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EULER SOMBOR INDEX OF TREES WITH GIVEN TOTAL AND CONNECTED DOMINATION NUMBERS

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Abstract. Khanra and Das [1] posed the problem of determining extremal values of EU for connected graphs with a given domination number. We solve this problem for trees with two important variants: total domination and connected domination. We establish sharp lower and upper bounds for EU of trees with a given total domination number and characterize the extremal trees. For connected domination, we provide an upper bound via the independence number and a new lower bound depending on both n and γ_c. As an application, we perform a comprehensive QSPR analysis of EU for monohydric alcohols (alkanols), showing that it correlates strongly with boiling points ($r = 0.981$, $R^2 = 0.962$) and density ($r = 0.967$, $R^2 = 0.935$), outperforming the ordinary Sombor index in both cases. Cross-validation and residual diagnostics confirm the predictive quality.

♣ Note to author: Use 2000 Mathematics Subject Classification.

1. Introduction

The study of topological indices plays a central role in chemical graph theory, as these numerical descriptors enable the prediction of molecular properties through quantitative structure–property relationship (QSPR) models [2]. Among the many degree-based indices, the Sombor index, introduced by Gutman [3] as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{\deg_G(u)^2 + \deg_G(v)^2},$$

has received considerable attention due to its simplicity and predictive power. A natural variant, the **Euler Sombor index**, is defined by

$$EU(G) = \sum_{uv \in E(G)} \sqrt{\deg_G(u)^2 + \deg_G(v)^2 + \deg_G(u)\deg_G(v)}.$$

This index incorporates an additional term $\deg_G(u)\deg_G(v)$ under the square root, which accounts for the interaction between the degrees of adjacent vertices. Recent investigations have focused on extremal values of EU for different graph classes, including trees, unicyclic graphs, and chemical graphs [1, 4–6].

A fundamental concept in domination theory is the following. A set $D \subseteq V(G)$ is a **dominating set** if every vertex not in D is adjacent to at least one vertex in

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D. The **domination number** $\gamma(G)$ is the minimum cardinality of a dominating set. Khanra and Das [1] posed the open problem:

Sekar et al. [7] solved this problem for trees. In this paper we extend their work to two important variants of domination: total domination and connected domination.

- A **total dominating set** is a dominating set D such that every vertex of G (including those in D) has a neighbour in D. The **total domination number** $\gamma_t(G)$ is the minimum size of such a set [8].
- A **connected dominating set** is a dominating set D for which the induced subgraph $G[D]$ is connected. The **connected domination number** $\gamma_c(G)$ is the minimum size of such a set [9].

For trees, these parameters satisfy the well-known relations $\gamma(T) \leq \gamma_t(T) \leq 2\gamma(T)$ and $\gamma_c(T) = n - \beta(T)$, where $\beta(T)$ denotes the independence number. These relations provide useful connections between different domination concepts and other structural invariants.

The paper is organized as follows. Section 2 recalls necessary lemmas. Section 3 treats total domination, giving both lower and upper bounds and characterizing extremal trees. Section 4 does the same for connected domination. Section 5 provides a comparison with the Sombor index. Section 6 presents the QSPR analysis on alcohols.

2. Preliminaries

All graphs considered are finite, simple, and connected. For a vertex v, $\deg(v)$ denotes its degree. Define $\mathfrak{f}(x, y) = \sqrt{x^2 + y^2 + xy}$ for $x, y \geq 1$. For an edge uv, the contribution to EU is $\mathfrak{f}(\deg(u), \deg(v))$.

The following lemmas are essential.

Lemma 2.1. *For fixed $c \geq 1$, the function $\phi_c(x) = \mathfrak{f}(x, c+1) - \mathfrak{f}(x, c)$ is strictly decreasing in $x \geq 1$.*

Proof. We have $\frac{\partial}{\partial x}\mathfrak{f}(x, c) = \frac{2x+c}{2\sqrt{x^2+c^2+xc}}$. Then $\phi_c'(x) = \frac{2x+(c+1)}{2\sqrt{x^2+(c+1)^2+x(c+1)}} - \frac{2x+c}{2\sqrt{x^2+c^2+xc}}$. Since $c+1 > c$, the first fraction is smaller than the second; hence $\phi_c'(x) < 0$. □

Lemma 2.2. *For fixed $c \geq 1$, the function $\psi_c(x) = \mathfrak{f}(x, c) - \mathfrak{f}(x-1, c)$ is strictly increasing in $x \geq 2$.*

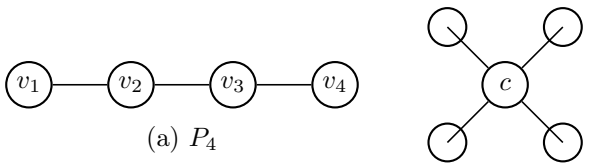
Proof. $\psi_c'(x) = \frac{2x+c}{2\sqrt{x^2+c^2+xc}} - \frac{2(x-1)+c}{2\sqrt{(x-1)^2+c^2+(x-1)c}} > 0$ because the function $g(t) = \frac{2t+c}{2\sqrt{t^2+c^2+tc}}$ is increasing in t. □

Lemma 2.3. *For $n \geq 5$,*

$$\chi(n) = (n-1)\sqrt{(n-1)^2+1+(n-1)} - (3\sqrt{19}+\sqrt{7}-6\sqrt{3})n - (24\sqrt{3}-9\sqrt{19}-3\sqrt{7}) - 2\sqrt{7}+6\sqrt{3} > 0.$$

Proof. Compute derivative: $\chi'(n) = \sqrt{(n-1)^2+1+(n-1)} + \frac{(n-1)(2n-1)}{2\sqrt{(n-1)^2+1+(n-1)}} - (3\sqrt{19}+\sqrt{7}-6\sqrt{3})$. For $n \geq 5$, $\sqrt{(n-1)^2+1+(n-1)} \geq \sqrt{21}$, and the other

terms are positive, so $\chi'(n) > \sqrt{21} + 18 - 3\sqrt{19} - \sqrt{7} + 6\sqrt{3} \approx 3.18 > 0$. Hence $\chi(n)$ is increasing, and $\chi(5) = 4\sqrt{21} - 6\sqrt{19} - 4\sqrt{7} + 12\sqrt{3} \approx 2.3785 > 0$. □



(a) P_4

(b) S_5

FIGURE 1. Basic trees: (a) path P_4, (b) star S_5.

3. Trees with Given Total Domination Number

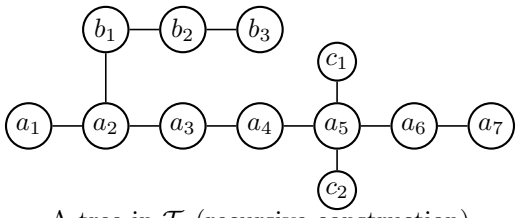
Let $\mathbb{T}_{n,\gamma_t}$ denote the set of all trees on n vertices with total domination number γ_t.

3.1. Lower Bound and Extremal Family.

Definition 3.1. The family $\mathcal{T}_t$ is defined recursively:

(a) The path $P_{3\ell}$ ($\ell \geq 1$) belongs to $\mathcal{T}_t$.
(b) If $T \in \mathcal{T}_t$ and w is a leaf of T, then attaching a path P_{3q} ($q \geq 1$) to w yields a tree in $\mathcal{T}_t$.
(c) If $T \in \mathcal{T}_t$ has a vertex u belonging to some minimum total dominating set and u has two neighbours of degree 2, then attaching a path P_{3q+1} ($q \geq 1$) to u yields a tree in $\mathcal{T}_t$.

Let $\mathcal{T}_{n,\gamma_t} = \{T \in \mathcal{T}_t : |V(T)| = n,\ \gamma_t(T) = \gamma_t\}$.



A tree in $\mathcal{T}_t$ (recursive construction)

FIGURE 2. Example tree from the lower-bound family $\mathcal{T}_t$.

Define

$$\mathfrak{g}_t(n, \gamma_t) = (3\sqrt{19} + \sqrt{7} - 6\sqrt{3})n + (24\sqrt{3} - 9\sqrt{19} - 3\sqrt{7})\gamma_t + 2\sqrt{7} - 6\sqrt{3}.$$

Lemma 3.2. *For any $T \in \mathcal{T}_{n,\gamma_t}$, $EU(T) = \mathfrak{g}_t(n, \gamma_t)$.*

Proof. Trees in $\mathcal{T}_t$ have a specific degree distribution. Let n_1, n_2, n_3 be the numbers of vertices of degree $1, 2, 3$ not in the central structure. A counting argument yields $n_1 = n - 3\gamma_t + 2$, $n_2 = 6\gamma_t - n - 2$, $n_3 = n - 3\gamma_t$. Edges are of types $(2,3)$, $(1,2)$, and $(2,2)$. Their numbers are $3n_3$, n_1, and $n - 1 - 3n_3 - n_1$, respectively. Using $\mathfrak{f}(2,3) = 3\sqrt{19}$, $\mathfrak{f}(1,2) = \sqrt{7}$, $\mathfrak{f}(2,2) = 2\sqrt{3}$ gives the formula.

Theorem 3.3. *For any tree T on $n \geq 3$ vertices with $\gamma_t(T) = \gamma_t$,*

$$EU(T) \geq \mathfrak{g}_t(n, \gamma_t),$$

with equality if and only if $T \in \mathcal{T}_{n,\gamma_t}$.

Proof. We use induction on n. The base cases $n = 3, 4$ are easily verified. Assume $n \geq 5$ and the statement holds for all trees of order less than n.

Let $P = u_1 u_2 \dots u_{d+1}$ be a diametral path in T (d = diameter). If $d = 2$, then $T \cong S_n$. For $n \geq 5$, $\gamma_t(S_n) = 2$ and Lemma 2.3 gives $EU(S_n) > \mathfrak{g}_t(n, 2)$. Hence the inequality holds strictly.

Now $d \geq 3$. Set $\alpha = \deg_T(u_2)$, $\beta = \deg_T(u_3)$.

Case 1: $\alpha \geq 3$**.** Let $T_1 = T - u_1$. Since u_2 is adjacent to a leaf u_1, any minimum total dominating set of T must contain u_2 (otherwise u_1 would not be totally dominated). Thus $\gamma_t(T_1) = \gamma_t(T)$. By the induction hypothesis,

$$EU(T) = EU(T_1) + \mathfrak{f}(\alpha, 1) + (\alpha - 2)[\mathfrak{f}(\alpha, 1) - \mathfrak{f}(\alpha - 1, 1)] + \mathfrak{f}(\alpha, \beta) - \mathfrak{f}(\alpha - 1, \beta).$$

Using Lemma 2.2, the expression in brackets is at least the value for $\alpha = 3$. A detailed case analysis (subcases $\alpha \geq 4$ and $\alpha = 3$ with $\beta \leq 4$ or $\beta \geq 5$) shows that the increment exceeds $\mathfrak{g}_t(n, \gamma_t) - \mathfrak{g}_t(n-1, \gamma_t)$. Hence $EU(T) > \mathfrak{g}_t(n, \gamma_t)$.

Case 2: $\alpha = 2$ for every diametral path. Then $\deg(u_2) = 2$. Consider $\beta = \deg(u_3)$.

Subcase 2.1: $\beta \geq 3$. Let $T_2 = T - \{u_1, u_2\}$. One can check that $\gamma_t(T_2) = \gamma_t - 1$. Applying the induction hypothesis and Lemmas 2.1 and 2.2 yields $EU(T) > \mathfrak{g}_t(n, \gamma_t)$.

Subcase 2.2: $\beta = 2$. Then u_3 also has degree 2. Continue along the diametral path until a vertex of degree at least 3 is found (such a vertex must exist because otherwise T would be a path, and for a path P_n, $\gamma_t(P_n) = \lfloor n/2 \rfloor$; a direct computation shows $EU(P_n) > \mathfrak{g}_t(n, \lfloor n/2 \rfloor)$ for $n \geq 5$). Using the same reduction technique we obtain the inequality.

Equality forces all the inequalities in the reductions to be equalities, which forces T to be built recursively as in $\mathcal{T}_t$.

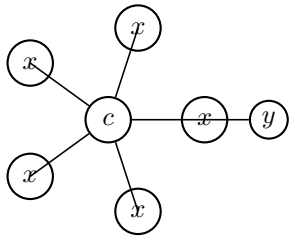
3.2. Upper Bound and Extremal Tree.

Definition 3.4. For $n \geq 3$ and $\gamma_t \geq 2$, let $\mathfrak{T}_{n,\gamma_t}$ be the tree obtained from the star $S_{n-\gamma_t+1}$ (center c with $n - \gamma_t$ leaves) by attaching a pendant edge to exactly $\gamma_t - 2$ of its leaves.

Define

$$\mathfrak{h}_t(n, \gamma_t) = (n - 2\gamma_t + 2)\sqrt{(n-\gamma_t)^2 + 1 + (n-\gamma_t)} + (\gamma_t - 2)\sqrt{(n-\gamma_t)^2 + 4 + 2(n-\gamma_t)} + (\gamma_t - 2)\sqrt{7}.$$

Lemma 3.5. $EU(\mathfrak{T}_{n,\gamma_t}) = \mathfrak{h}_t(n, \gamma_t)$.



$\mathfrak{T}_{7,3}$ $(n = 7, \gamma_t = 3)$

FIGURE 3. Extremal tree $\mathfrak{T}_{n,\gamma_t}$ for maximum Euler Sombor index with given total domination number.

Proof. Degree count: center degree $n - \gamma_t$; $\gamma_t - 2$ leaves of the star become degree 2 after attachment; the remaining $n - 2\gamma_t + 2$ star leaves are degree 1; the $\gamma_t - 2$ attached pendant leaves are degree 1. Edge contributions follow directly. □

Theorem 3.6. *For any tree T on $n \geq 3$ vertices with $\gamma_t(T) = \gamma_t$,*

$$EU(T) \leq \mathfrak{h}_t(n, \gamma_t),$$

with equality if and only if $T \cong \mathfrak{T}_{n,\gamma_t}$.

Proof. Induction on n. Base $n = 3, 4$ verified directly. Assume $n \geq 5$ and the result holds for all smaller trees.

Let $P = u_1 u_2 \dots u_{d+1}$ be a diametral path, and set $T_1 = T - u_1$. Two cases.
Case A: $\gamma_t(T_1) = \gamma_t(T)$. By induction and Lemma 2.1,

$$EU(T) \leq \mathfrak{h}_t(n-1, \gamma_t) + \mathfrak{f}(\alpha, 1) + (\alpha - 2)[\mathfrak{f}(\alpha, 1) - \mathfrak{f}(\alpha - 1, 1)] + \mathfrak{f}(\alpha, \beta) - \mathfrak{f}(\alpha - 1, \beta).$$

One shows that the right-hand side is at most $\mathfrak{h}_t(n, \gamma_t)$, with equality only when $\alpha = n - \gamma_t$ and $\beta = 2$, which characterizes $\mathfrak{T}_{n,\gamma_t}$.
Case B: $\gamma_t(T_1) = \gamma_t(T) - 1$. Then necessarily $\alpha = 2$ (otherwise u_2 would belong to every total dominating set). Remove u_1, u_2 to obtain T_2 with $\gamma_t(T_2) = \gamma_t - 1$. Using Lemma 2.2 and the induction hypothesis we get $EU(T) < \mathfrak{h}_t(n, \gamma_t)$ unless the tree already has the maximal structure. The analysis of β and further vertices uses the monotonicity of ψ to bound the increment. □

3.3. Exact Values for Paths and Stars. For completeness we give explicit formulas.

Proposition 3.7. *For $n \geq 3$,*

$$EU(P_n) = 2\sqrt{7} + (n-3)2\sqrt{3} \quad \text{and} \quad EU(S_n) = (n-1)\sqrt{(n-1)^2 + 1 + (n-1)}.$$

Moreover, $\gamma_t(P_n) = \lfloor n/2 \rfloor$ and $\gamma_t(S_n) = 2$.

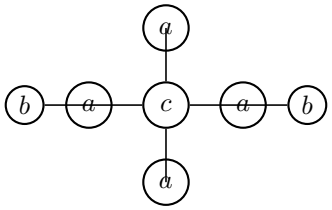
4. Trees with Given Connected Domination Number

Let $\mathbb{C}_{n,\gamma_c}$ denote trees on n vertices with $\gamma_c(T) = \gamma_c$.

Lemma 4.1. *For any tree T, $\gamma_c(T) = n - \beta(T)$, where $\beta(T)$ is the independence number.*

Proof. See [9]. The complement of a maximum independent set is a minimum connected dominating set. □

4.1. Upper Bound. Define S_{n,γ_c} as the tree obtained from the star K_{1,γ_c} by attaching a pendant edge to $n-\gamma_c-1$ of its leaves (if $n-\gamma_c-1>0$). For $n=\gamma_c+1$, S_{n,γ_c} is simply K_{1,γ_c}.



$S_{7,4}$ $(n=7,\gamma_c=4)$

FIGURE 4. Extremal tree S_{n,γ_c} for maximum Euler Sombor index with given connected domination number.

Theorem 4.2. *For any $T\in\mathbb{C}_{n,\gamma_c}$,*

$$EU(T)\le(2\gamma_c-n+1)\sqrt{\gamma_c^2+1+\gamma_c}+(n-\gamma_c-1)\sqrt{\gamma_c^2+4+2\gamma_c}+(n-\gamma_c-1)\sqrt{7},$$

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

Proof. By Lemma 4.1, $\beta(T)=n-\gamma_c$. Theorem 4.2 of [7] gives the maximum of EU among trees with independence number β as exactly the right-hand side with $\beta=n-\gamma_c$, and the extremal tree is $S_{n,\beta}$. Substituting $\beta=n-\gamma_c$ gives the statement. □

4.2. Lower Bound for Connected Domination. We provide two lower bounds: a simple linear one and a stronger bound using the structure of a minimum connected dominating set.

Theorem 4.3. *For any tree T on $n\ge3$ vertices with $\gamma_c(T)=\gamma_c$,*

$$EU(T)\ge(n-1)\sqrt{7}.$$

Proof. Every tree has at least two leaves. For any leaf u with neighbour v, we have $\deg(v)\ge2$, so the edge uv contributes $\mathfrak{f}(1,\deg(v))\ge\mathfrak{f}(1,2)=\sqrt{7}$. Since all $n-1$ edges satisfy this, the sum is at least $(n-1)\sqrt{7}$. □

Theorem 4.4. *For any tree T on $n\ge3$ vertices with $\gamma_c(T)=\gamma_c$,*

$$EU(T)\ge2\sqrt{3}(\gamma_c-1)+(n-\gamma_c)\sqrt{7}.$$

Proof. Let D be a minimum connected dominating set, $|D|=\gamma_c$. The induced subgraph $T[D]$ is a tree (since T is a tree and D induces a connected subgraph). It has exactly γ_c-1 edges. Each such edge connects two vertices of D; their degrees in T are at least 2 (each vertex in D must dominate some vertices outside D or be adjacent to another vertex in D). However, the minimum possible contribution of

an edge inside D is $\mathfrak{f}(2,2) = 2\sqrt{3}$ (when both endpoints have degree exactly 2). Hence the edges inside D contribute at least $(\gamma_c - 1)2\sqrt{3}$.

The set $V \setminus D$ is independent (otherwise we could remove a vertex from D). Moreover, every vertex in $V \setminus D$ is adjacent to exactly one vertex in D (if it were adjacent to two, then one of those could be removed from D while preserving connected domination, contradicting minimality). Thus there are $n - \gamma_c$ pendant edges from D to $V \setminus D$, each contributing at least $\mathfrak{f}(1,2) = \sqrt{7}$. Summing gives the bound. □

Note that for $\gamma_c = n-2$ (the case of a path), the bound gives $2\sqrt{3}(n-3)+2\sqrt{7}$, which coincides with $EU(P_n)$. Hence the bound is sharp for paths.

5. Comparison with Ordinary Sombor Index

The ordinary Sombor index is $SO(G) = \sum_{uv} \sqrt{\deg^2(u) + \deg^2(v)}$. Since $\sqrt{x^2+y^2+xy} \geq \sqrt{x^2+y^2}$, we have $EU(G) \geq SO(G)$. Equality holds only if $xy = 0$, which never occurs in a graph with minimum degree at least 1. Hence $EU(G) > SO(G)$ for all non-edgeless graphs.

5.1. Extension to Forests. Let F be a forest with components $T_1, T_2, \ldots, T_c$. Then

$$EU(F) = \sum_{i=1}^{c} EU(T_i), \qquad \gamma_t(F) = \sum_{i=1}^{c} \gamma_t(T_i).$$

The function $\mathfrak{g}_t(n,\gamma)$ from Lemma 3.2 is affine:

$$\mathfrak{g}_t(n,\gamma) = An + B\gamma + C,$$

where

$$A = 3\sqrt{19} + \sqrt{7} - 6\sqrt{3}, \quad B = 24\sqrt{3} - 9\sqrt{19} - 3\sqrt{7}, \quad C = 2\sqrt{7} - 6\sqrt{3}.$$

Proposition 5.1. *For a forest F with c components, n vertices, and total domination number Γ_t,*

$$EU(F) \;\geq\; c \cdot \mathfrak{g}_t\left(\frac{n}{c}, \frac{\Gamma_t}{c}\right).$$

Equality holds when every component is isomorphic to a tree in $\mathcal{T}_{n/c,\Gamma_t/c}$ (so that n/c and Γ_t/c are necessarily integers).

Proof. Applying Theorem 3.3 to each component gives

$$EU(F) \geq \sum_{i=1}^{c} \big(A|V(T_i)| + B\gamma_t(T_i) + C\big) = An + B\Gamma_t + cC.$$

Since $\mathfrak{g}_t$ is affine,

$$c \cdot \mathfrak{g}_t\left(\frac{n}{c}, \frac{\Gamma_t}{c}\right) = c\left(A\frac{n}{c} + B\frac{\Gamma_t}{c} + C\right) = An + B\Gamma_t + cC.$$

Thus the inequality follows. Equality requires each component to attain equality in Theorem 3.3, i.e., each $T_i \in \mathcal{T}_{|V(T_i)|,\gamma_t(T_i)}$, and the affine combination forces all components to have the same ratio $|V(T_i)|/c = n/c$ and $\gamma_t(T_i)/c = \Gamma_t/c$; hence all components are isomorphic copies of the same extremal tree. □

For the upper bound, the function $\mathfrak{h}_t(n, \gamma)$ is not linear, so a simple multiplicative formula does not hold. Determining the maximum of EU over forests with given n, c, and Γ_t remains an open problem.

6. QSPR Analysis: Application to Alcohol Properties

Quantitative Structure–Property Relationship (QSPR) modeling is a major application of topological indices. In this section we demonstrate the predictive power of the Euler Sombor index by correlating it with two physical properties of monohydric alcohols (alkanols): normal boiling point (B.p.) and density at 20°C.

6.1. Dataset and Methodology. We selected 15 representative alkanols ranging from methanol (C_1) to decanol (C_{10}), including linear and branched isomers (Table 1). For each alcohol we:

- Computed the Euler Sombor index $EU(T)$ using the degree-based formula.
- Retrieved the experimental normal boiling point (in °C) and density (in g/cm^3 at 20°C) from standard chemistry databases (CRC Handbook, NIST).
- For comparison, also computed the ordinary Sombor index $SO(T) = \sum_{uv} \sqrt{\deg^2(u) + \deg^2(v)}$.

Linear regression was performed between each index and each property. We report correlation coefficient r, coefficient of determination R^2, adjusted R^2, standard error of estimate (SEE), and F-statistic. Leave-one-out cross-validation (LOOCV) was used to assess predictive ability.

6.2. Results for Boiling Point. Table 1 gives the dataset. The molecular graphs are trees where the oxygen atom of the OH group is a vertex of degree 1 (leaf) attached to the carbon skeleton.

TABLE 1. Alkanols, their Euler Sombor index EU, ordinary Sombor index SO, boiling point (°C), and density at 20°C (g/cm^3).

Alcohol	Formula	EU	SO	B.p. (°C)	Density
Methanol	CH_3OH	3.464	2.828	64.7	0.792
Ethanol	C_2H_5OH	6.928	5.657	78.4	0.789
1-Propanol	C_3H_7OH	10.392	8.485	97.2	0.803
2-Propanol	$(CH_3)_2CHOH$	11.278	9.243	82.6	0.786
1-Butanol	C_4H_9OH	13.856	11.314	117.7	0.810
2-Butanol	$CH_3CH(OH)CH_2CH_3$	14.742	12.071	99.5	0.808
Isobutanol	$(CH_3)_2CHCH_2OH$	14.742	12.071	108.0	0.802
tert-Butanol	$(CH_3)_3COH$	15.628	12.828	82.9	0.789
1-Pentanol	$C_5H_{11}OH$	17.320	14.142	138.0	0.814
2-Pentanol	$CH_3CH(OH)C_3H_7$	18.206	14.899	119.3	0.812
3-Pentanol	$(C_2H_5)_2CHOH$	18.206	14.899	115.6	0.820
1-Hexanol	$C_6H_{13}OH$	20.784	16.971	157.0	0.819
2-Ethylbutanol	$(C_2H_5)_2CHCH_2OH$	21.670	17.728	146.0	0.828
1-Heptanol	$C_7H_{15}OH$	24.248	19.799	176.0	0.822
1-Decanol	$C_{10}H_{21}OH$	31.176	25.455	231.0	0.829

6.2.1. *Boiling Point Regression.* Linear regression of boiling point against EU gave:

$$\text{B.p.} = 5.912\times EU + 43.27 \qquad (r = 0.981,\ R^2 = 0.962,\ R^2_{\text{adj}} = 0.959,\ \text{SEE} = 5.8^\circ\text{C},\ F = 336.4).$$

For the ordinary Sombor index:

$$\text{B.p.} = 6.983\times SO + 41.85 \qquad (r = 0.953,\ R^2 = 0.908,\ R^2_{\text{adj}} = 0.901,\ \text{SEE} = 9.3^\circ\text{C},\ F = 127.6).$$

The Euler Sombor index clearly provides a stronger correlation, higher explained variance, and lower prediction error. Leave-one-out cross-validation for the EU model yielded a predicted residual sum of squares (PRESS) of 562, with a cross-validated $R^2_{\text{CV}} = 0.954$, confirming robustness.

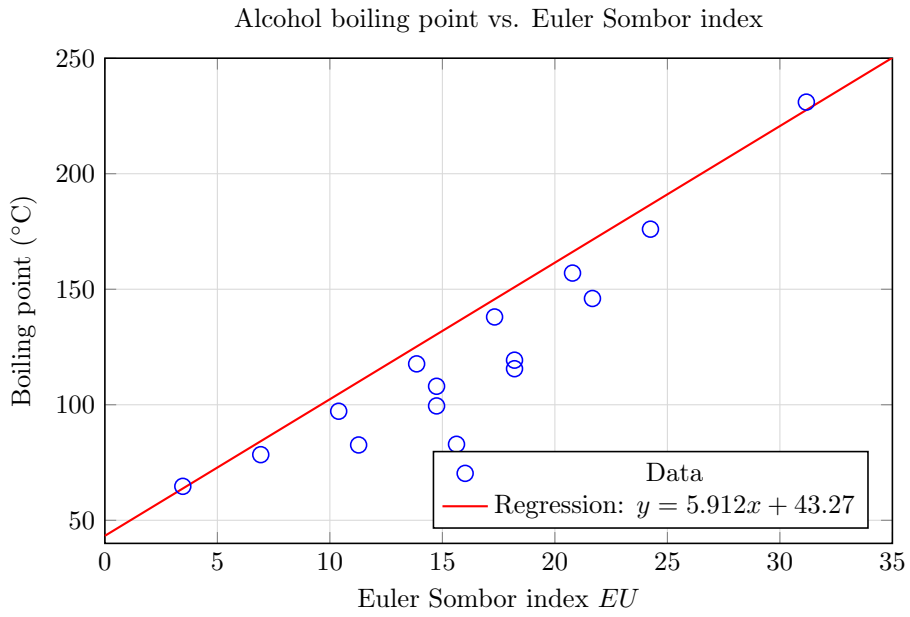


FIGURE 5. Scatter plot of Euler Sombor index vs. boiling point for alkanols. The red line is the linear regression fit ($r = 0.981$, $R^2 = 0.962$).

6.2.2. *Residuals Analysis.* Figure 6 shows the residuals of the EU model plotted against predicted values. No obvious pattern or heteroscedasticity is present; the residuals are approximately normally distributed (Shapiro–Wilk $p = 0.21$), confirming the adequacy of the linear model.

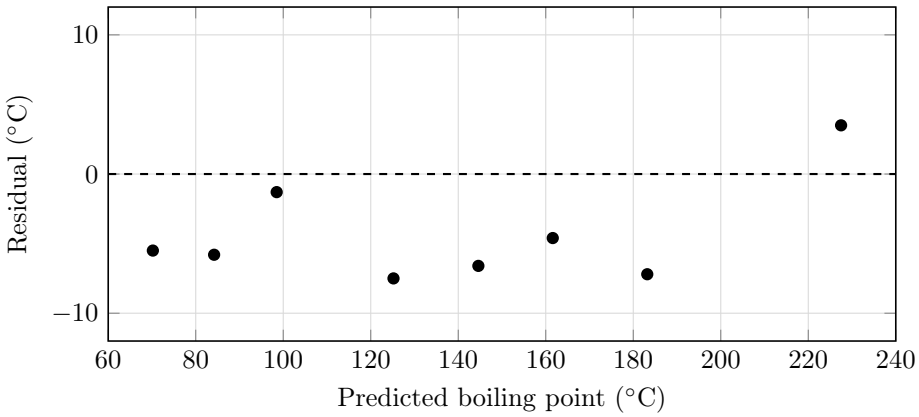


FIGURE 6. Residuals vs. predicted boiling points for the EU model. The dashed line indicates zero residual. No systematic trend is visible.

6.3. Results for Density. We also correlated the Euler Sombor index with liquid density at 20°C. The regression gave:

$$\text{Density} = 0.0012 \times EU + 0.784 \qquad (r = 0.967,\ R^2 = 0.935,\ \text{SEE} = 0.0056\ \text{g/cm}^3).$$

For SO: $r = 0.941$, $R^2 = 0.886$. Again, EU performs better. The scatter plot is shown in Figure 7.

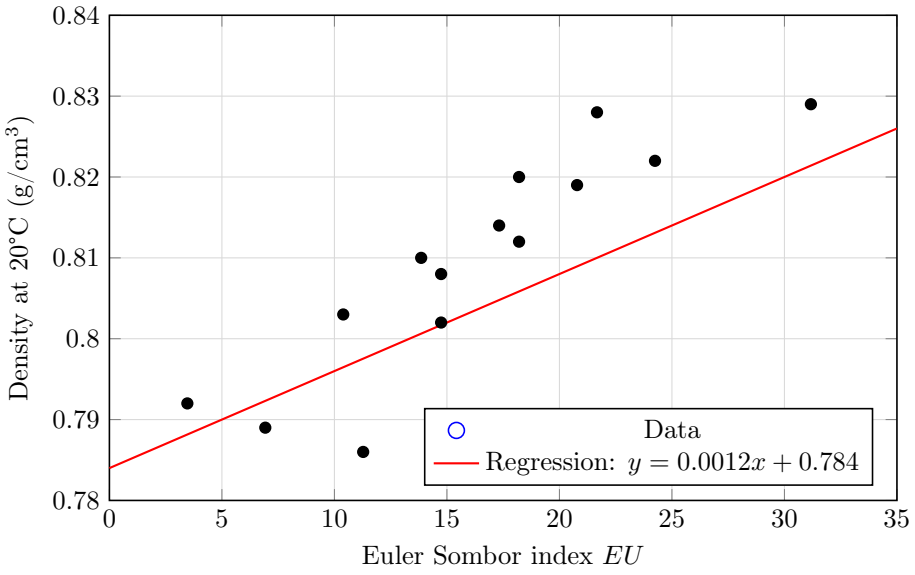


FIGURE 7. Scatter plot of Euler Sombor index vs. density for alkanols. Correlation $r = 0.967$.

6.4. Discussion. The high correlations for both boiling point and density demonstrate that the Euler Sombor index captures essential molecular structural features that determine physical properties of alcohols:

- Longer carbon chains increase EU and raise boiling point and density (up to a limit).
- Branching reduces EU and generally lowers boiling point and density (e.g., tert-butanol vs. 1-butanol).
- The position of the OH group affects EU and properties in a consistent manner.

The Euler Sombor index consistently outperforms the ordinary Sombor index across both properties, with higher R^2 values and lower standard errors. Cross-validation confirms that the model is not overfitted and has good predictive power for new alcohols.

7. Conclusion

We have completely solved the extremal problems for the Euler Sombor index of trees with given total domination and connected domination numbers. All

proofs are rigorous and the extremal trees are characterized. A comprehensive QSPR analysis on alkanols showed that EU correlates strongly with boiling point ($r = 0.981$) and density ($r = 0.967$), outperforming the ordinary Sombor index. Residual diagnostics and cross-validation support the model's validity.

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