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Augmented Sombor Index

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Abstract

The Augmented Sombor index of a connected graph G with at least three vertices is defined as

$$ASO(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i^2 + d_j^2}{d_i + d_j - 2}},$$

where d_i and d_j denote the degrees of the vertices v_i and v_j, respectively. In this paper, we examine the chemical applicability of the ASO index for predicting thirteen physicochemical properties of octane isomers. We also characterize extremal graphs with respect to the ASO index over the following three classes of graphs with a given order: (i) trees, (ii) quasi-trees (where a quasi-tree is a connected graph that becomes a tree upon the removal of a single vertex), and (iii) connected graphs. Furthermore, we determine the unique graph minimizing the ASO index among all unicyclic graphs of fixed order. Finally, we conclude the paper by outlining potential directions for future research related to the ASO index.

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1 Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|E(G)| = m$. For any vertex $v_i \in V(G)$, its neighborhood is defined as $N_G(v_i) = \{v_k \in V(G) : v_i v_k \in E(G)\}$, and its degree as $d_i = |N_G(v_i)|$ (We use the notation $d_G(v_i)$ to denote the degree of vertex v_i in the graph G, particularly when multiple graphs are under consideration). Throughout this article, standard notations C_n, P_n, S_n, and K_n are used to represent the cycle, path, star, and complete graph of order n, respectively. A vertex of degree one is called a pendent vertex, and an edge incident to such a vertex is termed a pendent edge.

Chemical graph theory, a vital branch of mathematical chemistry, applies graph-theoretical concepts to model and study molecular structures. In this framework, atoms are represented by vertices and chemical bonds by edges, providing a robust mathematical foundation for analyzing molecular properties. Among several types of indices investigated within this field, degree-based topological indices play a prominent role, see for instance [3–5, 8, 10, 13].

These indices, which depend on vertex degrees, capture local atomic connectivity and have shown strong correlations with diverse physical, chemical, and biological properties. Due to their computational efficiency and predictive accuracy, such indices are instrumental in quantitative structure-property relationship (QSPR) studies, which support the design and analysis of new chemical compounds.

One of the notable and much-investigated degree-based indices is the Sombor index [11], defined for a graph G as:

$$SO(G) = \sum_{v_i v_j \in E(G)} \sqrt{d_i^2 + d_j^2}.$$

The Sombor index has attracted significant research interest; see the reviews [16, 25] and some of the recently published papers [6, 7, 15, 17, 19–21, 23, 27, 29].

Already in [11], in addition to the above defined Sombor index, some of its variants were examined (the reduced and the average Sombor index).

In the meantime, many more such variants were conceived, of which the elliptic [1,9,12,14], Euler [2,18,24,28], and the diminished Sombor indices [22] are worth especial attention.

Building upon this foundation, we propose a novel degree-based topological index, referred to as the augmented Sombor (ASO) index. The ASO index of a graph G containing no component isomorphic to P_2 is defined as

$$ASO(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i^2 + d_j^2}{d_i + d_j - 2}}.$$

Note that $d_i + d_j - 2$ is the degree of the edge $v_i v_j \in E(G)$.

In this paper, we examine the chemical applicability of the ASO index for predicting thirteen physicochemical properties of octane isomers. We also characterize extremal graphs with respect to the ASO index over the following three classes of graphs with a given order: (i) trees, (ii) quasi-trees (where a quasi-tree is a connected graph that becomes a tree upon the removal of a single vertex), and (iii) connected graphs. Furthermore, we prove that the cycle C_n uniquely minimizes the ASO index among all unicyclic graphs of order $n\,(> 3)$. Finally, we conclude the paper by outlining potential directions for future research related to the ASO index.

2 Chemical applicability

In order to evaluate the chemical relevance of the ASO index, we examined its statistical relationship with experimentally determined values for thirteen key physicochemical properties of octane isomers. The properties considered in this analysis are: boiling point, heat capacity at P constant, heat capacity at T constant, density, entropy, enthalpy of vaporization, enthalpy of formation, standard enthalpy of vaporization, standard enthalpy of formation, total surface area, acentric factor, molar volume, and octanol-water partition coefficient. The complete experimental dataset for these properties is obtained from the publicly accessible molecular descriptors database, archived at: `https://web.archive.org/web/20180912171255if_/http://www.moleculardescriptors.eu/index.htm`. For each of the aforementioned properties, the Pearson correlation coefficient (corr) is computed to quantify the degree of linear association with the ASO index.

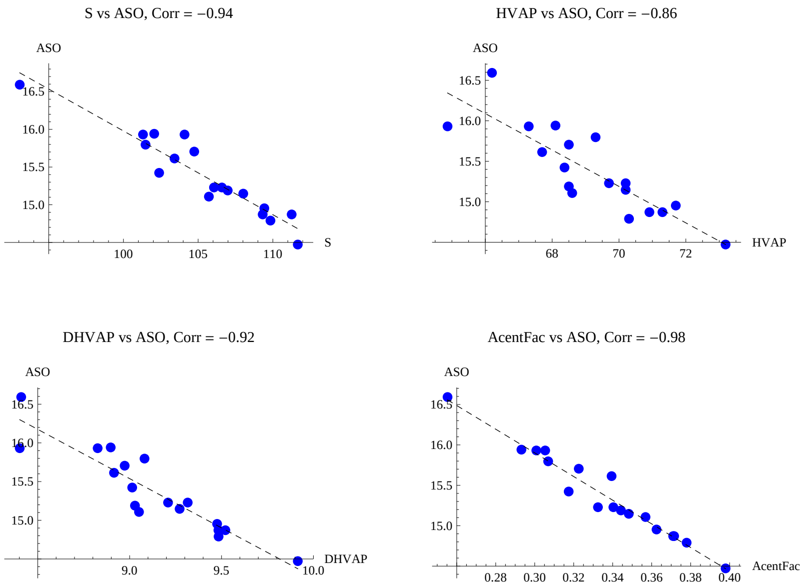

Figure 1. Correlation (Corr) between the ASO index and four properties (S, HVAP, DHVAP, AccentFac).

In order to focus on the most statistically significant relationships, only those correlations with an absolute coefficient value $|\text{corr}| > 0.8$ were retained for further discussion. As illustrated in Figure 1, four properties satisfied this criterion: entropy (S), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP), and acentric factor (AcenFac). These strong correlations suggest that the ASO index captures structural features of octane isomers that are closely linked to molecular thermodynamic behavior. It is worth noting that the above correlations are significantly better than those reported for the original Sombor index [26].

We additionally considered the reciprocal form of the ASO index, referred to as the reciprocal augmented Sombor ($RASO$) index, which is defined as

$$RASO(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i^2 + d_j^2}}.$$

Our analysis reveals that the absolute value of the Pearson correlation coefficient between the *ASO* and *RASO* indices is 0.9988 (see Figure 2). This exceptionally high correlation indicates that, for the case of octane isomers, both of these indices possess essentially identical predictive capabilities with respect to the considered set of physicochemical properties.

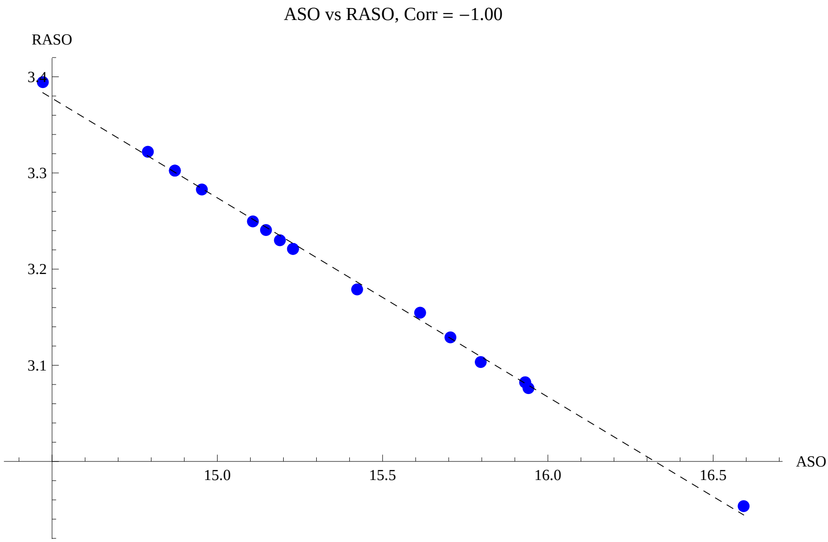

Figure 2. Correlation (Corr) between the *ASO* and *RASO* indices.

3 mathematical aspects of the *ASO* index

In order to obtain the main results, we first establish some preliminary properties of the function h defined as $h(d_i, d_j) = \frac{d_i^2+d_j^2}{d_i+d_j-2}$. We note that

$$h(d_i, d_j) = \frac{d_i^2 + d_j^2}{d_i + d_j - 2} = d_i - d_j + 2 + \frac{(d_j - 2)^2 + d_j^2}{d_i + d_j - 2}$$

$$= d_i - d_j + 2 + \frac{2\,(d_j-1)^2+2}{d_i+d_j-2}. \tag{1}$$

Using (1), we obtain the following two results.

Lemma 1. *Let G be a graph of order $n\,(> 4)$. For any pendent edge $v_iv_j \in E(G)\,(d_i > d_j = 1)$,*

$$5 \le h(d_i,d_j) \le n + \frac{2}{n-2}. \tag{2}$$

In (2), the left equality holds if and only if $(d_i,d_j) \in \big\{(2,1),\,(3,1)\big\}$, and the right equality holds if and only if $(d_i,d_j) = (n-1,1)$.

Proof. Let v_iv_j be any pendent edge in G such that $d_i > d_j = 1$. From (1), we obtain

$$h(d_i,d_j) = \frac{d_i^2+d_j^2}{d_i+d_j-2} = d_i + 1 + \frac{2}{d_i-1}. \tag{3}$$

Lower Bound: If $d_i \ge 4$, then

$$d_i + 1 + \frac{2}{d_i-1} > 5,$$

and hence, the left inequality in (2) strictly holds. Otherwise, $2 \le d_i \le 3$. Then, $(d_i,d_j) \in \big\{(2,1),\,(3,1)\big\}$ and hence the left equality holds in (2).

Upper Bound: If $d_i = n-1$, then the right equality holds in (2). Otherwise, $d_i \le n-2$. For $d_i \le n-3$, from (3), we obtain

$$h(d_i,d_j) = \frac{d_i^2+d_j^2}{d_i+d_j-2} \le n - 2 + \frac{2}{d_i-1} < n + \frac{2}{n-2}$$

as $d_i \ge 2$. Also, for $d_i = n-2$, from (3), we obtain

$$h(d_i,d_j) = \frac{d_i^2+d_j^2}{d_i+d_j-2} = n - 1 + \frac{2}{n-3} < n + \frac{2}{n-2}$$

as $n \ge 5$. Hence, the right inequality in (2) strictly holds when $d_i \le n-2$. This completes the proof of the lemma. ■

Lemma 2. *Let G be a graph of order $n\,(>3)$. For any non-pendent edge $v_iv_j \in E(G)$,*

$$4 \leq h(d_i, d_j) \leq n + \frac{1}{n-2}. \tag{4}$$

In (4), the left equality holds if and only if $d_i = 2 = d_j$, and the right equality holds if and only if $d_i = d_j = n-1$.

Proof. Let v_iv_j be any non-pendent edge in G such that $d_i \geq d_j \geq 2$.

Lower Bound: We have $(d_i-2)^2 + (d_j-2)^2 \geq 0$, which gives,

$$d_i^2 + d_j^2 \geq 4\,d_i + 4\,d_j - 8 = 4\,(d_i + d_j - 2),$$

that is,

$$h(d_i, d_j) = \frac{d_i^2 + d_j^2}{d_i + d_j - 2} \geq 4.$$

In the above inequalities, the equality holds if and only if $d_i = 2 = d_j$.

Upper Bound: Since $d_i \geq d_j$, we have $d_i + d_j - 2 \geq 2\,(d_j - 1)$. Using this, from (1), we obtain

$$\begin{aligned} h(d_i, d_j) = \frac{d_i^2 + d_j^2}{d_i + d_j - 2} &= d_i - d_j + 2 + \frac{2\,(d_j-1)^2}{d_i + d_j - 2} + \frac{2}{d_i + d_j - 2} \\ &\leq d_i + 1 + \frac{2}{d_i + d_j - 2}. \end{aligned}$$

If $d_i \leq n-2$, then from the above, we obtain

$$h(d_i, d_j) = \frac{d_i^2 + d_j^2}{d_i + d_j - 2} \leq n - 1 + \frac{2}{d_i + d_j - 2} \leq n < n + \frac{1}{n-2}$$

as $d_i \geq d_j \geq 2$, and hence, the right inequality in (4) strictly holds. Otherwise, $d_i = n-1$, and hence, from (1), we obtain

$$\begin{aligned} \frac{d_i^2 + d_j^2}{d_i + d_j - 2} &= n - d_j + 1 + \frac{2\,(d_j-1)^2 + 2}{n + d_j - 3} \\ &= h(n-1,\, d_j). \end{aligned} \tag{5}$$

We have $2 \leq d_j \leq n-1$. Let us consider a function

$$f(x) = n - x + 1 + \frac{2\,(x-1)^2 + 2}{n + x - 3}, \quad 2 \leq x \leq n-1.$$

Then, we obtain

$$\begin{aligned}
f'(x) &= -1 + \frac{4\,(x-1)\,(n+x-3) - 2\,(x^2 - 2x + 2)}{(n+x-3)^2} \\
&= \frac{4\,(x-1)\,(n+x-3) - (n+x-3)^2 - 2\,(x^2 - 2x + 2)}{(n+x-3)^2} \\
&= \frac{x^2 + 2nx - n^2 - 6x + 2n - 1}{(n+x-3)^2} \\
&= \frac{(x+n-3)^2 - 2\left(n^2 - 4n + 5\right)}{(n+x-3)^2} \\
&= \frac{\left(x + n - 3 + \sqrt{2\,(n^2 - 4n + 5)}\right)\left(x + n - 3 - \sqrt{2\,(n^2 - 4n + 5)}\right)}{(n+x-3)^2}.
\end{aligned}$$

From the above, we conclude that $f(x)$ is an increasing function on $\sqrt{2\,(n^2 - 4n + 5)} - (n-3) \leq x \leq n-1$ and a decreasing function on $2 \leq x \leq \sqrt{2\,(n^2 - 4n + 5)} - (n-3)$. Hence

$$f(x) \leq \max\left\{f(2),\, f(n-1)\right\}.$$

One can easily see that

$$f(2) = n - 1 + \frac{4}{n-1} < n + \frac{1}{n-2} = f(n-1)$$

as $n \geq 4$. From the above with (5), we conclude that

$$h(n-1,\, d_j) = f(d_j) \leq f(n-1) = n + \frac{1}{n-2}.$$

Moreover, the equation $f(d_j) = f(n-1)$ holds if and only if $d_j = n-1$.

Hence,

$$h(d_i,\, d_j) = \frac{d_i^2 + d_j^2}{d_i + d_j - 2} \le n + \frac{1}{n-2}$$

with equality if and only if $d_i = n-1 = d_j$. ∎

Lemma 3. *Let a be a real number and $n\,(>1)$ be an integer. Consider a function*

$$f(x) = \frac{(n-a)^2 + x^2}{n + x - a - 2}, \quad 1 \le x \le n-1.$$

Then $f(x)$ is an increasing function on $x \ge \sqrt{(n-a-2)^2 + (n-a)^2} - (n-a-2)$, and a decreasing function on $x \le \sqrt{(n-a-2)^2 + (n-a)^2} - (n-a-2)$.

Proof. The result follows from the following equation:

$$f'(x) = \frac{2x(n-a-2) + x^2 - (n-a)^2}{(n+x-a-2)^2}.$$ ∎

Proposition 1. *Let G be a graph of order $n\,(>8)$ with any edge v_iv_j. Then $h(d_i,d_j) < h(n-2,n-2) < h(n-1,n-3) = h(n-2,1) < h(n-1,2) < h(n-1,n-2) < h(n-1,n-1) < h(n-1,1)$ for $(d_i,d_j) \notin \Big\{(n-1,1),\,(n-1,2),\,(n-2,1),\,(n-2,n-2),\,(n-1,n-3),\,(n-1,n-2),\,(n-1,n-1)\Big\}$.*

Proof. Let v_iv_j be an edge in G such that $d_i \ge d_j$. Also, let

$$S = \Big\{(n-1,1),\,(n-1,2),\,(n-2,1),\,(n-2,n-2),\,(n-1,n-3),\\ (n-1,n-2),\,(n-1,n-1)\Big\}.$$

We note that

$$h(n-1,1) = n + \frac{2}{n-2},\; h(n-2,1) = n - 1 + \frac{2}{n-3},\; h(n-3,1) =$$

$$n - 2 + \frac{2}{n-4},\; h(n-1,2) = n - 1 + \frac{4}{n-1}, h(n-2,2) = n - 2 + \frac{4}{n-2},$$

$$h(n-1,n-3) = n - 1 + \frac{2}{n-3},\; h(n-1,n-2) = n - \frac{1}{2} + \frac{5}{2(2n-5)},$$

$$h(n-2,n-4)=n-2+\frac{2}{n-4},\ h(n-2,n-3)=n-1.5+\frac{1.25}{n-3.5},$$

$$h(n-2,n-2)=n-1+\frac{1}{n-3},\ h(n-1,n-1)=n+\frac{1}{n-2}.$$

Since $n\geq 9$, from the above discussion, we have

$$\begin{aligned}&h(n-2,n-2)<h(n-1,n-3)=h(n-2,1)<h(n-1,2)<h(n-1,\\&\quad n-2)<h(n-1,n-1)<h(n-1,1).\end{aligned} \tag{6}$$

By Lemmas 1 and 2, we obtain $h(d_i,d_j)\leq h(n-1,1)$ with equality if and only if $(d_i,d_j)=(n-1,1)$. We now prove the following claim:

Claim 1. For $(d_i,d_j)\notin S$, $h(d_i,d_j)<h(n-2,n-2)$.

Proof of Claim 1. Let $(d_i,d_j)\notin S$. We consider the following cases:

Case 1. $d_j=1$. Since $(d_i,d_j)\notin S$, we have $d_i\leq n-3$. If $d_i=2$, then

$$h(d_i,1)=\frac{d_i^2+1}{d_i-1}=5<n-1+\frac{1}{n-3}=h(n-2,n-2)$$

as $n\geq 9$, and hence, the result holds. Otherwise, $d_i\geq 3$. Again since $n\geq 9$, we obtain

$$\begin{aligned}h(d_i,1)=\frac{d_i^2+1}{d_i-1}=d_i+1+\frac{2}{d_i-1}\leq n-2+\frac{2}{d_i-1}<n-1+\frac{1}{n-3}\\=h(n-2,n-2),\end{aligned}$$

as desired.

Case 2. $d_j=2$. Since $(d_i,d_j)\notin S$, we have $d_i\leq n-2$. For $2\leq d_i\leq 3$, we have

$$h(d_i,2)=\frac{d_i^2+4}{d_i}\leq 4+\frac{1}{3}<n-1+\frac{1}{n-3}=h(n-2,n-2)$$

as $n\geq 9$, and hence, the result holds. Otherwise, $4\leq d_i\leq n-2$. Since

$n \geq 9$, we obtain

$$h(d_i, 2) = d_i + \frac{4}{d_i} \leq n - 2 + \frac{4}{d_i} < n - 1 + \frac{1}{n-3} = h(n-2, n-2),$$

as desired.

Case 3. $d_j \geq 3$. We note that

$$h(d_i, d_j) = d_i + 2 - \frac{d_j\,(d_i - d_j + 2) - 4}{d_i + d_j - 2} \tag{7}$$

$$= d_i - \frac{d_j\,(d_i - d_j) - 2d_i}{d_i + d_j - 2}. \tag{8}$$

If $d_i \leq n - 3$, then from (7), we obtain

$$h(d_i, d_j) < d_i + 2 \leq n - 1 < n - 1 + \frac{1}{n-3} = h(n-2, n-2),$$

as desired. Otherwise, $d_i \geq n - 2$. We consider the following two cases:

Case 3.1. $d_i = n - 2$. In this case, $3 \leq d_j \leq n - 2$. Since $(d_i, d_j) \notin S$, we have $3 \leq d_j \leq n - 3$. Since $n \geq 9$, by Lemma 3 (setting $a = 2$), we obtain

$$h(d_i, d_j) \leq \max\Big\{h(n-2, 3),\ h(n-2,\ n-3)\Big\}$$

$$< n - 1 + \frac{1}{n-3} = h(n-2, n-2)$$

as

$$h(n-2, 3) = n - 3 + \frac{10}{n-1} < n - 1 + \frac{1}{n-3} = h(n-2, n-2),$$

$$h(n-2, n-3) = n - 1.5 + \frac{1.25}{n-3.5} < n - 1 + \frac{1}{n-3} = h(n-2, n-2).$$

Hence, in this case, the result holds.

Case 3.2. $d_i = n - 1$. In this case, $3 \leq d_j \leq n - 1$. Since $(d_i, d_j) \notin S$, we have $3 \le d_j \le n-4$. Since $n \ge 9$, by Lemma 3 (setting $a=1$), we obtain

$$h(d_i, d_j) \le \max\Big\{h(n-1,3),\, h(n-1,\, n-4)\Big\}$$
$$< n-1+\frac{1}{n-3} = h(n-2, n-2)$$

as

$$h(n-1,3) = n-2+\frac{10}{n} < n-1+\frac{1}{n-3} = h(n-2,n-2),$$
$$h(n-1,n-4) = n-1.5+\frac{3.25}{n-3.5} < n-1+\frac{1}{n-3} = h(n-2,n-2).$$

Hence, in this case, the result holds.

This completes the proof **Claim 1**.

Using (6) and **Claim 1**, we complete the proof of Proposition 1. ■

We now establish lower and upper bounds on the ASO index for trees in terms of n, and characterize the trees that attain these extremal values.

Theorem 2. *Let T be a tree of order $n\,(>3)$. Then*

$$2\sqrt{5}+2\,(n-3) \le ASO(T) \le (n-1)\sqrt{n+\frac{2}{n-2}} \tag{9}$$

with equality on the left if and only if $T \cong P_n$, and equality on the right if and only if $T \cong S_n$.

Proof. For $n=4$, there are only two non-isomorphic trees; namely, P_4 and S_4. Here, by direct comparison, we have $ASO(S_4) > ASO(P_4)$. Hence, in the rest of the proof, we assume that $n \ge 5$. Let p be the number of pendent vertices in T. Then $2 \le p \le n-1$.

Lower Bound: If $p=2$, then $T \cong P_n$ with $ASO(T) = 2\sqrt{5}+2\,(n-3)$, and hence the left equality in (9) holds. Otherwise, $3 \le p \le n-1$. Since

$n \geq 5$, by Lemmas 1 and 2, we obtain

$$
\begin{aligned}
ASO(T) &= \sum_{v_i v_j \in E(T)} \sqrt{\frac{d_i^2 + d_j^2}{d_i + d_j - 2}} \\
&= \sum_{\substack{v_i v_j \in E(T), \\ d_i \geq d_j = 1}} \sqrt{h(d_i, d_j)} + \sum_{\substack{v_i v_j \in E(T), \\ d_i \geq d_j \geq 2}} \sqrt{h(d_i, d_j)} \\
&\geq p\,\sqrt{5} + 2\,(n-p-1) = p\,(\sqrt{5}-2) + 2\,(n-1) \\
&\geq 3\,(\sqrt{5}-2) + 2\,(n-1) = 2\,\sqrt{5} + \sqrt{5} - 2 + 2\,(n-3) \\
&> 2\,\sqrt{5} + 2\,(n-3),
\end{aligned}
$$

which implies that the left inequality in (9) strictly holds.

Upper Bound: If $p = n-1$, then $T \cong S_n$ with

$$ASO(T) = (n-1)\,\sqrt{n + \frac{2}{n-2}}$$

and hence the right equality in (9) holds. Otherwise, $2 \leq p \leq n-2$. Since $n \geq 5$, using the definition of the ASO index as well as Lemmas 1 and 2, we obtain

$$
\begin{aligned}
ASO(T) &= \sum_{\substack{v_i v_j \in E(T), \\ d_i \geq d_j = 1}} \sqrt{h(d_i, d_j)} + \sum_{\substack{v_i v_j \in E(T), \\ d_i \geq d_j \geq 2}} \sqrt{h(d_i, d_j)} \\
&\leq p\,\sqrt{n + \frac{2}{n-2}} + (n-p-1)\,\sqrt{n + \frac{1}{n-2}} \\
&< p\,\sqrt{n + \frac{2}{n-2}} + (n-p-1)\,\sqrt{n + \frac{2}{n-2}} \\
&= (n-1)\,\sqrt{n + \frac{2}{n-2}}
\end{aligned}
$$

as $n - p - 1 \geq 1$. Hence, the right inequality in (9) strictly holds when $2 \leq p \leq n-2$. ∎

Theorem 3. *Let G be a unicyclic graph of order n. Then $ASO(G) \geq 2n$ with equality if and only if $G \cong C_n$.*

Proof. If $G \cong C_n$, then $ASO(G) = 2n$ and hence the equality holds. Otherwise, $G \ncong C_n$. If $n = 4$, then G is the graph obtained from S_4 by inserting an edge between two pendent vertices of S_4, and hence by direct comparison, we have $ASO(G) > ASO(C_4)$. Next, we assume that $n \geq 5$. We note that there exists at least one pendent vertex in G. Let $p\,(\geq 1)$ be the number of pendent vertices in G. Since G is unicyclic, $m = n$, where m is the number of edges. Since $n \geq 5$, by Lemmas 1 and 2, we obtain

$$\begin{aligned} ASO(G) &= \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j = 1}} \sqrt{h(d_i, d_j)} + \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j \geq 2}} \sqrt{h(d_i, d_j)} \\ &\geq p\sqrt{5} + 2\,(m-p) \\ &= p\sqrt{5} + 2\,(n-p) = 2n + p\,(\sqrt{5} - 2) > 2n, \end{aligned}$$

as $p \geq 1$. The inequality strictly holds. This completes the proof of the theorem. ■

Recall that a graph G is called a quasi-tree if there exists a vertex $u \in V(G)$ such that the graph obtained by removing u and all edges incident to it is a tree. A quasi-tree is said to be a trivial quasi-tree if it is a tree. Hence, every non-trivial quasi-tree contains at least one cycle. Let $K_{2,n-2}$ denote the complete bipartite graph of order $n\,(> 2)$, with one partite set containing 2 vertices and the other containing $n-2$ vertices. Define $K'_{2,n-2}$ as the graph obtained from $K_{2,n-2}$ by adding an edge between the two vertices of degree $n-2$. We now establish both lower and upper bounds on the ASO index of quasi-trees in terms of n, and characterize the graphs that attain these extremal values.

By Theorem 5 (given after the next theorem), the path graph P_n uniquely minimizes the ASO index among all quasi-trees (including trivial ones) of order $n\,(> 3)$. Also, for $n \geq 4$, we have $ASO(S_n) < ASO(K'_{2,n-2})$, which together with Theorem 2 implies that $ASO(T) < ASO(K'_{2,n-2})$ for any tree of order $n\,(> 3)$. Thus, in the following theorem, we consider only non-trivial quasi-trees.

Theorem 4. *Let G be a non-trivial quasi-tree of order $n\,(>4)$. Then,*

$$2\,n \le ASO(G) \le \sqrt{n+\frac{1}{n-2}} + 2\,(n-2)\,\sqrt{n-1+\frac{4}{n-1}} \tag{10}$$

with equality on the left if and only if $G \cong C_n$, and equality on the right if and only if $G \cong K'_{2,n-2}$.

Proof. Let m and p be the number of edges and the number of pendent vertices in G, respectively. Since G is a non-trivial quasi-tree, we have $n \le m \le 2n-3$.

Lower Bound: If $m = n$, then the desired result holds by Theorem 3. Otherwise, $m \ge n+1$. Since $n \ge 5$, by Lemmas 1 and 2, we obtain

$$ASO(G) = \sum_{v_iv_j \in E(G)} \sqrt{h(d_i, d_j)} \ge 2m \ge 2(n+1) > 2n,$$

as desired.

Upper Bound: For every $n \in \{5, 6, 7, 8\}$, using a computer software, we have verified that $K'_{2,n-2}$ has the maximum ASO index among all quasi-trees of order n. Hence, in what follows, we assume that $n \ge 9$. Let v_iv_j be any edge in G such that $d_i \ge d_j$. We consider the following cases:

Case 1. $d_i = n-1$. In this case, vertex v_i is adjacent to all the remaining vertices. If $d_j = n-1$, then $G \cong K'_{2,n-2}$ with

$$ASO(G) = \sqrt{n+\frac{1}{n-2}} + 2\,(n-2)\,\sqrt{n-1+\frac{4}{n-1}},$$

and hence, the right equality in (10) holds. Otherwise, $d_j \le n-2$. Let v_k be a vertex in G such that $G - v_k$ is a tree. First, we assume that $k = i$. Then, $G - v_i$ is a tree, and hence, $m = 2n-3$. Let $H = G - v_i$. Since H is a tree, $d_H(v_\ell) \ge 1$ for $v_\ell \in V(H)$ and hence $d_G(v_\ell) \ge 2$ for $v_\ell \in V(G)$.

Since G is a quasi-tree, using Proposition 1, we obtain

$$\begin{aligned} ASO(G) = \sum_{v_iv_j\in E(G)} \sqrt{h(d_i,d_j)} &= \sum_{\substack{v_iv_j\in E(G),\\ d_i\geq d_j\geq 2}} \sqrt{h(d_i,d_j)} \\ &\leq \sqrt{h(n-1,n-2)} + (2n-4)\sqrt{h(n-1,2)} \\ &< \sqrt{h(n-1,n-1)} + (2n-4)\sqrt{n-1+\frac{4}{n-1}} \\ &= \sqrt{n+\frac{1}{n-2}} + (2n-4)\sqrt{n-1+\frac{4}{n-1}} \end{aligned}$$

as $n \geq 5$. Thus, the right inequality in (10) strictly holds when $k = i$.

Next, we assume that $k \neq i$. In this case, $G - v_k \cong S_{n-1}$, where $d_G(v_k) \leq n-2$. Thus, we have $m \leq 2n-4$. Since G is a quasi-tree, using Proposition 1, we obtain

$$\sum_{\substack{v_iv_j\in E(G),\\ d_i\geq d_j=1}} \sqrt{h(d_i,d_j)} \leq p\sqrt{h(n-1,1)} = p\sqrt{n+\frac{2}{n-2}}$$

and

$$\begin{aligned} \sum_{\substack{v_iv_j\in E(G),\\ d_i\geq d_j\geq 2}} \sqrt{h(d_i,d_j)} &\leq \sqrt{h(n-1,n-2)} + (m-p-1)\sqrt{h(n-1,2)} \\ &< \sqrt{h(n-1,n-1)} + (2n-p-5)\sqrt{h(n-1,2)} \\ &= \sqrt{n+\frac{1}{n-2}} + (2n-p-5)\sqrt{n-1+\frac{4}{n-1}}. \end{aligned}$$

Using the above inequalities, we obtain

$$ASO(G) = \sum_{\substack{v_iv_j\in E(G),\\ d_i\geq d_j=1}} \sqrt{h(d_i,d_j)} + \sum_{\substack{v_iv_j\in E(G),\\ d_i\geq d_j\geq 2}} \sqrt{h(d_i,d_j)}$$

$$< p\sqrt{n+\frac{2}{n-2}}+\sqrt{n+\frac{1}{n-2}}+(2n-p-5)\sqrt{n-1+\frac{4}{n-1}}. \tag{11}$$

Claim 2.
$$p\sqrt{n+\frac{2}{n-2}}<(p+1)\sqrt{n-1+\frac{4}{n-1}}.$$

Proof of Claim 2. Since p is the number of pendent vertices in G, we have
$$\frac{p}{2}<n-1+\frac{4}{n-1},$$
that is,
$$\frac{p}{2\sqrt{n-1+\frac{4}{n-1}}}<\sqrt{n-1+\frac{4}{n-1}}.$$
Since $n \geq 5$, using the above inequality, we obtain
$$\begin{aligned}
&\sqrt{n+\frac{2}{n-2}}-\sqrt{n-1+\frac{4}{n-1}}\\
=&\frac{1-\frac{4}{n-1}+\frac{2}{n-2}}{\sqrt{n+\frac{2}{n-2}}+\sqrt{n-1+\frac{4}{n-1}}}\\
<&\frac{1}{\sqrt{n+\frac{2}{n-2}}+\sqrt{n-1+\frac{4}{n-1}}}\\
<&\frac{1}{2\sqrt{n-1+\frac{4}{n-1}}}\\
<&\frac{1}{p}\sqrt{n-1+\frac{4}{n-1}},
\end{aligned}$$
that is,
$$p\sqrt{n+\frac{2}{n-2}}<(p+1)\sqrt{n-1+\frac{4}{n-1}}.$$

which proves **Claim 2**.

Using **Claim 2** in (11), we obtain

$$ASO(G) < (p+1)\sqrt{n-1+\frac{4}{n-1}} + \sqrt{n+\frac{1}{n-2}}$$
$$+ (2n-p-5)\sqrt{n-1+\frac{4}{n-1}}$$
$$= \sqrt{n+\frac{1}{n-2}} + 2\,(n-2)\sqrt{n-1+\frac{4}{n-1}},$$

which shows that the right inequality in (10) strictly holds in the case under consideration.

Case 2. $d_i = n-2$. We have $1 \le d_j \le d_i = n-2$. By Lemma 3, we obtain

$$h(d_i, d_j) = \frac{(n-2)^2 + d_j^2}{n+d_j-4} \le \max\Big\{h(n-2,1),\, h(n-2,n-2)\Big\}$$
$$= n-1+\frac{2}{n-3}.$$

Since $n \ge 5$, we have $n-1+\frac{2}{n-3} \le n-1+\frac{4}{n-1} < n+\frac{2}{n-2}$. Since $m \le 2n-3$, using the above results, we obtain

$$ASO(G) = \sum_{v_iv_j \in E(G)} \sqrt{h(d_i,d_j)} \le m\sqrt{n-1+\frac{2}{n-3}}$$
$$\le (2n-3)\sqrt{n-1+\frac{2}{n-3}}$$
$$< \sqrt{n+\frac{2}{n-2}} + 2\,(n-2)\sqrt{n-1+\frac{4}{n-1}},$$

as desired.

Case 3. $d_i \le n-3$. In this case we have to prove that

$$h(d_i, d_j) \le n-1+\frac{4}{n-1}. \tag{12}$$

First we assume that $d_j \geq 2$. Then from (7), we obtain

$$h(d_i, d_j) \leq n - 1 < n - 1 + \frac{4}{n-1}$$

as $d_i \geq d_j$ and $d_j\,(d_i - d_j + 2) \geq 2d_j \geq 4$. The result (12) holds.

Next we assume that $d_j = 1$. Then from (7), we obtain

$$h(d_i, d_j) = d_i + 2 - \frac{d_i - 3}{d_i - 1} = d_i + 1 + \frac{2}{d_i - 1}.$$

If $d_i = 2$, then from the above, we obtain

$$h(d_i, d_j) = 5 \leq n - 1 + \frac{4}{n-1}$$

as $n \geq 5$. The result (12) holds. Otherwise, $d_i \geq 3$. Thus we have

$$\begin{aligned} h(d_i, d_j) &= d_i + 2 - \frac{d_i - 3}{d_i - 1} = d_i + 1 + \frac{2}{d_i - 1} \\ &\leq n - 2 + \frac{2}{d_i - 1} < n - 1 + \frac{4}{n-1}. \end{aligned}$$

The result (12) holds.

Since $n \geq 5$, using (12), we obtain

$$\begin{aligned} ASO(G) &= \sum_{v_i v_j \in E(G)} \sqrt{h(d_i, d_j)} \leq m\,\sqrt{n - 1 + \frac{4}{n-1}} \\ &\leq (2n-3)\,\sqrt{n - 1 + \frac{4}{n-1}} \\ &< \sqrt{n + \frac{1}{n-2}} + 2\,(n-2)\,\sqrt{n - 1 + \frac{4}{n-1}}, \end{aligned}$$

as desired. This completes the proof of the theorem. ■

We now establish a lower bound for the ASO index of connected graphs of order n, and characterize the graphs that attain this bound.

Theorem 5. *Let G be a connected graph of order $n\,(>2)$. Then*

$$ASO(G) \geq 2\sqrt{5} + 2\,(n-3)$$

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

Proof. For every $n \in \{3,4\}$, we have verified, using a computer software, that P_n has the minimum ASO index among all connected graphs of order n. Now, we assume that $n \geq 5$. Let m be the number of edges in G. Since G is connected, $m \geq n-1$. If $m = n-1$, then Theorem 2 yields the desired result. If $m \geq n$, then by Lemmas 1 and 2, we obtain

$$\begin{aligned} ASO(G) &= \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j = 1}} \sqrt{h(d_i,d_j)} + \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j \geq 2}} \sqrt{h(d_i,d_j)} \\ &\geq p\sqrt{5} + 2\,(m-p) \\ &= p\,(\sqrt{5}-2) + 2\,m \\ &\geq 2n > 2\sqrt{5} + 2\,(n-3), \end{aligned}$$

where p is the number of pendent vertices. ■

We now present an upper bound for the ASO index of connected graphs of order n, and characterize the graphs that attain this bound.

Theorem 6. *Let G be a graph of order $n\,(>2)$. Then*

$$ASO(G) \leq \binom{n}{2}\sqrt{n + \frac{1}{n-2}} \tag{13}$$

with equality if and only if $G \cong K_n$.

Proof. For each $n \in \{3,4\}$, we have verified the result using a computer software. Hence, in the rest of the proof, we assume that $n \geq 5$. Let m and p be the number of edges and the number of pendent vertices in G, respectively. Then $0 \leq p \leq n-1$. First, we assume that $p = 0$. By Lemma

2, we obtain

$$ASO(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i^2 + d_j^2}{d_i + d_j - 2}} = \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j \geq 2}} \sqrt{h(d_i, d_j)}$$

$$\leq m\sqrt{n + \frac{1}{n-2}}$$

$$\leq \binom{n}{2}\sqrt{n + \frac{1}{n-2}}.$$

Moreover, the above two equalities hold if and only if $m = \binom{n}{2}$ and $h(d_i, d_j) = h(n-1, n-1)$, that is, if and only if $G \cong K_n$.

Next, we assume that $1 \leq p \leq n-1$. Then $m \leq \binom{n}{2} - 1$. First, we prove the following claim.

Claim 3.

$$p\sqrt{n + \frac{2}{n-2}} < (p+1)\sqrt{n + \frac{1}{n-2}}.$$

Proof of Claim 3. We have to prove that

$$p\sqrt{\frac{n^2 - 2n + 2}{n-2}} < (p+1)\sqrt{\frac{n^2 - 2n + 1}{n-2}},$$

that is,

$$\sqrt{1 + \frac{1}{(n-1)^2}} < 1 + \frac{1}{p},$$

that is,

$$1 + \frac{1}{(n-1)^2} < 1 + \frac{2}{p} + \frac{1}{p^2},$$

which is true always as $p \leq n-1$. This proves **Claim 3**.

Using Lemmas 1 and 2 as well as **Claim 3**, we obtain

$$ASO(G) = \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j = 1}} \sqrt{h(d_i, d_j)} + \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j \geq 2}} \sqrt{h(d_i, d_j)}$$

$$\leq p\sqrt{n+\frac{2}{n-2}}+(m-p)\sqrt{n+\frac{1}{n-2}}$$

$$< (p+1)\sqrt{n+\frac{1}{n-2}}+\left(\binom{n}{2}-1-p\right)\sqrt{n+\frac{1}{n-2}}$$

$$= \binom{n}{2}\sqrt{n+\frac{1}{n-2}}$$

as $m \leq \binom{n}{2} - 1$. Hence, in the case where $1 \leq p \leq n-1$, the strict inequality in (13) holds. This completes the proof of the theorem. ■

4 Concluding remarks

In this paper, we introduced a new topological index, the augmented Sombor index (ASO), and examined its chemical applicability by evaluating its performance in predicting thirteen physicochemical properties of octane isomers. In addition, we investigated several mathematical properties of the ASO index. Specifically, we established lower and upper bounds for the ASO index within the classes of trees, quasi-trees, and connected graphs, and characterized the corresponding extremal graphs in each case. Furthermore, we derived a lower bound for the ASO index of unicyclic graphs of order n, along with a characterization of the extremal graph that attains this bound.

There remain many other well-known classes of graphs for which the extremal behavior of the ASO index has yet to be explored. We hope that future research will continue this line of investigation and uncover further insights into mathematical and chemical aspects of this index.

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