

Diminished Sombor Index

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Abstract

The diminished Sombor index of a graph G is defined as

$$DSO(G) = \sum \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v},$$

where d_u and d_v are the degrees of vertices u and v , and the summation goes over all pairs of adjacent vertices. Although DSO was introduced as early as in 2021, its properties were not studied so far. The present paper is aimed at filling this gap. We obtain bounds on DSO , characterize the extremal graphs, and establish Nordhaus–Gaddum-type relations. In addition, we report results of numerical studies of the structure-dependency of DSO and its chemical applicability.

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1 Introduction

The Sombor index is a vertex-degree-based graph invariant introduced in 2021 [4], which eventually gained much popularity. Its mathematical properties and applications in chemistry and other areas were studied in great detail. It is defined as

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2}. \quad (1)$$

As early as in 2021, Rajathagiri [11] considered a variant of Sombor index, defined as

$$DSO = DSO(G) = \sum_{uv \in \mathbf{E}(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} \quad (2)$$

which we prefer to be called “*diminished Sombor index*”. No later publication (known to the present authors) considers this graph invariant, and neither in [11] nor in any other place any property of DSO has been established. The present paper is aimed at filling this gap.

In Eqs. (1), (2), and later in this paper, G denotes a simple graph whose vertex and edge sets are $\mathbf{V}(G)$ and $\mathbf{E}(G)$, respectively. The order of G (the number of its vertices) is $|\mathbf{V}(G)| = n$ and its size of G (the number of its edges) is $|\mathbf{E}(G)| = m$. The edge connecting the vertices u and v is denoted by uv .

The degree of a vertex $u \in \mathbf{V}(G)$, denoted d_u , is the count of vertices of the graph G , directly connected to u . Let $\Delta = \max\{d_u : u \in \mathbf{V}(G)\}$ and $\delta = \min\{d_u : u \in \mathbf{V}(G)\}$. An edge connecting vertices of degree a and b is said to be an (a, b) -edge.

The complement of the graph G is denoted by $\overline{G}$. As usual, the standard graphs: cycle, path, star, and complete graph of order n are denoted by C_n , P_n , S_n , and K_n , respectively. The complete bipartite graph of order $p + q$ is denoted by $K_{p,q}$. Recall that $S_n \equiv K_{n-1,1}$.

The wheel W_n is the graph obtained by connecting all vertices of C_{n-1} to a new vertex. The generalized Dutch windmill graph $D_p^{(q)}$, (where $p \geq 2$ and $q \geq 3$), is formed by taking p cycles, each of length q , and joining them at a single common vertex. Notably, when the cycle length q is equal to 3

(resulting in triangles), then one has a friendship graph, denoted by F_p .

Graph-theoretical definitions and notions, not specified above, can be found in the books [7, 13].

2 Preparations

We start by listing expressions for diminished Sombor index of a few simple graphs. Their proofs are straightforward and therefore omitted.

Proposition 1. *Let G be a graph of order n and size m with maximum and minimum vertex degrees Δ and δ .*

- 1) *For the complete graph K_n , $DSO(K_n) = \frac{\sqrt{2}}{4}n(n-1)$.*
- 2) *For the cycle C_n , $DSO(C_n) = \frac{\sqrt{2}}{2}n$.*
- 3) *For the path P_n , $DSO(P_n) = \frac{2\sqrt{5}}{3} + \frac{\sqrt{2}}{2}(n-3)$.*
- 4) *For the complete bipartite graph $K_{p,q}$, $DSO(K_{p,q}) = \frac{m}{n}\sqrt{p^2+q^2}$.*
- 5) *For the star S_n , $DSO(S_n) = \frac{n-1}{n}\sqrt{(n-1)^2+1}$.*
- 6) *If G is the k -dimensional cube Q_k , then $DSO(Q_k) = \sqrt{2} \cdot 2^{k-2}k$.*
- 7) *For the wheel W_n , $DSO(W_n) = (n-1)\left(\frac{\sqrt{2}}{2} + \frac{\sqrt{n^2-2n+10}}{n+2}\right)$.*
- 8) *If G is the Dutch windmill $D_p^{(q)}$, $p \geq 3, q \geq 2$, then*

$$DSO(D_p^{(q)}) = 2p \left[\frac{\sqrt{p^2+1}}{q+1} + \frac{\sqrt{2}}{4}(q-2) \right].$$

- 9) *For the friendship graph F_p , $DSO(F_p) = 2p \left[\frac{\sqrt{p^2+1}}{p+1} + \frac{\sqrt{2}}{4} \right]$.*

From Eq. (2), we see that the term $\frac{\sqrt{d_u^2+d_v^2}}{d_u+d_v}$ is the contribution of the edge uv to the diminished Sombor index of the graph G . Bearing this in mind, we consider the function

$$\gamma(x, y) = \frac{\sqrt{x^2+y^2}}{x+y}$$

recalling that the variables x and y must belong to the interval $[1, n-1]$ and, of course, assume integral values.

We first note that whenever $y = x$, then $\gamma = 1/\sqrt{2}$, irrespective of the actual value of x, y .

By direct calculation we get

$$\frac{\partial}{\partial x} \gamma(x, y) = \frac{y(x-y)}{(x+y)^2 \sqrt{x^2+y^2}}$$

and

$$\frac{\partial}{\partial y} \gamma(x, y) = -\frac{x(x-y)}{(x+y)^2 \sqrt{x^2+y^2}}.$$

This implies that for $x > y$, $\gamma(x, y)$ is a monotonously increasing function of x and a monotonously decreasing function of y . Thus, in the interval $[1, n-1]$, the maximum value of $\gamma(x, y)$ is attained for x as large as possible and y as small as possible, i.e.,

$$\gamma(x, y)_{max} = \gamma(n-1, 1) = \frac{1}{n} \sqrt{(n-1)^2 + 1}. \quad (3)$$

It also follows that minimum possible value of γ is

$$\gamma(x, y)_{min} = \gamma(x, x) = \frac{1}{\sqrt{2}} \quad \text{for } x = 1, 2, \dots, n-1. \quad (4)$$

3 Main results

Theorem 2. *Let G be a graph of size m . Then*

$$\frac{\sqrt{2}}{2}m \leq DSO(G) \leq m.$$

Equality on the left-hand side holds if and only if G consists of components, each of which is a regular graph (not necessarily of equal degree). Equality on the right-hand side holds if and only if $m = 0$, i.e. if $G \cong \overline{K_n}$.

Proof. In the theory of Sombor index, the inequalities

$$\frac{1}{\sqrt{2}}(x+y) \leq \sqrt{x^2+y^2} < x+y \quad (5)$$

were used many times [5, 6, 9]. Equality on the left-hand side holds if and only if $x = y$. Equality on the right-hand side would hold only if $x = 0$ or $y = 0$ (or both). Assuming that $x, y \in [1, n - 1]$, from (5) it immediately follows

$$\frac{1}{\sqrt{2}} \leq \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} < 1$$

which after summation over all pairs of adjacent vertices of the graph G directly implies Theorem 2. ■

Corollary 1. *Among graphs of size m , those consisting of components, each of which is a regular graph (not necessarily of same degree) have minimal DSO. Among connected graphs of size m , regular graphs (of any degree) have minimal DSO.*

Proof. All edges of the graphs specified in Corollary 1 satisfy condition (4). ■

Corollary 2. *Among connected regular graphs of order $n \geq 3$, the cycle C_n has minimal DSO. Among disconnected regular graphs of order $n \geq 4$ without isolated vertices,*

- (a) *if n is even, then the graph consisting of $n/2$ isolated edges has minimal DSO, and*
- (b) *if n is odd, then the graph consisting of $(n - 3)/2$ isolated edges and a triangle has minimal DSO.*

Proof. The graphs specified in Corollary 2 are those from Corollary 1 possessing n vertices and minimum number of edges. ■

Corollary 3. *Let G be a simple graph of order n with maximum vertex degree Δ and minimum vertex degree δ . Then*

$$\frac{\sqrt{2}}{4}n\delta \leq DSO(G) \leq \frac{n\Delta}{2}.$$

Proof. By using the handshaking lemma, we have $n\delta \leq \sum_{u \in V} d_u = 2m \leq$

$n\Delta$. Therefore, by applying Theorem 2, we get

$$\frac{\sqrt{2}}{2} \left(\frac{n\delta}{2} \right) \leq \frac{\sqrt{2}}{2} m \leq DSO(G) \leq m \leq \frac{n\Delta}{2}. \quad \blacksquare$$

Theorem 3. *Let G be a graph of order n . Then*

- i) $DSO(G) > DSO(G - e) + \frac{|d_u - d_v|}{\sqrt{2}(2n-2)}$, for any edge $e = uv \in \mathbf{E}(G)$,
- ii) $DSO(G + e) > DSO(G) + \frac{|d_u - d_v|}{\sqrt{2}(2n-2)}$, where $e = uv$ such that the vertices u and v are not adjacent in G .

Proof. It is sufficient to prove case (i). Let $e = uv$ be an edge in the graph G . By removing it from G , we obtain the subgraph $G - e$. Now we add the edge $e = uv$ back to $G - e$. Then the terms $\frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v}$ adds to $DSO(G - e)$. Since $\sqrt{d_u^2 + d_v^2} > \frac{|d_u - d_v|}{\sqrt{2}}$, and since $d_u + d_v \leq 2n - 2$ holds for any edges $e = uv$, it follows that

$$\begin{aligned} DSO(G) &> DSO(G - e) + \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} \\ &> DSO(G - e) + \frac{|d_u - d_v|}{\sqrt{2}(d_u + d_v)} \\ &> DSO(G - e) + \frac{|d_u - d_v|}{\sqrt{2}(2n - 2)}. \end{aligned}$$

The proof of case (ii) follows in an analogous manner. $\blacksquare$

Theorem 4. *Let v be a vertex of the graph G . Denote by $\mathbf{E}(G, v)$ the set of edges of G whose one endpoint is v . Then for a graph G of order n ,*

$$DSO(G - v) < DSO(G) - \frac{1}{\sqrt{2}(2n - 2)} \sum_{uv \in \mathbf{E}(G, v)} |d_u - d_v|.$$

Proof. By removing a vertex $v \in \mathbf{V}(G)$ along with all its incident edges, we obtain the graph $G - v$. We now add the vertex v back to $G - v$ together with all edges that were originally incident to v . From the previous proof we know that for any edge $uv \in \mathbf{E}(G)$, $\sqrt{d_u^2 + d_v^2} > \frac{|d_u - d_v|}{\sqrt{2}}$ and $d_u + d_v \leq$

$2n - 2$ hold. Therefore,

$$\begin{aligned}
 DSO(G) &> DSO(G - v) + \sum_{uv \in \mathbf{E}(G, v)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} \\
 &> DSO(G - v) + \sum_{uv \in \mathbf{E}(G, v)} \frac{|d_u - d_v|}{\sqrt{2}(d_u + d_v)} \\
 &> DSO(G - v) + \frac{1}{\sqrt{2}(2n - 2)} \sum_{uv \in \mathbf{E}(G, v)} |d_u - d_v|. \quad \blacksquare
 \end{aligned}$$

We add here that if $u \notin \mathbf{V}(G)$, then, $DSO(G) \leq DSO(G + u)$, with equality if and only if u is an isolated vertex.

The following theorem is a Nordhaus–Gaddum type relation for the diminished Sombor index [1].

Theorem 5. *Let G be a simple graph of order n . Then*

$$DSO(G) + DSO(\overline{G}) \geq \frac{\sqrt{2}}{4}n(n - 1).$$

Equality holds if and only if $G \cong K_n$.

Proof. Let G be a simple graph of order n and size m . If d_u is the degree of vertex $u \in \mathbf{V}(G)$, then $n - 1 - d_u$ is the degree of this vertex in $\overline{G}$. Setting $a = (n - 1 - d_u)^2$ and $b = (n - 1 - d_v)^2$ into the inequality (5), we get for any $uv \in \mathbf{E}(G)$,

$$\frac{\sqrt{2}}{2} \left(\frac{\sqrt{(n-1-d_u)^2} + \sqrt{(n-1-d_v)^2}}{(n-1-d_u) + (n-1-d_v)} \right) \leq \frac{\sqrt{(n-1-d_u)^2 + (n-1-d_v)^2}}{(n-1-d_u) + (n-1-d_v)}.$$

Therefore,

$$DSO(\overline{G}) \geq \frac{\sqrt{2}}{2} \sum_{uv \in \mathbf{E}(G)} 1 = \frac{\sqrt{2}}{2} m'$$

where m' is the number of edges of $\overline{G}$. On the other hand, using Theorem 2, $DSO(G) \geq \frac{\sqrt{2}}{2}m$. Therefore,

$$DSO(G) + DSO(\overline{G}) \geq \frac{\sqrt{2}}{2}(m + m')$$

and Theorem 5 follows by $m + m' = n(n - 1)/2$. ■

Theorem 6. *Let G be a graph of order n and size m . Then*

$$DSO(G) \cdot DSO(\overline{G}) \geq \frac{1}{2}m \left(\frac{n(n-1)}{2} - m \right).$$

Proof. This result is easily derived from Theorems 2 and 5. ■

Theorem 7. *Let G be a graph of size m with the maximum degree Δ and the minimum degree δ . Then*

$$DSO(G) \leq \frac{\sqrt{\Delta^2 + \delta^2}}{\Delta + \delta} m.$$

Equality holds if and only if G is a regular graph or a complete bipartite graph.

Proof. Recalling that $\gamma(x, y)$ is a monotonously increasing function of x and a monotonously decreasing function of y , we conclude that in our case the greatest possible contribution of an edge to $DSO(G)$ is $\gamma(\Delta, \delta)$. Thus

$$\gamma(\Delta, \delta) = \frac{\sqrt{\Delta^2 + \delta^2}}{\Delta + \delta} \geq \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v}$$

holds for all edges $uv \in \mathbf{E}(G)$. ■

The following lemma will be used in the next result.

Lemma 1. [10] *If $F : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is a convex function and $x_i > 0$ for $1 \leq i \leq m$, then*

$$F\left(\frac{x_1 + \cdots + x_m}{m}\right) \leq \frac{1}{m}(F(x_1) + \cdots + F(x_m)).$$

Theorem 8. *Let G be a simple graph of size m with the maximum degree Δ and the minimum degree δ . Then for $\alpha \geq \frac{1}{2}$,*

$$DSO(G) \leq m^{2\alpha} \left(\frac{\delta\Delta}{\delta^2 + \Delta^2} \right)^\alpha.$$

Proof. We begin by proving that for any two vertices $u, v \in \mathbf{V}(G)$,

$$\frac{2\Delta\delta}{\Delta^2 + \delta^2} \leq \frac{2d_u d_v}{d_u^2 + d_v^2}. \quad (6)$$

Assume that $f(x) = \frac{2x}{x^2+1}$ where $x > 0$. We have $f'(x) = \frac{2(1-x^2)}{x^2+1}$ and consequently, $f(x)$ is an increasing function on $[0, 1]$ and a decreasing function on $[1, \infty]$. Therefore, the minimum value of $f(x)$ on $[\frac{\delta}{\Delta}, \frac{\Delta}{\delta}]$ occurs at the end points. Therefore, for any $x, y \in [\delta, \Delta]$ where $\frac{x}{y} \in [\frac{\delta}{\Delta}, \frac{\Delta}{\delta}]$, we get $f\left(\frac{x}{y}\right) \geq f\left(\frac{\delta}{\Delta}\right)$. Hence

$$\frac{2\left(\frac{x}{y}\right)}{\frac{x^2}{y^2} + 1} \geq \frac{2\left(\frac{\delta}{\Delta}\right)}{\frac{\delta^2}{\Delta^2} + 1}$$

and we get

$$\frac{2xy}{x^2 + y^2} \geq \frac{2\Delta\delta}{\delta^2 + \Delta^2}$$

from which inequality (6) follows.

Thus, for any $d_u, d_v \in [\delta, \Delta]$ we have $\frac{\Delta\delta}{\Delta^2 + \delta^2} \leq \frac{d_u d_v}{d_u^2 + d_v^2}$, with equality if and only if $\{d_u, d_v\} \in [\delta, \Delta]$. Since

$$\frac{d_u^2 + d_v^2}{(d_u + d_v)^2} \leq \frac{d_u^2 + d_v^2}{d_u d_v} \leq \frac{\delta^2 + \Delta^2}{\delta\Delta}$$

we get

$$\sum_{uv \in \mathbf{E}(G)} \left(\frac{d_u^2 + d_v^2}{(d_u + d_v)^2} \right)^\alpha \leq \sum_{uv \in \mathbf{E}(G)} \left(\frac{\delta^2 + \Delta^2}{\delta\Delta} \right)^\alpha.$$

For $\alpha \geq \frac{1}{2}$, the function $h(x) = x^{2\alpha}$ is convex and using Lemma 1 we get

$$\begin{aligned} DSO(G)^{2\alpha} &= m^{2\alpha} \left(\sum_{uv \in \mathbf{E}(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} \right)^{2\alpha} \\ &\leq m^{2\alpha} \left(\frac{1}{m} \sum_{uv \in \mathbf{E}(G)} \left(\frac{d_u^2 + d_v^2}{(d_u + d_v)^2} \right)^\alpha \right) \leq m^{2\alpha} \left(\frac{1}{m} \sum_{uv \in \mathbf{E}(G)} \left(\frac{\delta^2 + \Delta^2}{\delta\Delta} \right)^\alpha \right) \end{aligned}$$

and Theorem 8 follows. ■

Theorem 9. *Let G be a connected graph of order n and size m with ϵ pendent edges. Then*

$$DSO(G) \geq \sqrt{2} \left[\frac{\epsilon}{2(n-1)} + \frac{m-\epsilon}{(n-1-\frac{\epsilon}{2})^2} \right].$$

Proof. Since $0 < \frac{1}{d_u} \leq 1$ for any $u \in \mathbf{V}(G)$, it holds $\frac{1}{d_u} + \frac{1}{d_v} \leq 2$ and thus,

$$\frac{2}{d_u + d_v} \geq \frac{1}{d_u d_v}. \quad (7)$$

For any pendent edge $uv \in \mathbf{E}(G)$, we have $\frac{1}{d_u d_v} \geq \frac{1}{n-1}$. If uv is a non-pendent edge, then $d_u + d_v \leq 2(n-1) - \epsilon$ and consequently

$$d_u d_v \leq \left(\frac{d_u + d_v}{2} \right)^2 \leq \left(n-1 - \frac{\epsilon}{2} \right)^2.$$

Therefore, for such a case and by using (7),

$$\frac{2}{d_u + d_v} \geq \frac{1}{d_u d_v} \geq \frac{1}{(n-1-\frac{\epsilon}{2})^2}$$

and we get

$$\begin{aligned} DSO(G) &= \sum_{uv \in \mathbf{E}(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u + d_v} = \frac{1}{2} \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2} \left(\frac{2}{d_u + d_v} \right) \\ &\geq \frac{1}{2} \left[\frac{\epsilon \sqrt{1+1}}{n-1} + \frac{(m-\epsilon) \sqrt{2^2+2^2}}{(n-1-\frac{\epsilon}{2})^2} \right] = \frac{1}{2} \left[\frac{\sqrt{2}\epsilon}{n-1} + \frac{2\sqrt{2}(m-\epsilon)}{(n-1-\frac{\epsilon}{2})^2} \right]. \end{aligned}$$

■

4 Graphs extremal with respect to diminished Sombor index

In order to avoid trivialities, throughout this section it is assumed that the graphs are connected. We always consider graphs having a given order

n . For such graphs we establish those with minimal and maximal DSO . Some other extremality-related results are given above in Corollaries 1 and 2.

Theorem 10. *Among all connected graphs with $n \geq 2$ vertices,*

$$DSO(P_n) \leq DSO(G) \leq DSO(K_n).$$

Equalities holds if and only if $G \cong P_n$ and $G \cong K_n$.

Proof. The upper bound is obtained directly from the definition of DSO and Theorem 3(ii).

By Theorem 3, by deleting an edge from the graph G , $DSO(G)$ decreases. Therefore, the connected graph with minimum DSO -value is a tree. In a trivial manner, for $n = 2, 3$, this tree is the path. We thus suppose that $n \geq 4$.

Consider now any other tree $T \not\cong P_n$. Then it has at least three pendent edges. Replacing one of these pendent edges so that it becomes a $(2,2)$ -edge, we obtain a tree T' with no more pendent edges than T . Bearing in mind the result (4), it must be $DSO(T') < DSO(T)$. Repeating this transformation, we must arrive at a tree with exactly two pendent edges, i.e., at the path. ■

Theorem 11. *For any tree T of order n ,*

$$DSO(P_n) \leq DSO(T) \leq DSO(S_n).$$

Equality holds if and only if $T \cong P_n$ and $T \cong S_n$.

Proof. The left-hand side of Theorem 11 follows from Theorem 10.

Earlier we established that the maximal possible contribution of an edge to the DSO -value of any graph is $\gamma(n-1, 1)$, cf. Eq. (3). Since all edges of the star S_n are $(n-1, 1)$ -edges, we arrive at the upper bound. ■

For characterizing cyclic graphs with minimal DSO , we will need an argument stated in the next proposition. We used it already in the proof of Theorem 10.

Proposition 12. *For $c \geq 1$, c -cyclic graphs with minimal DSO-value have no pendent edges.*

Proof. Let G be a graph and v its vertex. Let a branch (a tree) Θ be attached to v . Let Θ has t edges of which at least one must be pendent. Replace one of the pendent edges of Θ into any other part of the graph G , so that it becomes a (2,2)-edge.

Denote the newly obtained graph by G' . Then the branch attached to v in G' has $t - 1$ edges of which at least one is pendent (except when $t - 1 = 0$). The graphs G and G' have the same number of vertices and the same number of edges, and therefore equal cyclomatic numbers, i.e., equal number of cycle. Bearing in mind (4), $DSO(G') < DSO(G)$.

Repeating the transformation $G \Rightarrow G'$ sufficient number of times, we completely eliminate the branch Θ , arriving at a graph G^* without branch Θ . The graphs G and G^* have equal number of cycles and $DSO(G^*) < DSO(G)$. ■

Denote by U_n the unicyclic graph obtained from a star S_n by connecting two pendent vertices with an edge.

Theorem 13. *Among unicyclic graphs of order n ,*

$$DSO(C_n) \leq DSO(G) \leq DSO(U_n).$$

Equalities holds if and only if $G \cong C_n$ and $G \cong U_n$.

Proof. The lower bound is a special case of Proposition 12. U_n is the unicyclic graph with maximum number of $(n - 1, 1)$ -edges, which implies the upper bound. ■

Theorem 14. *Among bicyclic graphs of order n , minimal DSO have the graphs*

- (a) *obtained by inserting an edge into C_n , and*
- (b) *obtained by connecting two disjoint cycles by an edge, both having DSO equal to*

$$4\gamma(3, 2) + \gamma(3, 3) + (n - 4)\gamma(2, 2) = \frac{1}{\sqrt{2}}n + \left(\frac{4}{5}\sqrt{13} - \frac{3}{2}\sqrt{2}\right).$$

Proof. Taking into account Proposition 12, we need to focus our attention to the graphs of the type $\mathcal{A}_0$, $\mathcal{A}_1$, and $\mathcal{A}_2$ shown in Figure 1

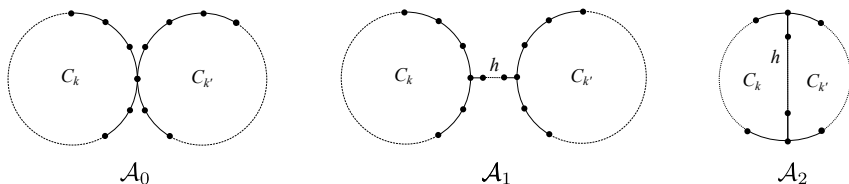


Figure 1. Bicyclic graphs without branches.

In order to minimize DSO , in $\mathcal{A}_1$ and $\mathcal{A}_2$ one should choose $h = 0$, because then we get a $(3,3)$ -edge. If so, then $\mathcal{A}_0$ has four $(2,4)$ -edges, whereas the rest are $(2,2)$ -edges, $\mathcal{A}_1$ has four $(2,3)$ -edges, whereas the rest are $(2,2)$ - and $(3,3)$ -edges, and $\mathcal{A}_2$ has four $(2,3)$ -edges, whereas the rest are $(2,2)$ - and $(3,3)$ -edges. It can be immediately verified that $\gamma(2,4) > \gamma(2,3)$. Therefore, the bicyclic graphs with minimal DSO are $\mathcal{A}_1$ and $\mathcal{A}_2$, both with $h = 0$ and with the same DSO -value. ■

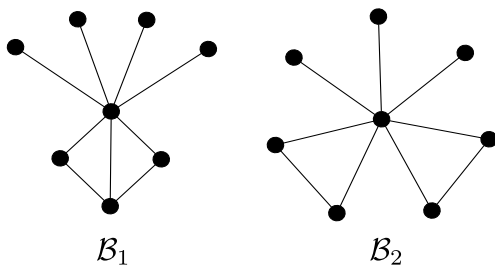


Figure 2. Bicyclic graphs considered in Theorem 15.

Denote by $\mathcal{B}_1$ the bicyclic graph obtained by connecting by two edges three pendent vertices of the star S_n , see Figure 2.

Theorem 15. *Among bicyclic graphs of order n , $\mathcal{B}_1$ has maximal DSO -value.*

Proof. Among bicyclic graphs, $\mathcal{B}_1$ has the greatest number of $(n-1, 1)$ -edges.

To be on the safe side, we compare the *DSO*-values of the two graphs depicted in Figure 2. The fact that the difference

$$DSO(\mathcal{B}_1) - DSO(\mathcal{B}_2) = [\gamma(n-1, 1) + \gamma(n-1, 3)] - 2\gamma(n-1, 2)$$

is positive-valued for all $n \geq 5$ can be checked by direct calculation. ■

We conclude this section by conjecturing that the tricyclic graphs with minimal *DSO* are those obtained by connecting two disjoint cycles by two edges, so that a quadrangle is formed.

5 Numerical work

To assess the features of the diminished Sombor index, we performed a comparative numerical analysis of this index and its predecessors. In particular, we compared the diminished Sombor index (*DSO*) with the Sombor index (*SO*), the reduced Sombor index (*RSO*), the average Sombor index (*ASO*), the Euler Sombor index (*EuSO*), and the elliptic Sombor index (*ESO*). Here, the results on prediction ability, intercorrelations, degeneracy, and the structure sensitivity of the *DSO* compared to the other Sombor indices are presented.

5.1 On prediction ability

Nowadays, it has become a common procedure to assess the prediction quality of a topological index on the set of physicochemical properties of octanes. Dataset with physicochemical properties of octanes are taken from [14]. Among them, we selected the boiling point (T_B), the enthalpy of formation (ΔH_f), the enthalpy of vaporization (ΔH_{vap}), the entropy (S), and the acentric factor (ω), to be used for an assessment of the predicting ability of the *DSO*. These particular properties were selected because the correlation coefficients obtained with the diminished Sombor index are higher than 0.8. This value is a limit below which one can consider that there is no correlation between the index and the property.

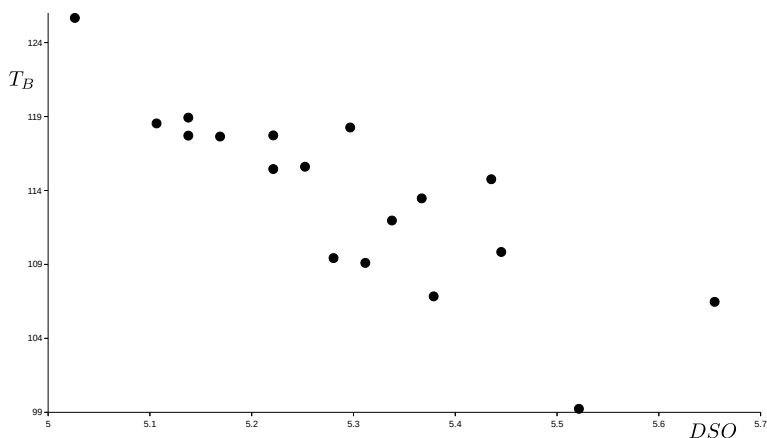
A Python script was used to calculate the values of the Sombor indices for the octanes, and to compute the correlation coefficients between the Sombor indices and the physicochemical properties. The results of the correlation analysis are presented in Table 1.

Correlation coefficients R inscribed into Table 1 reveal that the diminished Sombor index DSO demonstrated significantly stronger correlations with the T_B , ΔH_f , and the ΔH_{vap} of octanes than the other Sombor indices.

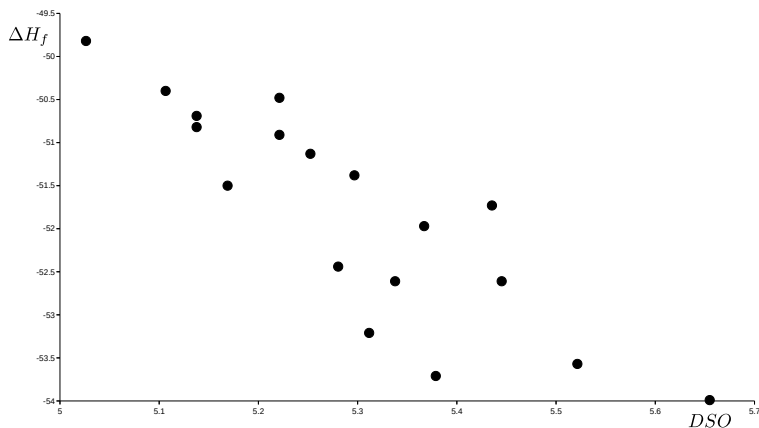
Table 1. Correlation coefficients R between the Sombor indices and physicochemical properties of octanes.

	Correlation coefficients R					
	SO	RSO	ASO	$EuSO$	ESO	DSO
T_B	-0.7497	-0.7579	-0.7333	-0.7332	-0.6844	-0.8265
ΔH_f	-0.7937	-0.7979	-0.7600	-0.7763	-0.7398	-0.8564
ΔH_{vap}	-0.9032	-0.9097	-0.8966	-0.8936	-0.8600	-0.9474
S	-0.9465	-0.9446	-0.9460	-0.9514	-0.9576	-0.9114
ω	-0.9594	-0.9597	-0.9791	-0.9674	-0.9744	-0.9180

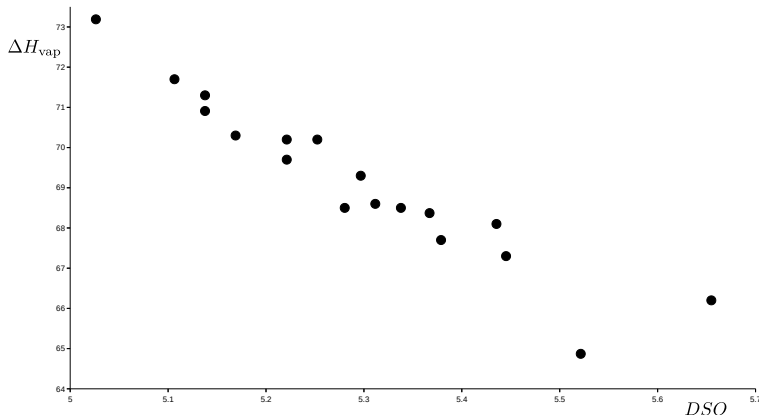
In order to avoid a possibility of specious correlations, these for the boiling point (T_B), the heat of formation (ΔH_f), and the heat of vaporization (ΔH_{vap}) are presented in Figs. 3a, 3b, and 3c, respectively.



(a) Correlation between the diminished Sombor index and the boiling point of octanes.



(b) Correlation between the diminished Sombor index and the heat of formation of octanes.



(c) Correlation between the diminished Sombor index and the heat of vaporization of octanes.

The diminished Sombor index DSO has passed this preliminary test and justified its introduction. In other words, in some cases it exhibits better prediction ability than other well-established Sombor indices.

5.2 On intercorrelations

Assuming a linear relationship among the Sombor indices, we performed a correlation analysis. The obtained correlation matrix is presented in Figure 4.

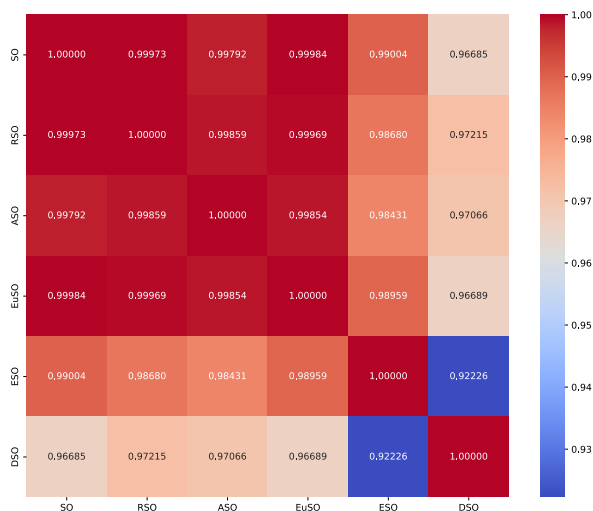


Figure 4. Correlation matrix.

The first observation is that the Sombor indices are highly correlated with each other. This is particularly expressed in the group of indices SO , RSO , ASO , and $EuSO$. The correlation coefficients between these indices are higher than 0.99, which indicates that they are very similar to each other. A slightly lower correlation is observed between the elliptic Sombor index ESO and the other Sombor indices, with correlation coefficients ranging from 0.92 to 0.99. The lowest correlation is observed between the diminished Sombor index DSO and the other Sombor indices, with correlation coefficients ranging from 0.92 to 0.97. Although, this test reveals a high correlation between the diminished Sombor index and the other Sombor indices, it is still lower than the correlation between the other Sombor indices themselves. This indicates that the diminished Sombor index captures some additional information that is not present in the other Sombor indices.

5.3 On degeneracy

Degeneracy of a topological index is an indicator of its ability to discriminate among different graphs. The property was introduced in [8]. We used this property to compare the diminished Sombor index with the other Sombor indices. The results are shown in Figure 5 for the case of all trees with 10 vertices.

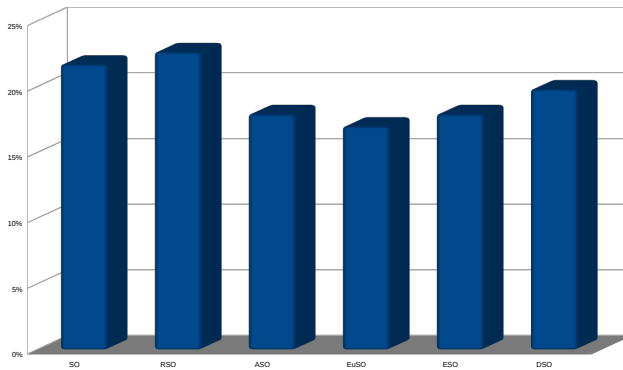


Figure 5. Degeneracy of the Sombor indices.

Figure 5 shows that the degeneracy of the *DSO* is comparable with other Sombor indices. In particular, the degeneracy of the diminished Sombor index is approaching 20% in the case of trees with 10 vertices. The Sombor and reduced Sombor indices are more degenerate than *DSO*, but the average Sombor index, the Euler Sombor index, and the elliptic Sombor index are less degenerate. The Euler Sombor index is the least degenerate among all Sombor indices in the case of 10-vertex trees with the degeneracy equal to 16.98%, while the highest degeneracy is observed with the reduced Sombor index, reaching the degeneracy of 22.64%. Thus, the diminished Sombor index *DSO*, with degeneracy of 19.81%, is placed in the middle of the Sombor indices in terms of degeneracy.

5.4 On structure sensitivity

The structure sensitivity of a topological index measures its response to structural changes. It is expected that the value of a topological descriptor

will gradually change with a gradual change in the structure of a molecule. This quality of a topological index is not easy to quantify. To the best knowledge of the authors, there are two approaches to quantify structure sensitivity [3, 12]. In both of them, two parameters need to be calculated. One is called structure sensitivity (*SS*) and the other is abruptness (*Abr*). Structure sensitivity measures the response of a topological index to minor structural changes, while abruptness detects abnormalities in the values of a topological index when the structure is just a mildly changed (unexpectedly high leaps in values for a minor structural modification). Recently, a third parameter *SA* was introduced, which is the ratio between structure sensitivity and abruptness [2].

Both procedures for quantifying structure sensitivity has pros and cons. Here we chose the second method [12] because of its lower computational complexity, but its domain is limited to only molecular graphs.

Following closely the procedure described in [12], we performed a structure sensitivity analysis of the diminished Sombor index *DSO* and compared it with the other Sombor indices. We used a set of all decanes. The results of the structure sensitivity analysis are summarized in Table 2 and Figure 6.

Table 2. Structure sensitivity of the Sombor indices tested on a set of all decanes.

	<i>SS</i>	<i>Abr</i>	<i>SA</i>
<i>SO</i>	0.19317	0.39619	0.48757
<i>RSO</i>	0.19250	0.39298	0.48983
<i>ASO</i>	0.18231	0.37609	0.48475
<i>EuSO</i>	0.19117	0.38768	0.49311
<i>ESO</i>	0.18798	0.38973	0.48232
<i>DSO</i>	0.20578	0.41723	0.49321

The data in Table 2, as well as Figure 6 show that there is no significant difference in structure sensitivity and abruptness among the Sombor indices. In particular, the lowest value of the *SS* was obtained for the average Sombor index, while the highest one is detected in the case of the diminished Sombor index. The same is obtained in the case of abruptness. Superficial reasoning would conclude that the diminished Sombor index is

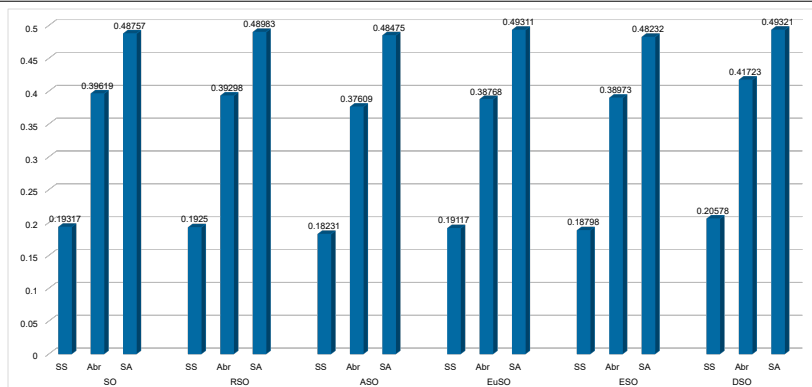


Figure 6. Structure sensitivity of the Sombor indices tested on a set of all decanes.

the one with the best structure sensitivity among tested Sombor indices. However, the high value of the abruptness calls for an attention. Probably, the most convenient way for comparing these indices in the case of index sensitivity is by ranking them using the novel *SA* measure. This measure shows that the diminished and the Euler Sombor indices are more sensitive on slight structural changes than other Sombor indices. Furthermore, by inspecting the abruptness of these two indices, the first pick would certainly be the Euler Sombor index.

6 Conclusion

The diminished Sombor index *DSO* is a mathematical invariant that was introduced in the same year as the original Sombor index *SO*. However, until now it has not been properly investigated. The aim of this paper was to fill this gap and to provide a comprehensive study of the diminished Sombor index. We have shown that the diminished Sombor index has a number of interesting mathematical properties. Additionally, it exhibits a good prediction ability and for some properties it supersedes other Sombor indices. We trust that the diminished Sombor index will find its place in the family of Sombor indices and that it will be used in future research in mathematical chemistry.

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