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Trees with Extremal Values of the Sombor–Index–Like Graph Invariants

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Abstract

A new geometric background of graph invariants was introduced by Gutman, using the triangle formed by the degree-point, dual-degree-point, and the origin of the coordinate system, a number of new Sombor-index-like VDB invariants, denoted by $SO_1, SO_2, \ldots, SO_6$, were constructed by means of geometric arguments. In this paper, the chemical applicability of these Sombor-index-like graph invariants is investigated, and it is shown that almost all of these six indices are useful in predicting physicochemical properties with high accuracy compared to some well-established and often used indices. Also, we obtain a bound for some of the Sombor-index-like graph invariants among all (molecular) trees with fixed numbers of vertices, and characterize those (molecular) trees achieving the extremal value.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$, and denote by $n = |V(G)|$ and $m = |E(G)|$ the number of vertices and edges, respectively. The degree of a vertex v in G, denoted by $d_G(v)$ or $d(v)$, is the number of its neighbors. If the vertices u and v are adjacent,

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then the edge connecting them is labeled by $e = uv$. In the mathematical and chemical literature, several dozens of vertex-degree-based (VDB) graph invariants (usually referred to as "topological indices") have been introduced and extensively studied [6–8, 10, 16]. Their general formula is

$$TI(G) = \sum_{uv \in E} F(d_G(u), d_G(v)),$$

where $F(x, y)$ is a function with the property $F(x, y) = F(y, x)$.

The Sombor index [7] is also a VDB topological index actually conceived by using the geometric considerations, and soon attracted much attention. Numerous mathematical properties and chemical applications of the Sombor index have been established [1,4,9,11–13], but the geometry-based features of the Sombor index were ignored. Recently in [8] Gutman showed that geometry-based reasoning reveal the geometric background of several classical topological indices (Zagreb index, Albertson index and Sombor index) and introduced a series of new Sombor-index-like VDB invariants, denoted below by $SO_k (k = 1, 2, \cdots, 6)$. These Sombor-index-like graph invariants are defined as

$$\begin{aligned}
SO_1 &= SO_1(G) = \frac{1}{2} \sum_{uv \in E} |d_G^2(u) - d_G^2(v)| \\
SO_2 &= SO_2(G) = \sum_{uv \in E} \frac{|d_G^2(u) - d_G^2(v)|}{d_G^2(u) + d_G^2(v)} \\
SO_3 &= SO_3(G) = \sum_{uv \in E} \sqrt{2} \frac{d_G^2(u) + d_G^2(v)}{d_G(u) + d_G(v)} \pi \\
SO_4 &= SO_4(G) = \frac{1}{2} \sum_{uv \in E} \left(\frac{d_G^2(u) + d_G^2(v)}{d_G(u) + d_G(v)} \right)^2 \pi \\
SO_5 &= SO_5(G) = \sum_{uv \in E} \frac{2|d_G^2(u) - d_G^2(v)|}{\sqrt{2} + 2\sqrt{d_G^2(u) + d_G^2(v)}} \pi \\
SO_6 &= SO_6(G) = \sum_{uv \in E} \left(\frac{d_G^2(u) - d_G^2(v)}{\sqrt{2} + 2\sqrt{d_G^2(u) + d_G^2(v)}} \right)^2 \pi.
\end{aligned} \tag{1}$$

Also, Gutman pointed out at the end of the paper [8] that it would be interesting to examine the properties of these geometry-based topological indices, and see if these are usable in applications.

A molecular tree is a tree of maximum degree at most four. In this paper, a bound for these Sombor-index-like graph invariants among all (molecular) trees with fixed numbers of vertices are obtained, and those molecular trees achieving the extremal values are characterized. Also, the chemical applicability of these Sombor-index-like graph invariants is investigated and it is shown that almost all of these six Sombor-index-like indices are useful in predicting physicochemical properties with high accuracy compared to some well-established and often used indices.

2 Extremal values of Sombor index like graph invariants

Let $G = (V, E)$ be a graph with order n and size m, δ and Δ the minimum and maximum degree, respectively. Denote by m_{ij} the number of edges with end vertices of degree i and j, and ω_{ij}^k the contribution of an edge with end vertices of degree i and j in G. By the definition (1) of the Sombor-index-like indices of a graph, we have

$$SO_k(G) = \sum_{\delta \le i \le j \le \Delta} m_{ij}\omega_{ij}^k, \tag{2}$$

where

$$\begin{aligned}
\omega_{ij}^1 &= \frac{1}{2}|i^2 - j^2| = \frac{1}{2}(max\{i^2, j^2\} - min\{i^2, j^2\}) \\
\omega_{ij}^2 &= \frac{|i^2 - j^2|}{i^2 + j^2}, \qquad \omega_{ij}^3 = \sqrt{2}\pi\frac{i^2 + j^2}{i + j}, \\
\omega_{ij}^4 &= \frac{\pi}{2}\left(\frac{i^2 + j^2}{i + j}\right)^2, \quad \omega_{ij}^5 = \frac{2\pi|i^2 - j^2|}{\sqrt{2} + 2\sqrt{i^2 + j^2}} \\
\omega_{ij}^6 &= \pi\left(\frac{i^2 - j^2}{\sqrt{2} + 2\sqrt{i^2 + j^2}}\right)^2.
\end{aligned} \tag{3}$$

Theorem 1. *Let G be a connected graph with order $n > 3$ and size m and*

the maximal degree Δ *and the minimal degree* δ*, then*
(I) $0 \leq SO_1(G) \leq m(\Delta^2 - \delta^2)$*, the left equality holds if and only if* G *is regular and the right equality holds if and only if* $max\{d_G(u), d_G(v)\} = \Delta$ *and* $min\{d_G(u), d_G(v)\} = \delta$ *for any edge* $uv \in E$*, i.e., all* $m_{ij} = 0$ *except* $m_{\delta\Delta}$*;*
(II) [15] $0 \leq SO_2(G) \leq m\frac{\Delta^2-\delta^2}{\Delta^2+\delta^2}$*, the left equality holds if and only if* G *is regular and the right equality holds if and only if* $\frac{max\{d_G(u),d_G(v)\}}{min\{d_G(u),d_G(v)\}} = \frac{\Delta}{\delta}$ *for any edge* $uv \in E$*;*
(III) $SO_3(G) \geq \frac{6n-8}{3}\sqrt{2}\pi$ *with equality if and only if* G *is the path* P_n*.*
(IV) $SO_4(G) \geq \frac{18n-29}{9}\pi$ *with equality if and only if* G *is the path* P_n*.*

Proof. By $SO_1(G) = \sum_{uv\in E}(max\{d_G^2(u), d_G^2(v)\} - min\{d_G^2(u), d_G^2(v)\})$, we can straightforwardly obtain (I).

Let $f(x) = \frac{a^2+x^2}{a+x}(0 < a \leq x)$, then $f(x)$ is increasing for $x > 0$, and $\frac{i^2+j^2}{i+j} > \frac{5}{2}$ for $i + j > 4$. Note that

$$\omega_{11}^3 < \omega_{12}^3 = \frac{5\sqrt{2}\pi}{3} < \omega_{22}^3 = 2\sqrt{2}\pi < \omega_{13}^3 = \frac{5\sqrt{2}\pi}{2} < \omega_{ij}^3 \ \ (i + j > 4)$$

we have

$$\begin{aligned} SO_3(G) &\geq m_{12}\omega_{12}^3 + m_{22}\omega_{22}^3 + (m - m_{12} - m_{22})\omega_{22}^3 \\ &= m_{12}\omega_{12}^3 + (m - m_{12})\omega_{22}^3 \\ &\geq m_{12}\omega_{12}^3 + m_{22})\omega_{22}^3 \end{aligned}$$

with equality if and only if $m = m_{12} + m_{22}$, i.e., $G = P_n$. So, $SO_3(G) \geq SO_3(P_n) = \frac{6n-8}{3}\sqrt{2}\pi$.

Similarly, we can prove (IV). ■

In the following, we will determine the extremal values of SO_1, SO_2, SO_3 and the corresponding extremal trees among all trees with n vertices.

From (1), we have

$$\begin{aligned} SO_3(G) &= \sum_{uv\in E} \sqrt{2}\pi \frac{d_G^2(u)+d_G^2(v)}{d_G(u)+d_G(v)} \\ &= \sum_{uv\in E} \sqrt{2}\pi(d_G(u)+d_G(v)) - \sum_{uv\in E} \sqrt{2}\pi \frac{2d_G(u)d_G(v)}{d_G(u)+d_G(v)} \\ &= \sqrt{2}\pi(M_1(G) - 2ISI(G)) \end{aligned} \tag{4}$$

where $M_1(G) = \sum_{uv\in E}(d_G(u)+d_G(v))$ is the first Zagreb index, $ISI(G) = \sum_{uv\in E} \frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)}$ is the inverse sum indeg of G.

Lemma 2.1. *[14] If T is a tree with n vertices, then*

$$ISI(T) \geq n + \frac{1}{n} - 2$$

with equality if and only if T is isomorphic to S_n.

Lemma 2.2. *[2] If T is a tree with n vertices, then*

$$M_1(T) \leq n(n-1)$$

with equality if and only if T is isomorphic to S_n.

Theorem 2. *Let T be a tree with $n > 2$ vertices, then*

$$3 \leq SO_1(T) \leq \frac{(n^2-2n)(n-1)}{2}$$

$$\frac{6}{5} \leq SO_2(T) \leq \frac{(n^2-2n)(n-1)}{n^2-2n+2}$$

$$\sqrt{2}\pi\frac{6n-8}{3} \leq SO_3(T) \leq \sqrt{2}\pi\frac{(n-1)(n^2-2n+2)}{n}$$

the left equality holds if and only if T is the path P_n and the right equality holds if and only if T is the star S_n.

Proof. From (1), we have

$$SO_1(T) = \frac{1}{2}\sum_{uv\in E}(max\{d_T^2(u), d_T^2(v)\} - min\{d_T^2(u), d_T^2(v)\})$$
$$\leq \frac{1}{2}\sum_{uv\in E}((n-1)^2 - 1^2) = \frac{(n-1)(n^2-2n)}{2}.$$

with equality if and only if $T \cong S_n$.

Let E_1 be the set of pendant edges in T and $E_2 = E - E_1$, then $|E_1| \geq 2$ and $|d_T^2(u) - d_T^2(v)| \geq 2^2 - 1 = 3$ for $uv \in E_2$. By (1), we have

$$SO_1(T) = \frac{1}{2}(\sum_{uv\in E_1} + \sum_{uv\in E-E_1})(max\{d_T^2(u), d_T^2(v)\} - min\{d_T^2(u), d_T^2(v)\})$$
$$\geq \frac{1}{2}\sum_{uv\in E_1}(max\{d_T^2(u), d_T^2(v)\} - min\{d_T^2(u), d_T^2(v)\}) \geq \frac{3|E_1|}{2} \geq 3.$$

with equality holds if and only if $T \cong P_n$.

From [15], we can see

$$\frac{6}{5} \leq SO_2(T) \leq \frac{(n^2-2n)(n-1)}{n^2-2n+2}$$

the left equality holds if and only if T is the path P_n and the right equality holds if and only if T is the star S_n.

From (4), Theorem 1 and Lemmas 2.1-2.2, we can obtain

$$\sqrt{2}\pi\frac{6n-8}{3} \leq SO_3(T) \leq \sqrt{2}\pi\frac{(n-1)(n^2-2n+2)}{n}$$

the left equality holds if and only if T is the path P_n and the right equality holds if and only if T is the star S_n. ■

3 The Sombor index like indices of molecular trees

In this section, we consider the extremal values of SO_1, SO_2, SO_3, SO_4 for molecular trees.

Let $\mathcal{C}T_n$ be the set of molecular trees with n vertices, $n_i = n_i(T)$ the number of vertices of degree i in $T \in \mathcal{C}T_n$, $i \in \{1, 2, 3, 4\}$. We can get the following system of six linear equations which are satisfied by all molecular trees

$$\begin{cases} n_1 + n_2 + n_3 + n_4 = n \\ n_1 + 2n_2 + 3n_3 + 4n_4 = 2n - 2 \\ m_{12} + m_{13} + m_{14} = n_1 \\ m_{12} + 2m_{22} + m_{23} + m_{24} = 2n_2 \\ m_{13} + m_{23} + 2m_{33} + m_{34} = 3n_3 \\ m_{14} + m_{24} + m_{34} + 2m_{44} = 4n_4 \end{cases} \tag{5}$$

Solving the system (5) with unknowns $m_{14}, m_{24}, n_1, n_2, n_3$ and n_4, we can obtain

$$\begin{cases} m_{14} = \frac{n+3}{2} - \frac{3m_{12}}{2} - \frac{7m_{13}}{6} - \frac{m_{22}}{2} - \frac{m_{23}}{6} + \frac{m_{33}}{6} + \frac{m_{34}}{3} + \frac{m_{44}}{2} \\ m_{24} = \frac{n-5}{2} + \frac{m_{12}}{2} + \frac{m_{13}}{6} - \frac{m_{22}}{2} - \frac{5m_{23}}{6} - \frac{7m_{33}}{6} - \frac{4m_{34}}{3} - \frac{3m_{44}}{2} \\ n_1 = \frac{n+3}{2} - \frac{m_{12}}{2} - \frac{m_{13}}{6} - \frac{m_{22}}{2} - \frac{m_{23}}{6} + \frac{m_{33}}{6} + \frac{m_{34}}{3} + \frac{m_{44}}{2} \\ n_2 = \frac{n-5}{4} + \frac{3m_{12}}{4} + \frac{7m_{13}}{12} + \frac{3m_{22}}{4} + \frac{m_{23}}{12} - \frac{7m_{33}}{12} - \frac{2m_{34}}{3} - \frac{3m_{44}}{4} \\ n_3 = \frac{m_{13}}{3} + \frac{m_{23}}{3} + \frac{2m_{33}}{3} + \frac{m_{34}}{3} \\ n_4 = \frac{n-1}{4} - \frac{m_{12}}{4} - \frac{m_{13}}{4} - \frac{m_{22}}{4} - \frac{m_{23}}{4} - \frac{m_{33}}{4} + \frac{m_{44}}{4} \end{cases} \tag{6}$$

Also, solving the system (5) with unknowns $m_{14}, m_{44}, n_1, n_2, n_3$ and n_4, we can obtain

$$\begin{cases} m_{14} = \dfrac{2n+2}{3} - \dfrac{4m_{12}}{3} - \dfrac{10m_{13}}{9} - \dfrac{2m_{22}}{3} - \dfrac{4m_{23}}{9} - \dfrac{m_{24}}{3} \\ \qquad - \dfrac{2m_{33}}{9} - \dfrac{m_{34}}{9} \\ m_{44} = \dfrac{n-5}{3} + \dfrac{m_{12}}{3} + \dfrac{m_{13}}{9} - \dfrac{m_{22}}{3} - \dfrac{5m_{23}}{9} - \dfrac{2m_{24}}{3} - \dfrac{7m_{33}}{9} - \dfrac{8m_{34}}{9} \\ n_1 = \dfrac{2n+2}{3} - \dfrac{m_{12}}{3} - \dfrac{2m_{22}}{3} - \dfrac{4m_{23}}{9} - \dfrac{m_{24}}{3} - \dfrac{m_{13}}{9} - \dfrac{2m_{33}}{9} - \dfrac{m_{34}}{9} \\ n_2 = \dfrac{m_{12}}{2} + m_{22} + \dfrac{m_{23}}{2} + \dfrac{m_{24}}{2} \\ n_3 = \dfrac{m_{13}}{3} + \dfrac{m_{23}}{3} + \dfrac{2m_{33}}{3} + \dfrac{m_{34}}{3} \\ n_4 = \dfrac{n-2}{3} - \dfrac{m_{12}}{6} - \dfrac{m_{22}}{3} - \dfrac{7m_{23}}{18} - \dfrac{m_{24}}{6} - \dfrac{2m_{13}}{9} - \dfrac{4m_{33}}{9} - \dfrac{2m_{34}}{9} \end{cases} \tag{7}$$

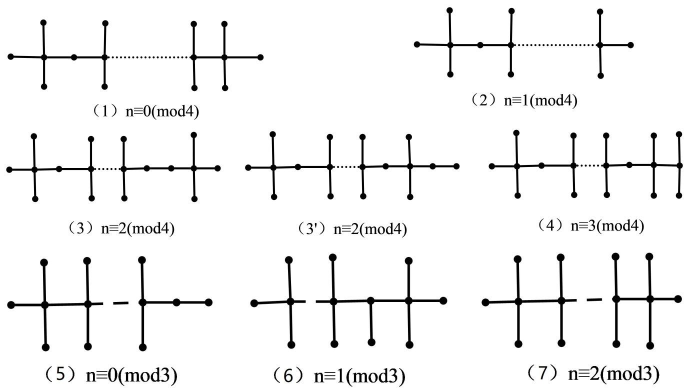

Figure 1. Eight types molecular trees with $n(n \geq 8)$ vertices

Next, we define seven types molecular trees.

Let $\mathcal{T}_1$ is the set of molecular trees T with $n \equiv 0(mod4)$ vertices, where T has no vertex with degree 3, every vertex of degree 2 is adjacent to two vertices of degree 4 in T and there is exactly a pair of vertices with degree 4 adjacent to each other, i.e., T is a tree on n vertices with $m_{14} = \frac{n+4}{2}$, $m_{24} = \frac{n-8}{2}$, $m_{44} = 1$, $m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$ (An example is shown in Figure 1 (1)).

Let $\mathcal{T}_2$ is the set of molecular trees T with $n \equiv 1(mod4)$ vertices, where

T has no vertex with degree 3, every vertex of degree 2 is adjacent to two vertices of degree 4 in T and no two vertices of degree 4 are mutually adjacent, i.e., T is a tree with $m_{14} = \frac{n+3}{2}$, $m_{24} = \frac{n-5}{2}$, $m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0$ (An example is shown in Figure 1 (2)).

Let $\mathcal{T}_3$ is the set of molecular trees T with $n \equiv 2(mod4)$ vertices, where T has no vertex with degree 3, exactly two of vertices of degree 2 are adjacent to a vertex of degree 4 and a vertex of degree 2, and other vertices of degree 2 are adjacent to two vertices of degree 4, i.e., T is a tree with $m_{14} = \frac{n+2}{2}$, $m_{24} = \frac{n-6}{2}$, $m_{22} = 1$, $m_{12} = m_{13} = m_{23} = m_{33} = m_{34} = m_{44} = 0$ (An example is shown in Figure 1 (3)).

Let $\mathcal{T}_{3'}$ is the set of molecular trees T with $n \equiv 2(mod4)$ vertices, where T has no vertex with degree 3, exactly one of vertices of degree 2 is adjacent to a vertex of degree 4 and a vertex of degree 1, and other vertices of degree 2 are adjacent to two vertices of degree 4, i.e., T is a tree with $m_{14} = \frac{n}{2}$, $m_{24} = \frac{n-4}{2}$, $m_{12} = 1$, $m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0$ (An example is shown in Figure 1 ($3'$)).

Let $\mathcal{T}_4$ is the set of molecular trees T with $n \equiv 3(mod4)$ vertices, where T has exactly one vertex of degree 3, which is adjacent to two vertices of degree 1 and one vertex of degree 4 and every vertex of degree 2 is adjacent to two vertices of degree 4, i.e., T is a tree with $m_{14} = \frac{n-1}{2}$, $m_{24} = \frac{n-7}{2}$, $m_{13} = 2$, $m_{34} = 1$, $m_{12} = m_{22} = m_{23} = m_{33} = m_{44} = 0$ (An example is shown in Figure 1 (4)).

Let $\mathcal{T}_5$ is the set of molecular trees T with $n \equiv 0(mod3)$ vertices, where T has exactly one 2-degree vertex, which is adjacent to one 4-degree vertex and one 1-degree vertex in T, and no 3-degree vertex, i.e., T is a tree on n vertices with $m_{14} = \frac{2n-3}{3}$, $m_{44} = \frac{n-6}{3}$, $m_{24} = 1$, $m_{12} = 1, m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$ (An example is shown in Figure 1 (5)).

Let $\mathcal{T}_6$ is the set of molecular trees T with $n \equiv 1(mod3)$ vertices, where T has exactly one 3-degree vertex, which is adjacent to two vertices of degree 4 and one 1-degree vertex in T, and no 2-degree vertex, i.e., T is a tree with $m_{14} = \frac{2n-2}{3}$, $m_{44} = \frac{n-10}{3}$, $m_{13} = 1, m_{34} = 2, m_{12} = m_{22} = m_{23} = m_{24} = m_{33} = 0$ (An example is shown in Figure 1 (6)).

Let $\mathcal{T}_7$ is the set of molecular trees T with $n \equiv 2(mod3)$ vertices, where

T has no vertex with degree 3 or degree 2, i.e., T is a tree with $m_{14} = \frac{2n+2}{3}$, $m_{44} = \frac{n-5}{3}$, $m_{12} = m_{13} = m_{22} = m_{23} = m_{24} = m_{33} = m_{34} = 0$ (An example is shown in Figure 1 (7)).

Theorem 3. *Let $T \in \mathcal{CT}_n$ with $n \geq 8$, then*

$$3 \leq SO_1(T) \leq \begin{cases} \frac{27n-36}{4} & n \equiv 0(mod4) \\ \frac{27n-15}{4} & n \equiv 1(mod4) \\ \frac{27n-42}{4} & n \equiv 2(mod4) \\ \frac{27n-53}{4} & n \equiv 3(mod4) \end{cases}$$

the left equality holds if and only if $T \cong P_n$ and the right equality holds if and only if $T \in \mathcal{T}_i$ for $n \equiv (i-1)(mod4)$ $(i = 1, 2, 4)$ and $T \in \mathcal{T}_3$ or $T \in \mathcal{T}_{3'}$ for $n \equiv 2(mod4)$.

Proof. By Theorem 2, we have $SO_1(T) \geq 3$ with equality if and only if $T \cong P_n$.

From the definition (1) of SO_1, we have

$$SO_1(T) = \frac{3}{2}m_{12} + 4m_{13} + \frac{15}{2}m_{14} + \frac{5}{2}m_{23} + 6m_{24} + \frac{7}{2}m_{34}. \tag{8}$$

Replacing m_{14} and m_{24} in (8) by (6), we have

$$\begin{aligned} SO_1(T) = \frac{27n-15}{4} - \frac{27m_{12}}{4} - \frac{15m_{13}}{4} - \frac{27m_{22}}{4} \\ -\frac{10m_{23}}{3} - \frac{23m_{33}}{4} - 2m_{34} - \frac{21m_{44}}{4} \end{aligned} \tag{9}$$

which is maximal for a fixed number of vertices when the values m_{12}, m_{13}, m_{22}, m_{23}, m_{33}, m_{34}, and m_{44} are equal to zero. However, in the case of molecular trees with n vertices, the condition

$$m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0 \tag{10}$$

can be satisfied only if $n \equiv 1(mod4)$.

Any molecular tree satisfying (10) has no vertices of degree 3, all its vertices of degree 2 are adjacent to two vertices of degree 4, and no two vertices of degree 4 are mutually adjacent (See (2) in Figure 1).

Hence, if $n \equiv 1(mod4)$, then for any molecular tree T with n vertices,

$$SO_1(T) \leq \frac{27n-15}{4}$$

with equality if and only if $T \in \mathcal{T}_2$.

If $n \not\equiv 1(mod4)$, then (10) cannot be satisfied by any molecular tree on n vertices. In order to find the molecular trees with the maximal SO_1-value, we have to find the values of the parameters $m_{12}, m_{13}, m_{22}, m_{23}, m_{33}, m_{34}$, and m_{44} as close to zero as possible compatible to the existence of a molecular tree, i.e., for which the right-hand sides of (6) are integers, and for which a graph exists and we have that $m_{13}+m_{23}+2m_{33}+m_{34}$ has to be a multiple of 3 from $n_3 = \frac{m_{13}}{3} + \frac{m_{23}}{3} + \frac{2m_{33}}{3} + \frac{m_{34}}{3}$.

By (9), we know that there is must be $n_3 = 0$ or $n_3 = 1$ for $n \not\equiv 1(mod4)$ if T is a molecular tree with the maximal $SO_1(T)$-value.

Case 1. If $n_3 = 0$, then $m_{13} = m_{23} = m_{33} = m_{34} = 0$, and

$$SO_1(T) = \frac{27n-15}{4} - \frac{27m_{12}}{4} - \frac{27m_{22}}{4} - \frac{21m_{44}}{4}. \tag{11}$$

To find the molecular tree(s) with the maximal $SO_1(T)$-value, we only need to consider $m_{12}+m_{22}+m_{44} = 1$.

If $n \equiv 2(mod4)$, there are two types of molecular trees such that $m_{12}+m_{22}+m_{44} = 1$, i.e., $m_{12} = 1, m_{22} = m_{44} = 0$ or $m_{12} = 0, m_{22} = 1, m_{44} = 0$. By simply computing and comparing, for any molecular tree T with $n \equiv 2(mod4)$ vertices, we have

$$SO_1(T) \leq \frac{27n-42}{4}$$

with equality if and only if $T \in \mathcal{T}_3$ or $T \in \mathcal{T}_{3'}$.

If $n \equiv 0(mod4)$, there is only one type of molecular trees such that $m_{12}+m_{22}+m_{44} = 1$, i.e., $m_{12} = m_{22} = 0, m_{44} = 1$. Then, for any molecular tree with $n \equiv 0(mod4)$ vertices,

$$SO_1(T) \leq \frac{27n-36}{4}$$

with equality if and only if $T \in \mathcal{T}_1$.

If $n \equiv 3(mod4)$, then there is no molecular trees such that $m_{12}+m_{22}+m_{44}=1$.

Case 2. If $n_3 = 1$, then $m_{13} + m_{23} + 2m_{33} + m_{34} = 3$. To find the molecular trees with the maximal $SO_1(T)$-value, we only need to consider all possible choices of $(m_{13}, m_{23}, m_{33}, m_{34})$ such that $m_{13}+m_{23}+2m_{33}+m_{34}=3$.

We hvae that a molecular tree on n vertices and $n_3 = 1$ with the maximal SO_2-value must satisfy

$$m_{12} = m_{22} = m_{44} = m_{23} = m_{33} = 0, m_{13} = 2, m_{34} = 1 \tag{12}$$

and it can be satisfied only if $n \equiv 3(mod4)$. Then, for any molecular tree with $n \equiv 3(mod4)$ vertices,

$$SO_1(T) \leq \frac{27n-53}{4}$$

with equality if and only if $T \in \mathcal{T}_4$. ■

For SO_2, we have

Theorem 4. *[15] Let $T \in \mathcal{C}T_n$ with $n \geq 8$, then*

$$\frac{6}{5} \leq SO_2(T) \leq \begin{cases} \frac{126n-108}{170} & n \equiv 0(mod4) \\ \frac{126n-30}{170} & n \equiv 1(mod4) \\ \frac{126n-102}{170} & n \equiv 2(mod4) \\ \frac{315n-281}{425} & n \equiv 3(mod4) \end{cases}$$

the left equality holds if and only if $T \cong P_n$ and the right equality holds *if and only if* $T \in \mathcal{T}_i$ *for* $n \equiv (i-1)(mod4)$ *(*$i = 1, 2, 4$*) and* $T \in \mathcal{T}_{3'}$ *for* $n \equiv 2(mod4)$*.*

Theorem 5. *Let* $T \in \mathcal{C}T_n$ *with* $n \geq 8$*, then*

$$\sqrt{2}\pi\frac{6n-8}{3} \leq SO_3(T) \leq \begin{cases} \sqrt{2}\pi\frac{18n-32}{5} & n \equiv 0(mod3) \\ \sqrt{2}\pi\frac{252n-417}{70} & n \equiv 1(mod3) \\ \sqrt{2}\pi\frac{18n-22}{5} & n \equiv 2(mod3) \end{cases}$$

$$\frac{18n-29}{9}\pi \leq SO_4(T) \leq \begin{cases} \frac{815n-3338}{225}\pi & n \equiv 0(mod3) \\ \frac{189080n-401491}{29000}\pi & n \equiv 1(mod3) \\ \frac{326n-474}{50}\pi & n \equiv 2(mod3) \end{cases}$$

the left equality holds if and only if $T \cong P_n$ *and the right equality holds if and only if* $T \in \mathcal{T}_i$ *for* $n \equiv (i-5)(mod3)$ *(*$i = 5, 6, 7$*).*

Proof. By Theorem 1, we have

$$SO_3(T) \geq \sqrt{2}\pi\frac{6n-8}{3}$$

and

$$SO_4(T) \geq \frac{18n-29}{9}\pi$$

with equality if and only if $T \cong P_n$.

From (2), we have

$$\begin{aligned} SO_3(T) = \sqrt{2}\pi(&\frac{5}{3}m_{12} + \frac{5}{2}m_{13} + \frac{17}{5}m_{14} + 2m_{22} + \frac{13}{5}m_{23} + \frac{10}{3}m_{24} \\ &+ 3m_{33} + \frac{25}{7}m_{34} + 4m_{44}). \\ SO_4(T) = \frac{\pi}{2}(&\frac{25}{9}m_{12} + \frac{25}{4}m_{13} + \frac{289}{25}m_{14} + 4m_{22} + \frac{169}{25}m_{23} + \frac{100}{9}m_{24} \\ &+ 9m_{33} + \frac{625}{49}m_{34} + 16m_{44}). \end{aligned} \tag{13}$$

Replacing m_{14} and m_{44} in (13) by (7), we have

$$\begin{aligned} SO_3(T) =&\sqrt{2}\pi\left[\frac{18n-22}{5}-\frac{23m_{12}}{15}-\frac{5m_{13}}{6}-\frac{8m_{22}}{5}-\frac{17m_{23}}{15}-\frac{7m_{24}}{15}\right.\\ &\left.-\frac{13m_{33}}{15}-\frac{38m_{34}}{105}\right]\\ SO_4(T) =&\frac{\pi}{2}\left[\frac{326n-474}{25}-\frac{1643m_{12}}{225}-\frac{289m_{13}}{60}-\frac{226m_{22}}{25}-\frac{109m_{23}}{15}\right.\\ &\left.-\frac{767m_{24}}{225}-\frac{578m_{33}}{225}-\frac{10112m_{34}}{3675}\right] \end{aligned} \tag{14}$$

which is maximal for a fixed number of vertices when the values m_{12}, m_{13}, m_{22}, m_{23}, m_{24}, m_{33}, and m_{34} are equal to zero. However, in the case of molecular trees with n vertices, the condition

$$m_{12} = m_{13} = m_{22} = m_{23} = m_{24} = m_{33} = m_{34} = 0 \tag{15}$$

can be satisfied only if $n \equiv 2(mod3)$.

Any molecular tree satisfying (15) has no vertices of degree 3 and degree 2, all its vertices of degree 1 are adjacent to vertices of degree 4 (See (7) in Figure 1).

Hence, if $n \equiv 2(mod3)$, then for any molecular tree with n vertices,

$$SO_3(T) \leq \sqrt{2}\pi\frac{18n-22}{5} \qquad SO_4(T) \leq \frac{326n-474}{50}\pi$$

with equality if and only if $T \in \mathcal{T}_7$.

If $n \not\equiv 2(mod3)$, then (15) cannot be satisfied by any molecular tree on n vertices. In order to find the molecular trees with the maximal SO_k-value ($k = 3, 4$), we have to find the values of the parameters $m_{12}, m_{13}, m_{22}, m_{23}$, m_{24}, m_{33} and m_{34} as close to zero as possible compatible to the existence of a molecular tree, i.e., for which the right-hand sides of (7) are integers, and for which a graph exists and we have that $m_{13} + m_{23} + 2m_{33} + m_{34}$ has to be a multiple of 3 and $m_{12} + 2m_{22} + m_{23} + m_{24}$ has to be a multiple of 2.

By (14), we know that there is must be either $n_3 = 0, n_2 = 1$ or

$n_3 = 1, n_2 = 0$ for $n \not\equiv 2(mod3)$ if T is a molecular tree with the maximal $SO_3(T)$-value $(k = 3, 4)$.

Case 1. If $n_3 = 0$ and $n_2 = 1$, i.e. $m_{22} = m_{13} = m_{23} = m_{33} = m_{34} = 0$ and $m_{12} + m_{24} = 2$, then

$$\begin{aligned} SO_3(T) &= \sqrt{2}\pi\left(\frac{18n-22}{5} - \frac{23m_{12}}{15} - \frac{7m_{24}}{15}\right). \\ SO_4(T) &= \frac{\pi}{2}\left(\frac{326n-474}{25} - \frac{1643m_{12}}{225} - \frac{767m_{24}}{225}\right) \end{aligned} \tag{16}$$

and n must satisfy $n \equiv 1(mod3)$. There is one type of molecular trees such that $m_{12} = 1, m_{24} = 1$. By simply computing, for any molecular tree T with $n \equiv 1(mod3)$ vertices,

$$SO_3(T) \leq \sqrt{2}\pi\frac{18n-32}{5}$$

$$SO_4(T) \leq \frac{815n-3338}{225}\pi$$

with equality if and only if $T \in \mathcal{T}_5$.

Case 2. If $n_3 = 1$ and $n_2 = 0$, i.e. $m_{13} + m_{34} = 3$ and $m_{12} = m_{22} = m_{23} = m_{24} = m_{33} = 0$, then

$$\begin{aligned} SO_3(T) &= \sqrt{2}\pi\left(\frac{18n-22}{5} - \frac{5m_{13}}{6} - \frac{38m_{34}}{105}\right) \\ SO_4(T) &= \frac{\pi}{2}\left(\frac{326n-474}{25} - \frac{289m_{13}}{60} - \frac{10112m_{34}}{3675}\right). \end{aligned} \tag{17}$$

and n must satisfy $n \equiv 0(mod3)$. There are two types of molecular trees such that $m_{13} = 2, m_{34} = 1$ or $m_{13} = 1, m_{34} = 2$. By simply computing and comparing, for any molecular tree T with $n \equiv 0(mod3)$ vertices,

$$SO_3(T) \leq \sqrt{2}\pi\frac{252n-417}{70}$$

$$SO_4(T) \leq \frac{189080n-401491}{29000}\pi$$

with equality if and only if $T \in \mathcal{T}_6$. ■

4 Conclusions and open problems

In this paper we have analyzed the Sombor-index-like graph invariants and their extremal properties. We show that almost all of these six indices are useful in predicting physicochemical properties with high accuracy compared to some well-established and often used indices. We have found the extremal values of some Sombor-index-like graph invariants and the extremal graphs in the classes of trees and molecular trees with given number of vertices. Here, we propose the following open problems which solution would make the study of the Sombor-index-like graph invariants more complete:

(1) Find the extremal values of SO_5, SO_6 in the set of trees and molecular trees with given number of vertices, respectively;

(2) Find the maximal value of SO_4 in the set of trees with given number of vertices;

(3) Find the extremal values of SO_5, SO_6 in the set of connected graphs with given number of vertices;

(4) Find the maximal values of SO_3, SO_4 in the set of connected graphs with given number of vertices.

The solution of these problems would be an important contribution to the mathematical theory of chemically relevant Sombor-index-like graph invariants.

Appendix: The chemical applicability of Sombor index like graph invariants

In this section, the chemical applicability of the SO-like indices are investigated. We consider the data set of octane isomers for such testing and corresponding experimental values of physico-chemical properties are collected from `http://www.moleculardescriptors.eu/dataset/dataset.htm`. First, we give experimental values of the SO-like indices of for octane isomers, which are listed in Table 1, where there are two pairs of octane isomers with identical values of the SO-like indices since they have the same degree coordinates.

Table 1. Values of SO-like indices of octane isomers

Molecule	SO_1	SO_2	SO_3	SO_4	SO_5	SO_6
octane	3	1.2	59.238	40.143	6.404	5 6.5282
2-methyl-heptane	12	2.5846	67.828	53.466	19.835	34.345
3-methyl-heptane	12	2.7692	66.79	1 52.348	20.184	28.4028
4-methyl-heptane	12	2.7692	66.791	52.348	20.184	28.4028
3-ethyl-hexane	12	2.9538	65.755	51.229	20.534	22.4606
2,2-dimethyl-hexane	30	3.8471	85.303	88.858	39.749	111.02
2,3-dimethyl-hexane	16	3.3846	74.492	64.855	26.33	47.7741
2,4-dimethyl-hexane	21	4.1538	75.381	65.672	33.615	56.2197
2,5-dimethyl-hexane	21	3.9692	76.418	66.79	33.266	62.1619
3,3-dimethyl-hexane	30	4.1647	83.526	86.233	40.474	100.85
3,4-dimethyl-hexane	16	3.5692	73.456	63.736	26.68	41.8319
2-methyl-3-ethyl-pentane	16	3.5692	73.456	63.736	26.68	41.8319
3-methyl-3-ethyl-pentane	30	4.4824	81.749	83.608	41.2	90.6835
2,2,3-trimethyl-pentane	34	4.7117	91.248	99.31	46.461	116.533
2,2,4-trimethyl-pentane	39	5.2317	93.893	102.18	53.18	138.837
2,3,3-trimethyl-pentane	34	4.8447	90.508	97.804	46.837	112.307
2,3,4-trimethyl-pentane	20	4	82.193	77.362	32.476	67.1454
2,2,3,3-tetramethylbutane	45	5.2941	108.41	134.08	58.536	181.782

By the experimental values of Acentric-factor (AcenFac), Entropy(S), SNar and HNar of octane isomers (from http://www.moleculardescriptors.eu/dataset/dataset.htm.) and Table 1, we find the correlation of AcenFac, S, SNar and HNar with the second Sombor index SO_2 for octane isomers. The data related to octanes are listed in Table 3. The following equations give the regression models for the SO-like indices $SO_i(i = 1, 2 \ldots, 6)$.

$$AcenFac = a_{1i} - b_{1i} \times SO_i \tag{18}$$

$$S = a_{2i} - b_{2i} \times SO_i \tag{19}$$

$$SNar = a_{3i} - b_{3i} \times SO_i \tag{20}$$

$$HNar = a_{4i} - b_{4i} \times SO_i \tag{21}$$

By corresponding experimental values [3], we have that correlation of SO_2 with some existing indices like the Sombor index (SO), the first (M_1) and second (M_2) Zagreb indices, forgotten topological index (F), connectivity index (R), sum connectivity index (SCI), symmetric division degree index (SDD) and neighborhood Zagreb index (M_N) are shown in Table 4.

From Table 3, it is obvious that SO_3, SO_4, SO_6 strongly correlate properties of Acentric-factor, Entropy, SNar and HNar of octane isomers, SO_2, SO_5 has slightly better predictive properties for Acentric-factor, SNar

Table 2. The coefficient of a_{ij} and b_{ij} for SO-like indices SO_i

$a_{i,j}$	1	2	3	4	5	6
1	0.3926	0.4536	0.5523	0.4417	0.4163	0.3845
2	112.6025	119.1755	132.77	118.844	115.2222	111.6405
3	4.0841	4.6576	5.6333	4.5441	4.3044	4.0032
4	1.5521	1.7137	1.9554	1.6695	1.6122	1.5293
$b_{i,j}$	1	2	3	4	5	6
1	-0.0027	-0.0314	-0.0028	-0.0014	-0.0024	-0.0007
2	-0.3378	-3.6697	-0.3476	-0.1799	-0.2979	-0.0869
3	-0.026	-0.3003	-0.0267	-0.0136	-0.0235	-0.0066
4	-0.0068	-0.0815	-0.007	-0.0035	-0.0062	-0.0017

Table 3. The square of correlation coefficient of the SO-like indices with AcenFac, S, SNar and HNar

Physico-chemical property	SO_1	SO_2	SO_3	SO_4	SO_5	SO_6
Acentric-factor (AcenFac)	0.75	0.8468	0.8991	0.8962	0.8655	0.8153
Entropy (S)	0.7384	0.7111	0.8838	0.8881	0.7908	0.8187
SNar	0.8023	0.8753	0.9588	0.9282	0.9028	0.864
HNar	0.7664	0.9048	0.9124	0.8683	0.8841	0.8027

Table 4. The square of correlation coefficient of SO-like indices with some existing indices

	M_1	M_2	F	R	SCI	SDD	M_N	SO
SO_1	0.8253	0.6711	0.8219	0.8174	0.8295	0.8273	0.7678	0.8364
SO_2	0.8467	0.7532	0.814	0.8044	0.8373	0.7779	0.8324	0.8428
SO_3	0.9904	0.8318	0.9885	0.9667	0.9826	0.9805	0.9338	0.9984
SO_4	0.9835	0.8363	0.9955	0.9321	0.9528	0.9621	0.9385	0.9906
SO_5	0.9325	0.7671	0.9307	0.8934	0.9185	0.9057	0.8879	0.9433
SO_6	0.937	0.7296	0.9603	0.9106	0.9239	0.9545	0.8677	0.9581

Abbreviations: SO, Sombor index; SCI, sum connectivity index; SDD, symmetric division degree index.

and HNar of octane isomers, and therefore, they may be a step forward in QSPR studies.

From Table 4, we learn the following results: (i) all the six Sombor-index-like indices are strongly correlated with the well-established and often used indices the first Zagreb index (M_1), forgotten topological index (F), connectivity index (R), sum connectivity index (SCI) and the Sombor index (SO); (ii) SO_3, SO_4, SO_5, SO_6 are strongly correlated with symmetric division degree index (SDD) and neighborhood Zagreb index (MN).

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