\tau_8}\leq 3$, take $\mathscr{T}_{18}=\mathscr{T}-\{y_1,z_1,v_1,v_2,v_3,v_4\}$. Then

$$\begin{aligned}R(\mathscr{T}) &= R(\mathscr{T}_{18})-\phi(d_{\tau_8},2)+\phi(d_{\tau_8},3)-\phi(2,2)+\phi(3,2)-\phi(2,2)\\ &\quad+\phi(3,3)+\phi(3,1)+\phi(3,2)+3\phi(2,2)+\phi(2,1)\\ &\leq \Phi_{n-6,\gamma_t-2}+2\phi(3,3)+\phi(3,2)+\phi(2,2)+\phi(3,1)+\phi(2,1)\\ &= \Phi_{n,\gamma_t}-2\Big(\frac{2+\sqrt{3}}{\sqrt{6}}-\frac{13}{12}\Big)-2+\frac{2}{3}+\frac{1}{\sqrt{6}}+\frac{1}{2}+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{2}}\\ &\approx \Phi_{n,\gamma_t}-0.0212<\Phi_{n,\gamma_t}.\end{aligned}$$

Case 2.2.2.2.1.2.2. Let $d_{\tau_8}\geq 4$.
Case 2.2.2.2.1.2.2.1. Take $\mathscr{T}_{19}$ and $\mathscr{T}_{20}$ as sub-trees of $\mathscr{T}-\tau_7\tau_8$ containing τ_7 and τ_8, respectively on the condition that $|N(\tau_8)\cap\mathscr{D}|\geq 2$. Then

$$\begin{aligned}R(\mathscr{T}) &= R(\mathscr{T}_{19})+R(\mathscr{T}_{20})-\phi(3,2)+\phi(3,3)-\phi(2,1)+\phi(3,1)+\phi(l,3)\\ &\quad-\phi(d_{\tau_9},l-1)+\phi(d_{\tau_9},l)+\sum_{m=1}^{l-2}[\phi(d_{x_m},l)-\phi(d_{x_m},l-1)]\\ &\leq \Phi_{n,\gamma_t}+\sqrt{2}-\frac{3}{2}+\phi(4,3)+\phi(3,1)+\phi(3,3)-\phi(2,1)-\phi(3,2)\\ &= \Phi_{n,\gamma_t}+\sqrt{2}-\frac{3}{2}+\frac{1}{\sqrt{12}}+\frac{1}{\sqrt{3}}+\frac{1}{3}-\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{2}}\\ &\approx \Phi_{n,\gamma_t}-0.0018<\Phi_{n,\gamma_t}.\end{aligned}$$

Case 2.2.2.2.1.2.2.2. Suppose $N(\tau_8) \cap \mathscr{D} = \{\tau_7\}$. Any path from τ_8 to a pendant vertex that passes through vertices of the form $\tau_8 x_m$, where $m \in \{1, 2, \ldots, l-2\}$, has length 4. Based on the previously established claims, it follows that $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.
Case 2.2.2.2.2. Suppose that $d_{y_m} = 2$ for all $m \in \{1, 2, \ldots, i-2\}$. Then, any path from τ_7 to a pendant vertex passing through vertices of the form $\tau_7 y_m$ has length 5. From the above cases and the condition $d_{\tau_7} \geq 3$, it follows that $d_{\tau_7} = 3$. Consequently, there exists a pendant path $\tau_7 y_1 b_1 b_2 b_3 b_4$ on six vertices attached at τ_7, where $d_{y_1} = d_{b_1} = d_{b_2} = d_{b_3} = 2$ and $d_{b_4} = 1$.
Case 2.2.2.2.2.1. For $d_{\tau_8} = 2$, take $\mathscr{T}_{21} = \mathscr{T} - \{z_1, v_1, v_2, v_3, v_4, y_1, a_1, a_2, a_3, a_4\}$. Then

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_{21}) - \phi(2,2) + \phi(3,3) - 2\phi(2,2) + 2\phi(3,2) + 6\phi(2,2) \\ &\quad + 2\phi(3,3) + 2\phi(2,1) \\ &\leq \Phi_{n-10,\gamma_t-4} + \phi(3,3) + 4\phi(3,2) + 3\phi(2,2) + 2\phi(2,1) \\ &= \Phi_{n,\gamma_t} - 2\Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 4 + \frac{1}{3} + \frac{4}{\sqrt{6}} + \frac{3}{2} + \sqrt{2} \\ &= \Phi_{n,\gamma_t}, \end{aligned}$$

with equality holding precisely when $\mathscr{T}_{21} \in \mathscr{T}_{n-10,\gamma_t-4}$. i.e., $\mathscr{T} \in \mathscr{H}_{n,\gamma_t}$ (see Fig. 2).
Case 2.2.2.2.2.2. Let $d_{\tau_8} \geq 3$.
Case 2.2.2.2.2.2.1. Consider $|N(\tau_8) \cap \mathscr{D}| \geq 2$. Let $\mathscr{T}_{22}$ and $\mathscr{T}_{23}$ be the subtrees of $\mathscr{T} - \tau_7\tau_8$ that contain τ_7 and τ_8, respectively. Assume further that $d_{x_m} \leq 3$ for all $m \in \{1, \ldots, l-2\}$. Then,

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_{22}) + R(\mathscr{T}_{23}) - \phi(3,2) + \phi(3,3) - \phi(2,2) + \phi(3,2) + \phi(l,3) \\ &\quad - \phi(d_{\tau_9}, l-1) + \phi(d_{\tau_9}, l) + \sum_{m=1}^{l-2} [\phi(d_{x_m}, l) - \phi(d_{x_m}, l-1)] \\ &< R(\mathscr{T}_{22}) + R(\mathscr{T}_{23}) + \phi(3,3) + \phi(3,2) - \phi(2,2) + \phi(3,3) - \phi(3,2) + \phi(3,3) - \phi(3,2) \\ &= 10\phi(2,2) + 3\phi(3,2) + 3\phi(2,1) + R(\mathscr{T}_{23}) + 3\phi(3,3) - \phi(3,2) - \phi(2,2) \\ &\leq \Phi_{n-17,\gamma_t-8} + 2\phi(3,2) + 3\phi(2,1) + 9\phi(2,2) + 3\phi(3,3) \\ &= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 8 + \frac{2}{\sqrt{6}} + \frac{3}{\sqrt{2}} + 1 + \frac{9}{2} \\ &\approx \Phi_{n,\gamma_t} - 0.00248 < \Phi_{n,\gamma_t}. \end{aligned}$$

Case 2.2.2.2.2.2.2. Assume that $N(\tau_8) \cap \mathscr{D} = \{\tau_7\}$. Then, any path from τ_8 to a pendant vertex that passes through vertices of the form $\tau_8 x_m$, where $m \in \{1, 2, \ldots, l-2\}$, has length 4. Based on the previously established claims, it follows that $R(\mathscr{T}) < \Phi_{n,\gamma_t}$.

Case 3. Let $d_{\tau_6} \geq 4$. For $d_{z_m} \leq 3$; $m \in \{1, \ldots, p-2\}$ and $d_{\tau_7} \geq 2$, take $\mathscr{T}_{24} = \mathscr{T} - \{\tau_1, \tau_2, \tau_3, \tau_4, \tau_5\}$.

$$\begin{aligned} R(\mathscr{T}) &= R(\mathscr{T}_{24}) - \phi(d_{\tau_7}, p-1) + \phi(d_{\tau_7}, p) + \phi(p, 2) + 3\phi(2,2) + \phi(2,1) \\ &\quad + \sum_{m=1}^{p-2} [\phi(d_{z_m}, p) - \phi(d_{z_m}, p-1)] \\ &\leq \Phi_{n-5,\gamma_t-2} + \phi(4,2) - \phi(3,2) + \phi(4,2) + 3\phi(2,2) + \phi(2,1) + 2[\phi(4,3) - \phi(3,3)] \\ &= \Phi_{n,\gamma_t} - \Big(\frac{2+\sqrt{3}}{\sqrt{6}} - \frac{13}{12}\Big) - 2 + \frac{2}{\sqrt{8}} + \frac{2}{\sqrt{12}} - \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{3}{2} - \frac{2}{3} \\ &\approx \Phi_{n,\gamma_t} - 0.0236 < \Phi_{n,\gamma_t}. \end{aligned}$$

□

Remark 2.1. *In* [10]*, the authors established the following upper bound and identified the extremal trees that achieve it.*

$$R(T) \leq \frac{2n + (-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n + 1 - 2\gamma_t)\Big(\frac{\sqrt{14}-3}{2}\Big).$$

Let

$$\Phi^*_{n,\gamma_t} = \frac{2n + (-1)^n}{8} + \frac{\gamma_t}{2} + \sqrt{2} - \frac{13}{8} + (n + 1 - 2\gamma_t)\Big(\frac{\sqrt{14}-3}{2}\Big).$$

Without loss of generality, let n be odd so that

$$\Phi^*_{n,\gamma_t} = (n - 2\gamma_t)\Big(\frac{\sqrt{14}-3}{2} + \frac{1}{4}\Big) + \gamma_t + \sqrt{2} - \frac{3}{2} + \frac{\sqrt{14}}{2} - \frac{7}{4}.$$

Then,

$$\begin{aligned} \Phi^*_{n,\gamma_t} - \Phi_{n,\gamma_t} &= \Big\{(n - 2\gamma_t)\Big(\frac{\sqrt{14}-3}{2} + \frac{1}{4}\Big) + \gamma_t + \sqrt{2} - \frac{3}{2} + \frac{\sqrt{14}}{2} - \frac{7}{4}\Big\} \\ &\quad - \Big\{(n - 2\gamma_t)\Big(\frac{\sqrt{3}+2}{\sqrt{6}} - \frac{13}{12}\Big) + \gamma_t + \sqrt{2} - \frac{3}{2}\Big\} \\ &\approx (n - 2\gamma_t)(0.1805) + 0.1208 > 0. \end{aligned}$$

Hence, the bound proved in Theorem 2.1 is stronger than that obtained in [10] *whenever* $\frac{n}{2} > \gamma_t$.

3. QSPR analysis of alkanes

The structural composition of a molecule plays a crucial role in determining its biological and physicochemical properties, which can be analyzed and predicted using QSAR/QSPR modeling [2]. These methods employ mathematical and statistical techniques to identify and quantify the relationship between molecular characteristics and their associated properties [12, 24]. Regression models play a key role in linking physicochemical and biological characteristics to molecular descriptors [17, 18]. In this context, graph-theoretic topological indices are employed to transform chemical compounds into graphical representations. The objective of this section is to explore the relevance and implications of the newly derived bound. The experimental values for some selected physicochemical properties of 15 alkanes, such as the flash point-cc (FP), $\log P$, molar refraction (MR), molar volume (MV), parachor (PR), polarizability (α), boiling point (BP), and melting point (MP), are summarized in Table 1. These values are taken from existing literature source [14], PubChem [15], and ChemSpider [7]. The analysis and graphical representations were performed using Python and Microsoft Excel.

Sl. No.	Alkane	FP (°C)	$\log P$	MR (cm^3/mol)	MV (cm^3/mol)	PR	α (Å^3)	BP (°C)	MP (°C)
1	Pentane	-49	3.67	29.84	127.5	270.8	11.83	36	-129
2	Hexane	-22	4.21	34.47	144	310.6	13.66	69	-95
3	Heptane	-7	4.74	39.11	160.5	350.4	15.5	98.4	-90.6
4	Octane	13	5.28	43.74	177	390.2	17.34	126	-56.8
5	Nonane	31	5.82	48.37	193.6	430	19.17	150.8	-53.47
6	Decane	46	6.35	53.01	210.1	469.7	21.01	174.1	-29.7
7	Undecane	62	6.89	57.64	226.6	509.5	22.85	195.9	-25.54
8	Dodecane	74	7.42	62.27	243.1	549.3	24.28	216.3	-9.6
9	Tridecane	94	7.96	66.9	259.6	589.1	26.52	235.4	-5.5
10	Tetradecane	100	8.5	71.54	276.1	628.9	28.36	253.57	5.87
11	Pentadecane	132.2	9.03	76.17	292.6	668.7	30.19	270.6	9.95
12	Hexadecane	135	9.57	80.8	309.1	708.4	32.03	286.9	18.18
13	Heptadecane	149	10.1	85.44	325.6	748.2	33.87	303	21.97
14	Octadecane	166	10.64	90.07	342.1	788	35.7	316	28
15	Nonadecane	168	11.18	94.7	358.6	825.8	37.4	330	32

TABLE 1. Experimental physicochemical properties of alkanes

The chemical graphs of unbranched alkanes are structurally equivalent to path graphs. Chemical graphs are constructed from molecular structures by considering atoms as vertices and the bonds between them as edges, without accounting for hydrogen atoms or bond multiplicity [22]. Calculated values of R index, γ_t, Φ_{n,γ_t} and molecular weight (MW) for the candidate alkanes are displayed in Table 2.

Sl. No.	Alkane	n	γ_t	R	Φ_{n,γ_t}	MW (g/mol)
1	Pentane	5	3	2.4142	2.4739	72.15
2	Hexane	6	4	2.9142	3.0337	86.18
3	Heptane	7	4	3.4142	3.4739	100.2
4	Octane	8	4	3.9142	3.9142	114.23
5	Nonane	9	5	4.4142	4.4739	128.25
6	Decane	10	6	4.9142	5.0337	142.28
7	Undecane	11	6	5.4142	5.4739	156.31
8	Dodecane	12	6	5.9142	5.9142	170.33
9	Tridecane	13	7	6.4142	6.4739	184.36
10	Tetradecane	14	8	6.9142	7.0337	198.39
11	Pentadecane	15	8	7.4142	7.4739	212.41
12	Hexadecane	16	8	7.9142	7.9142	226.41
13	Heptadecane	17	9	8.4142	8.4739	240.5
14	Octadecane	18	10	8.9142	9.0337	254.5
15	Nonadecane	19	10	9.4142	9.4739	268.5

TABLE 2. Φ_{n,γ_t} values and corresponding basic parameters for the candidate alkanes

To assess whether the predictive ability of Φ_{n,γ_t} primarily arises from chain-length effects, comparative and partial correlation analyses were conducted using n, MW, and the R index as baseline descriptors. The linear correlations (r) of Φ_{n,γ_t} with these parameters are presented in Table 3. Furthermore, multiple linear regression analysis was performed

by incorporating n, MW, and the original R index alongside Φ_{n,γ_t} to evaluate the independent contribution of each variable, with the results for MV are summarized in Table 4.

	n	R	MW
Φ_{n,γ_t}	0.9998	0.9998	0.9998

TABLE 3. r values between Φ_{n,γ_t} and various basic parameters

Model No.	Multiple Regression Model		
1	$MV = 16.4757n + 0.0644\Phi_{n,\gamma_t} + 44.9805$		
2	$MV = 1.1792MW - 0.06398\Phi_{n,\gamma_t} + 42.5971$		
3	$MV = 32.9513R + 0.0644\Phi_{n,\gamma_t} + 47.8072$		
	Model 1	Model 2	Model 3
Multiple r	1	1	1
R^2	1	1	1
SE	0.03155	0.03678	0.03155
F-statistic	3.8E+07	2.8E+07	3.8E+07
p_F	1.5E-41	9.3E-41	1.5E-41

TABLE 4. Multiple linear regression using basic parameters for MV

3.1. **Regression models for the physicochemical properties.** Based on the linear correlation coefficients and scatter plot observations, linear regression analyses were performed for the selected alkanes to examine their relationships with physicochemical properties such as molar refractivity (MR), molar volume (MV), parachor (PR), $\log P$, and polarizability (α). For boiling point (BP), flash point (FP), and melting point (MP), cubic regression models were employed, with each property considered as the dependent variable and Φ_{n,γ_t} as the independent variable. The general forms of the regression models used are expressed as $Y = x_0 + x_1 Z$ for linear and $Y = x_0 + x_1 Z + x_2 Z^2 + x_3 Z^3$ for cubic relationships, where Y denotes the physicochemical property and Z represents Φ_{n,γ_t}. Model performance was evaluated using the coefficient of determination (R^2), mean absolute error (MAE), root mean square error (RMSE), standard error (SE), F-statistic and its probability (p_F). The results of these analyses are summarized in Tables 5 and 6, respectively. Since the dataset comprises 15 compounds, a Leave-One-Out (LOO) cross-validation (CV) was performed to evaluate model generalization and minimize the risk of overfitting. The cross-validated R^2 and RMSE values are reported alongside the results.

The predicted values of the physicochemical properties obtained from the above analysis are listed in Table 7. The scatter plots in Fig. 3–10 illustrate the graphical comparison between the experimental and predicted values for all the considered properties. For each corresponding scatter plot, the residual plots (shown in the same figure number) are provided to visualize the distribution of prediction errors and to assess the goodness of fit and model adequacy.

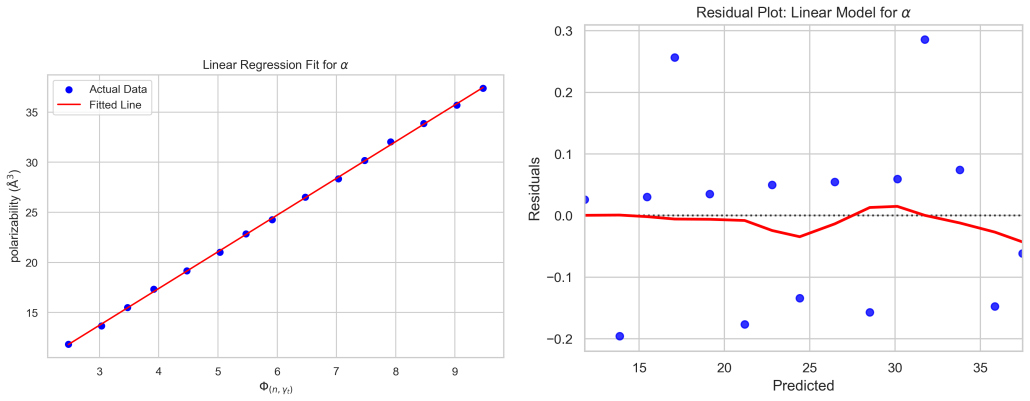
3.2. **Discussion.** Although Φ_{n,γ_t} exhibits strong correlations with the target properties, part of this trend may arise from chain-length dependence. To ensure its independent predictive capability, comparative and partial correlation analyses were performed against basic size descriptors such n, MW, and the R index (Table 4). The results confirm that

	log P	MR	MV	PR	α
R^2	0.9997	0.9996	0.9996	0.9996	0.9997
Adjusted R^2	0.9996	0.9996	0.9996	0.9996	0.9997
RMSE	0.043	0.3754	1.3382	3.245	0.142
MAE	0.0314	0.2748	0.9804	2.4429	0.1162
SE	0.0462	0.4032	1.4374	3.4857	0.1525
F-statistic	3.77E+04	3.70E+04	3.69E+04	3.64E+04	4.05E+04
p_F	6.82E-24	7.70E-24	7.75E-24	8.54E-24	4.28E-24
x_0	1.0166	6.9	45.7779	74.2972	2.7366
x_1	1.0718	9.2627	33.0041	79.4385	3.6653
R^2 (CV)	0.9995	0.9995	0.9995	0.9995	0.9996
RMSE (CV)	0.0493	0.4295	1.5315	3.7104	0.1633

TABLE 5. Linear regression analysis

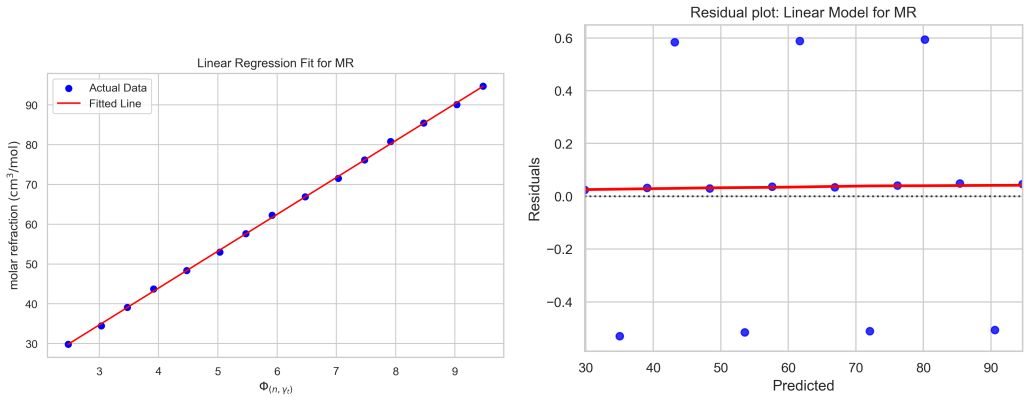
	BP	FP	MP
R^2	0.9996	0.996	0.992
Adjusted R^2	0.999	0.995	0.99
RMSE	1.8617	4.2958	4.1789
MAE	1.4263	3.07	3.1292
SE	2.174	5.0164	4.8799
F-statistic	8.50E+03	9.04E+02	4.83E+02
p_F	8.72E-19	1.93E-13	5.91E-12
x_0	-162.6724	-154.032	-296.3553
x_1	95.0985	47.1389	87.796
x_2	-6.5354	-1.4299	-8.6379
x_3	0.2097	0.0095	0.3202
R^2 (CV)	0.9993	0.9906	0.9872
RMSE (CV)	2.3675	6.564	5.4567

TABLE 6. Cubic regression analysis



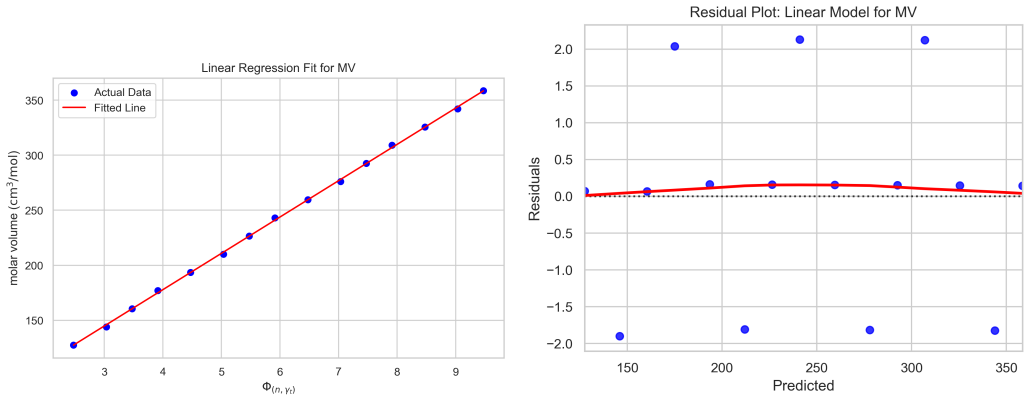
(a) (b)

FIGURE 3. Scatter and residual plots for linear regression models of α



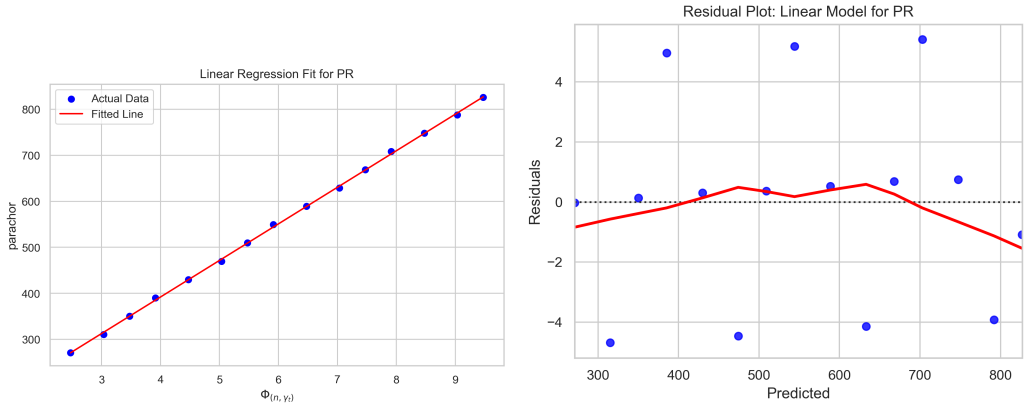
(a) (b)

FIGURE 4. Scatter and residual plots for linear regression models of MR



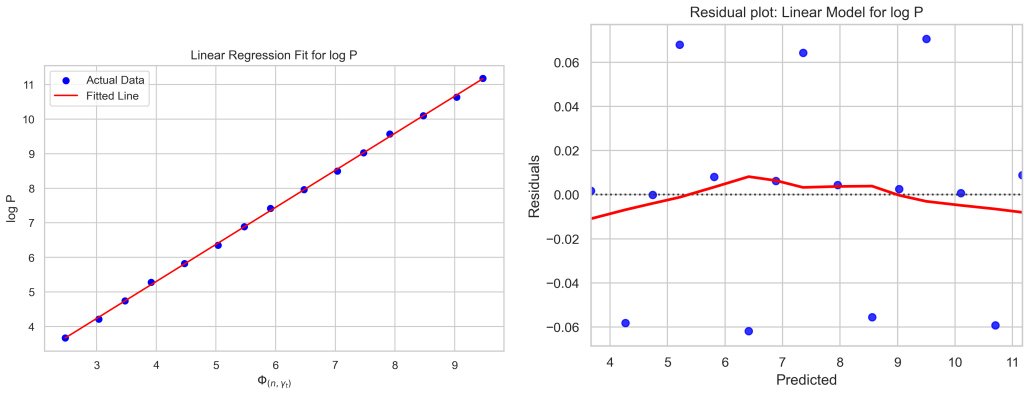
(a) (b)

FIGURE 5. Scatter and residual plots for linear regression models of MV



(a) (b)

FIGURE 6. Scatter and residual plots for linear regression models of PR



(a) (b)

FIGURE 7. Scatter and residual plots for linear regression models of log P

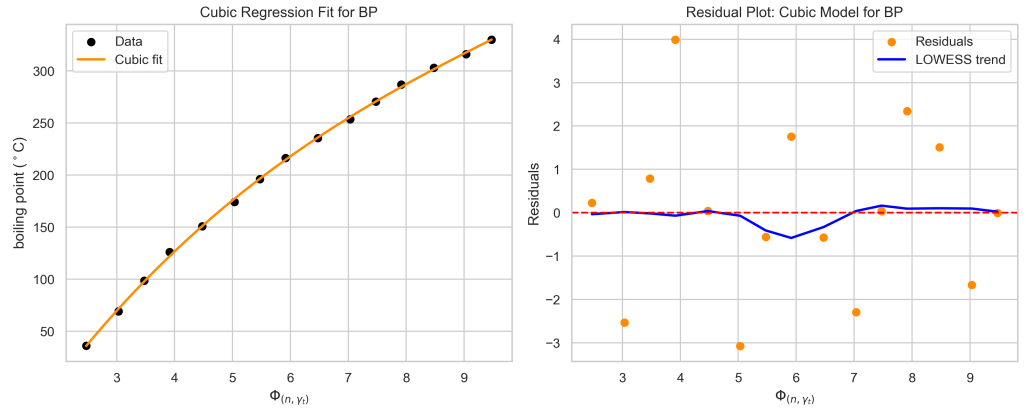


FIGURE 8. Scatter and residual plots for cubic regression models of BP

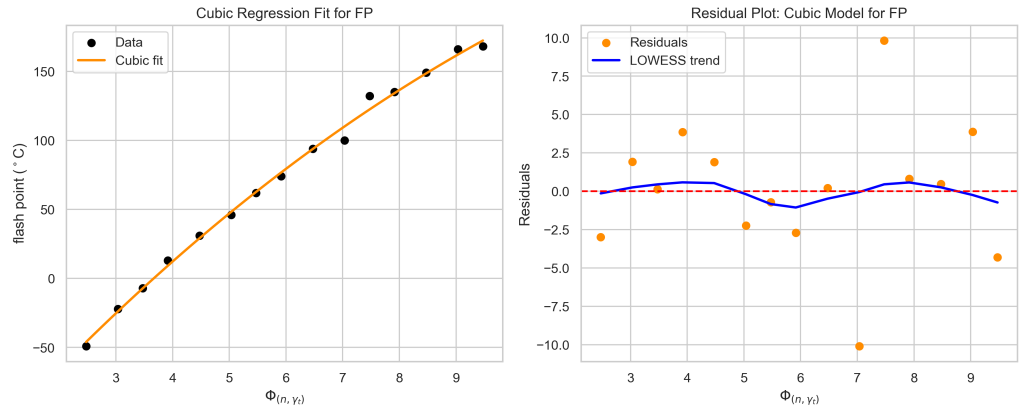


FIGURE 9. Scatter and residual plots for cubic regression models of FP

Φ_{n,γ_t} retains a statistically significant predictive contribution beyond these size-related effects.

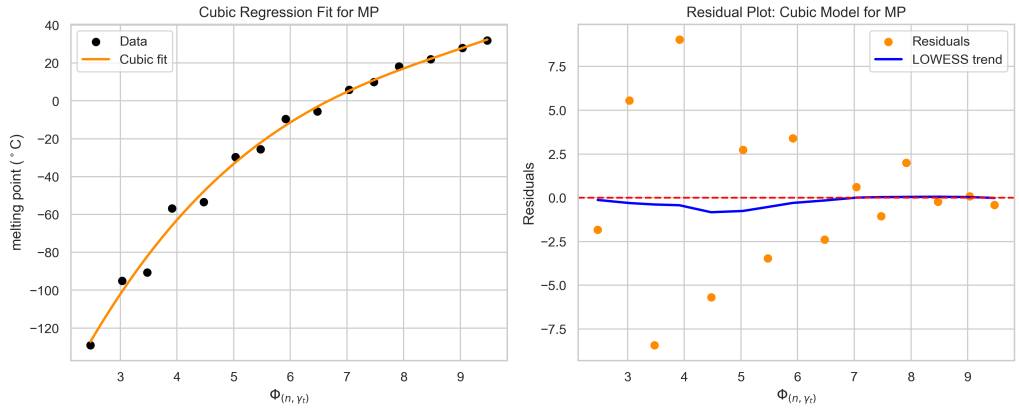


FIGURE 10. Scatter and residual plots for cubic regression models of MP

Name	log P		MR (cm^3/mol)		MV (cm^3/mol)		PR		α (Å^3)		BP (°C)		FP (°C)		MP (°C)	
Pentane	3.67	3.67	29.84	29.82	127.5	127.43	270.8	270.82	11.83	11.80	36	35.77	-49	-46.02	-129	-127.17
Hexane	4.21	4.27	34.47	35.00	144	145.90	310.6	315.29	13.66	13.86	69	71.53	-22	-23.92	-95	-100.57
Heptane	4.74	4.74	39.11	39.08	160.5	160.43	350.4	350.26	15.5	15.47	98.4	97.61	-7	-7.13	-90.6	-82.18
Octane	5.28	5.21	43.74	43.16	177	174.96	390.2	385.24	17.34	17.08	126	122.01	13	9.14	-56.8	-65.84
Nonane	5.82	5.81	48.37	48.34	193.6	193.44	430	429.70	19.17	19.13	150.8	150.76	31	29.09	-53.47	-47.78
Decane	6.35	6.41	53.01	53.53	210.1	211.91	469.7	474.16	21.01	21.19	174.1	177.17	46	48.23	-29.7	-32.45
Undecane	6.89	6.88	57.64	57.60	226.6	226.44	509.5	509.14	22.85	22.80	195.9	196.46	62	62.72	-25.54	-22.07
Dodecane	7.42	7.36	62.27	61.68	243.1	240.97	549.3	544.11	24.28	24.41	216.3	214.54	74	76.71	-9.6	-13.01
Tridecane	7.96	7.96	66.9	66.87	259.6	259.44	589.1	588.58	26.52	26.47	235.4	235.97	94	93.79	-5.5	-3.12
Tetradecane	8.5	8.56	71.54	72.05	276.1	277.92	628.9	633.04	28.36	28.52	253.57	255.86	100	110.09	5.87	5.26
Pentadecane	9.03	9.03	76.17	76.13	292.6	292.45	668.7	668.01	30.19	30.13	270.6	270.57	132.2	122.37	9.95	11.00
Hexadecane	9.57	9.50	80.8	80.21	309.1	306.98	708.4	702.99	32.03	31.74	286.9	284.56	135	134.18	18.18	16.18
Heptadecane	10.1	10.10	85.44	85.39	325.6	325.45	748.2	747.45	33.87	33.80	303	301.49	149	148.52	21.97	22.20
Octadecane	10.64	10.70	90.07	90.58	342.1	343.93	788	791.92	35.7	35.85	316	317.67	166	162.12	28	27.91
Nonadecane	11.18	11.17	94.7	94.65	358.6	358.46	825.8	826.89	37.4	37.46	330	330.00	168	172.30	32	32.40

TABLE 7. Comparison table for the actual and predicted physicochemical properties of alkanes using Φ_{n,γ_t}

The R^2 values obtained from the regression analysis demonstrate consistently strong relationships between Φ_{n,γ_t} and the selected physicochemical properties of alkanes, with adjusted R^2 and cross-validated values remaining close to R^2. Remarkably, all parameters show near-unity correlation coefficients, accompanied by small error terms, high F-statistic values, and statistically significant probabilities (Table 5 and 6). These findings indicate that Φ_{n,γ_t} provides excellent predictive performance across the examined properties.

Furthermore, Table 7 shows that the predicted values are in close agreement with the experimental data, exhibiting only minor deviations, particularly for FP and MP. The scatter plots in Fig. 3–10 illustrate this close correspondence between experimental and predicted values, while the accompanying residual plots (shown in the same figures) depict the random distribution of errors around zero, suggesting the absence of systematic bias. Together, these graphical and statistical observations confirm that the model achieves a high level of accuracy in predicting the physicochemical properties of alkanes.

4. CONCLUSION

This study refines the upper bound of the Randić index for trees by incorporating both the order and the total domination number, and it characterizes the extremal structures that attain this bound. The proposed bound was further evaluated through a QSPR analysis, which demonstrated strong predictive capability for the physicochemical properties of

alkanes. The high correlation coefficients and minimal deviations between predicted and experimental values confirm the effectiveness of Φ_{n,γ_t} in molecular property estimation. Although Φ_{n,γ_t} exhibits promising predictive performance, the present results are based on a limited dataset. Additional validation using larger and chemically diverse molecular systems would be valuable to establish its broader applicability.

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