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On the Augmented Sombor Index of Polycyclic Molecular Graphs

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Abstract: Let G be a graph with edge set $E(G)$. Recently, Das, Gutman and Ali introduced a new vertex-degree-based topological index, called the augmented Sombor index of G, defined as

$$ASO(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)^2 + d(v)^2}{d(u) + d(v) - 2}},$$

where $d(u)$ denotes the degree of vertex u. This paper establishes a linear model for predicting the physicochemical properties of benzenoid hydrocarbons using the augmented Sombor index. Moreover, we characterize all molecular graphs of order n and cyclomatic number ℓ that minimize the augmented Sombor index, under the condition that $n \geq 2(\ell - 1) \geq 4$.

Key Words: Augmented Sombor index, Smarandachely Sombor index, molecular graph, extremal value, cyclomatic number.

AMS(2010): 05C09, 05C07, 05C35, 05C92.

§1. Introduction

A molecular graph is defined in mathematical chemistry as a connected graph whose maximum vertex degree does not exceed four. It serves as an effective abstraction of the skeletal structure of compounds, with carbon atoms represented as vertices and covalent bonds as edges. This graphical framework allows the use of graph-theoretic invariants - termed topological indices - to quantify molecular architecture. Among these, the Sombor index family, which includes the original Sombor index [6], elliptic Sombor index [10], Euler Sombor index [20], diminished Sombor index [15], and augmented Sombor index [5], has attracted considerable research interest in recent years owing to its geometric motivation and strong predictive capability for physicochemical properties of molecular compounds. In Quantitative Structure Property Relationship (QSPR) and Quantitative Structure Activity Relationship (QSAR) studies, such indices are computed over specific molecular graph, for instance, benzenoid hydrocarbons and are correlated with target physicochemical descriptors (e.g., boiling point, π-electron energy,

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molecular weight), see for example [3, 13, 19]. This in silico methodology not only offers mechanistic insight into structure-property relationships but also constitutes a cost-efficient and rapid screening strategy before undertaking laborious experimental work.

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The order of G is denoted by n. For a vertex $u \in V(G)$, the set of its neighbors in G is denoted as $N(u) = \{v \in V(G) : uv \in E(G)\}$. The degree of u is the number of its neighbors, that is, $d_G(u) = d(u) = |N(u)|$. A vertex of degree one (at least three, respectively) is called a pendant vertex (branching vertex, respectively). An edge incident with a pendent vertex is called a pendent edge. The minimum and maximum degrees of a graph G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. The cyclomatic number of a graph is the smallest number of edges whose removal makes the graph acyclic.

In 2021, Gutman [8] introduced the Sombor index from a geometric perspective, and defined it as

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

This index has attracted considerable interest in both mathematics and theoretical chemistry, see, e.g., [6, 12, 14, 17, 18]. On this basis, scholars have proposed various versions related to the Sombor index, such as the first (to Sixth) Sombor-like index [9], the elliptic Sombor index [10], the Euler Sombor index [20], the hyperbolic Sombor index [2] and the diminished Sombor index [15].

Building upon the Sombor index, Das, Gutman, and Ali [5] further extended this metric by incorporating the degrees of line graph vertices, thereby proposing the augmented Sombor (ASO) index, which is defined as follows:

$$ASO(G) = \sum_{uv \in E(G)} \sqrt{\frac{d^2(u) + d^2(v)}{d(u) + d(v) - 2}},$$

and meanwhile, they established lower and upper bounds for the augmented Sombor index within the classes of trees, quasi-trees, and connected graphs, and characterized the corresponding extremal graphs in each case. Notice that the Sombor index $SO(G)$ and augmented Sombor index $ASO(G)$ are global properties on G. Generally, for an induced subgraph $H \prec G$ such as $K_3, K_3 + e, K_{1,3}, K_4 - e, \cdots$, a Smarandachely Sombor index $SSO_H(G)$ is defined by

$$SSO_H(G) = \sum_{uv \in E(G \setminus H)} \sqrt{\frac{d^2(u) + d^2(v)}{d(u) + d(v) - 2}}.$$

Clearly, if $H = \emptyset$ or there are no subgraphs $G' \simeq H$ in G, a Smarandachely Sombor index $SSO_H(G)$ of G is nothing else but the augmented Sombor index $ASO(G)$ of G. However, it characterizes the Sombor index on graph $G \setminus H$.

Alotaibi, Alanazi, Hassan, and Ali [1] determine all graphs that minimize the diminished Sombor index among molecular graphs of order n and with a cyclomatic number of at least three. Inspired by this, we investigate the chemical application of the augmented Sombor index to establish a linear model for predicting the physicochemical properties of benzenoid hydrocarbons (polycyclic molecular graphs). Furthermore, we characterize all molecular graphs of order n and cyclomatic number ℓ that minimize the ASO index, under the condition $n \geq 2(\ell - 1) \geq 4$.

§2. Applications of ASO Index to the Physicochemical Properties of Benzenoid Hydrocarbons

In this section, the chemical applicability of the ASO index is examined in the context of modeling several properties of benzenoid hydrocarbons. Linear regression models are developed for predicting boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR).

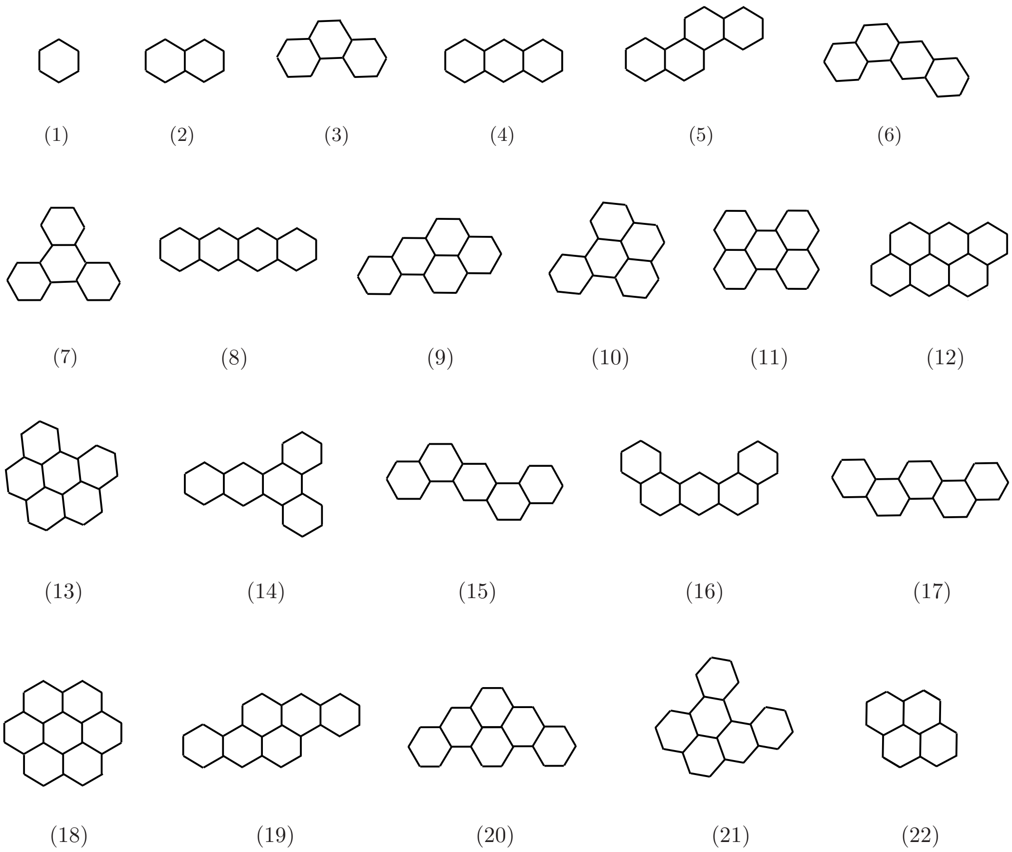

Figure 1. Molecular graphs

((1) Benzene, (2) Naphthalene, (3) Phenanthrene, (4) Anthracene, (5) Chrysene, (6) Benzo[a]anthracene, (7) Triphenylene, (8) Tetracene, (9) Benzo[a]pyrene, (10) Benzo[e]pyrene, (11) Perylene, (12) Anthanthrene, (13) Benzo[ghi]perylene, (14) Dibenz[a,c]anthracene, (15) Dibenz[a,h]anthracene, (16) Dibenz[a,j]anthracene, (17) Picene, (18) Coronene, (19) Dibenzo[a,h]pyrene, (20) Dibenzo[a,i]pyrene, (21) Dibenzo[a,l] pyrene, (22) Pyrene.)

The molecular graph and physicochemical properties of benzenoid hydrocarbons along with the computed ASO index are represented in Figure 1 and Table 1 respectively. For benzenoid hydrocarbons, the correlation coefficients (R) between the ASO index and various properties are as follows:

BP (0.9755), π-ele (0.9991), MW (0.9967), PO (0.9999), MV (0.9456), and MR (0.9999),

as summarized in Table 2. These strong correlations indicate that the ASO index is an effective descriptor for predicting these physicochemical properties.

Table 1. Experimental values of benzenoid hydrocarbons and the corresponding values of augmented Sombor index

Derivatives of benzene	BP	π-ele	MW	PO	MV	MR	ASO
Benzene	78.8	8	78.11	10.4	89.4	26.3	12
Naphthalene	221.5	13.683	128.17	17.5	123.5	44.1	22.4480
Phenanthrene	337.4	19.448	178.23	24.6	157.7	61.9	32.8540
Anthracene	337.4	19.314	178.23	24.6	157.7	61.9	32.8960
Chrysene	448	25.192	228.3	31.6	191.8	79.8	43.2599
Benzo[a]anthracene	436.7	25.101	228.3	31.6	191.8	79.8	43.3019
Triphenylene	425	25.275	228.3	31.6	191.8	79.8	43.2179
Tetracene	436.7	25.188	228.3	31.6	191.8	79.8	43.3440
Benzo[a]pyrene	495	28.222	252.3	35.8	196.1	90.3	49.6659
Benzo[e]pyrene	467.5	28.336	252.3	35.8	196.1	90.3	49.6239
Perylene	467.5	28.245	252.3	35.8	196.1	90.3	49.6239
Anthanthrene	497.1	31.253	276.3	40	200.4	100.8	56.0719
Benzo[ghi]perylene	501	31.425	276.3	40	200.4	100.8	56.0299
Dibenz[a,c]anthracene	518	30.942	278.3	38.7	225.9	97.6	53.6659
Dibenz[a,h]anthracene	524.7	30.881	278.3	38.7	225.9	97.6	53.7079
Dibenz[a,j]anthracene	524.7	30.88	278.3	38.7	225.9	97.6	53.7079
Picene	519	30.943	278.3	38.7	225.9	97.6	53.6659
Coronene	525.6	34.572	300.4	44.1	204.7	111.4	62.4358
Dibenzo[a,h]pyrene	552.3	33.928	302.4	42.9	230.2	108.1	60.0719
Dibenzo[a,i]pyrene	552.3	33.954	302.4	42.9	230.2	108.1	60.0719
Dibenzo[a,l]pyrene	552.3	34.031	302.4	42.9	230.2	108.1	60.0299
Pyrene	404	22.506	202.25	28.7	162	72.5	39.2599

Table 2. The correlation coefficient R from linear regression model between augmented Sombor index and physicochemical properties of benzenoid hydrocarbons

	BP	π-ele	MW	PO	MV	MR
ASO	0.9755	0.9991	0.9967	0.9999	0.9456	0.9999

The linear regression models linking the ASO index with the properties of boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR) were developed via the least squares fitting procedure, as illustrated in Figure 2. Regression analysis reveals that the properties considered in this study [11, 16] are strongly correlated with the ASO index.

§3. Minimum ASO Index of Molecular Graphs with Cyclomatic Number at Least 3

For an edge set $S \subseteq E(G)$, the graph $G - S$ is obtained by removing all edges in S from G. Similarly, $G + S$ is obtained by adding all edges in S to G. In particular, if $S = uv$, we simply write $G - uv$ and $G + uv$ instead of $G - \{uv\}$ and $G + \{uv\}$, respectively.

Let r, k and $a_1, a_2, \cdots, a_k$ be positive integers such that $1 \leqslant a_1 < a_2 < \cdots < a_k \leqslant \lfloor \frac{r}{2} \rfloor$.

Such a graph is called circulant graph. The circulant graph, denoted by $C(r; a_1, a_2, \cdots, a_k)$, is the graph with vertex set $\{v_0, v_1, v_2, \cdots, v_{r-1}\}$ and edge set

$$\left\{v_i v_{i+a_j} : 0 \leqslant i \leqslant r-1 \textit{ and } 1 \leqslant j \leqslant k,\ \textit{where } i+a_j \textit{ is taken modulo } r\right\}.$$

If $a_k < \frac{r}{2}$, then $C(r; a_1, a_2, \cdots, a_k)$ is $2k$-regular.

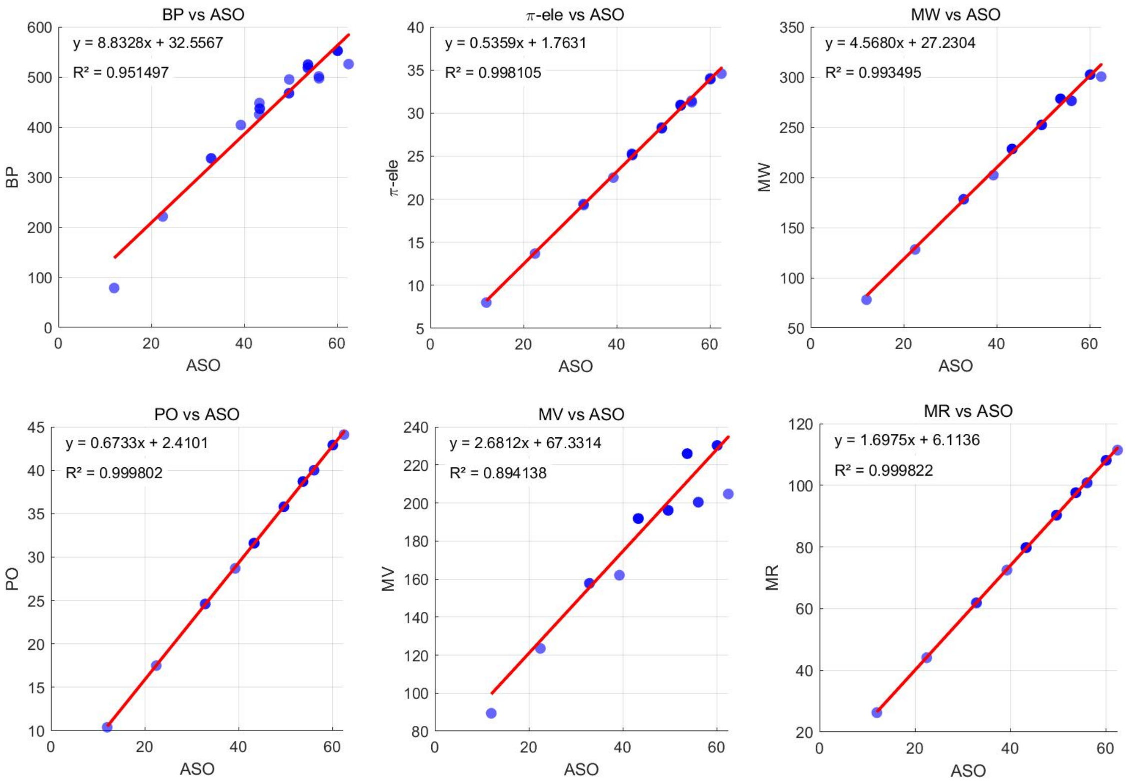

Figure 2. Scatter plots between physicochemical properties of benzenoid hydrocarbons and their ASO index

Lemma 3.1([4]) *The circulant graph $C_n(r; a_1, a_2, \cdots, a_k)$ is connected if and only if*

$$\gcd(a_1, a_2, \cdots, a_k, r) = 1.$$

Lemma 3.2 *Let G be a graph minimizing the ASO index among all n-order molecular graphs with cyclomatic number ℓ such that $4 \leqslant 2(\ell-1) \leqslant n$. Then, G contains no pendant edge incident to a vertex of degree 2.*

Proof This proof is by contradiction. Let G contain at least one pendant edge incident to a vertex of degree 2. Denote such an edge by $e = uv \in E(G)$, where $d_G(u) = 1$ and $d_G(v) = 2$. We consider a branching vertex $w \in V(G)$ such that the distance between w and u is minimized. Then, every vertex on the unique $u-w$ path P, except u and w, has degree 2 in G. Since $\ell \geqslant 3$,

w must be adjacent to at least two non-pendent vertices. Let $N_G(w) = \{w_1, w_2, \cdots, w_s\}$, where w_s lies on P and $s \in \{3, 4\}$. Let

$$d_G(w_1) = \max\{d_G(w_i) : 1 \leqslant i \leqslant s-1\}.$$

Case 1. $d_G(w) = 4$.

Since G is a molecular graph, by a direct computation, we have

$$\sqrt{\frac{16}{3}} - \sqrt{5} < \sqrt{5} - \sqrt{\frac{9}{2}} < \sqrt{\frac{17}{3}} - \sqrt{5} < \sqrt{5} - \sqrt{\frac{13}{3}},$$

$$\sqrt{\frac{16}{3}} - \sqrt{5} < \sqrt{\frac{17}{3}} - \sqrt{5} < \sqrt{5} - \sqrt{\frac{13}{3}} < \sqrt{5} - 2.$$

Let $G_1 = G - w_1w + w_1u$. Since $d_G(w_1) \geqslant 2$ and $1 \leqslant d_G(w_i) \leqslant d_G(w_1) \leqslant 4$ for each $i \in \{2, 3\}$, we have

$$\begin{aligned}
&ASO(G) - ASO(G_1)\\
&= \sum_{i=2}^{3}\left[\sqrt{\frac{4^2 + (d_G(w_i))^2}{4 + d_G(w_i) - 2}} - \sqrt{\frac{3^2 + (d_G(w_i))^2}{3 + d_G(w_i) - 2}}\right] + \sqrt{\frac{4^2+2^2}{4+2-2}} - \sqrt{\frac{3^2+2^2}{3+2-2}}\\
&\quad + \sqrt{\frac{1^2+2^2}{1+2-2}} - \sqrt{\frac{2^2+2^2}{2+2-2}} + \sqrt{\frac{4^2 + (d_G(w_1))^2}{4 + d_G(w_1) - 2}} - \sqrt{\frac{2^2 + (d_G(w_1))^2}{2 + d_G(w_1) - 2}}\\
&= \sum_{i=2}^{3}\left[\sqrt{\frac{16 + (d_G(w_i))^2}{2 + d_G(w_i)}} - \sqrt{\frac{9 + (d_G(w_i))^2}{1 + d_G(w_i)}}\right] + \sqrt{5} - \sqrt{\frac{13}{3}} + \sqrt{5} - 2\\
&\quad + \sqrt{\frac{16 + (d_G(w_1))^2}{2 + d_G(w_1)}} - \sqrt{\frac{4 + (d_G(w_1))^2}{d_G(w_1)}}\\
&\geqslant 2\left(\sqrt{\frac{16}{3}} - \sqrt{5}\right) + 2\sqrt{5} - \sqrt{\frac{13}{3}} - 2 + \sqrt{\frac{16}{3}} - \sqrt{5}\\
&> 0.61 > 0,
\end{aligned}$$

that is, $ASO(G) > ASO(G_1)$, a contradiction.

Case 2. $d_G(w) = 3$ and $(d_G(w_1), d_G(w_2)) \neq (4, 4)$.

By a direct computation, we have

$$0 = \sqrt{5} - \sqrt{5} < \sqrt{\frac{9}{2}} - \sqrt{\frac{13}{3}} < \sqrt{\frac{13}{3}} - 2.$$

Let $G_2 = G - w_1w + w_1u$. Since $d_G(w_1) \geqslant 2$, $1 \leqslant d_G(w_2) \leqslant d_G(w_1) \leqslant 4$ and

$$(d_G(w_1), d_G(w_2)) \neq (4, 4),$$

we have

$$\begin{aligned}
&ASO(G) - ASO(G_2)\\
&= \sqrt{\frac{3^2 + (d_G(w_2))^2}{3 + d_G(w_2) - 2}} - \sqrt{\frac{2^2 + (d_G(w_2))^2}{2 + d_G(w_2) - 2}} + \sqrt{\frac{3^2 + 2^2}{3 + 2 - 2}} - \sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}}\\
&\quad + \sqrt{\frac{1^2 + 2^2}{1 + 2 - 2}} - \sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} + \sqrt{\frac{3^2 + (d_G(w_1))^2}{3 + d_G(w_1) - 2}} - \sqrt{\frac{2^2 + (d_G(w_1))^2}{2 + d_G(w_1) - 2}}\\
&= \sqrt{\frac{9 + (d_G(w_2))^2}{1 + d_G(w_2)}} - \sqrt{\frac{4 + (d_G(w_2))^2}{d_G(w_2)}} + \sqrt{\frac{13}{3}} - 2 + \sqrt{5} - 2\\
&\quad + \sqrt{\frac{9 + (d_G(w_1))^2}{1 + d_G(w_1)}} - \sqrt{\frac{4 + (d_G(w_1))^2}{d_G(w_1)}}\\
&\geqslant \sqrt{5} - \sqrt{5} + \sqrt{\frac{13}{3}} - 2 + \sqrt{5} - 2 + \sqrt{5} - \sqrt{5}\\
&> 0.31 > 0,
\end{aligned}$$

that is, $ASO(G) > ASO(G_2)$, a contradiction.

Case 3. $d_G(w) = 3$ and $(d_G(w_1), d_G(w_2)) = (4, 4)$.

Subcase 3.1 Either w_1 or w_2 does not have three neighbors of degree 4.

Without loss of generality, let w_1 does not have three neighbors of degree 4. We choose a vertex $w_1' \in N_G(w_1) \setminus \{w\}$, such that it satisfies $d_G(w_1') = \min\{d_G(w') : w_1' \in N_G(w_1) \setminus \{w\}\}$. Therefore, $d_G(w_1') \leqslant 3$. Let $G_3 = G - w_1'w_1 + w_1'u$. Then, we have

$$\begin{aligned}
ASO(G) - ASO(G_3) = &\sum_{w' \in N_G(w_1)\setminus\{w, w_1'\}} \left[\sqrt{\frac{4^2 + ((d_G(w'))^2}{4 + d_G(w') - 2}} - \sqrt{\frac{3^2 + (d_G(w'))^2}{3 + d_G(w') - 2}}\right]\\
&+ \sqrt{\frac{1^2 + 2^2}{1 + 2 - 2}} - \sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} + \sqrt{\frac{3^2 + 4^2}{3 + 4 - 2}} - \sqrt{\frac{3^2 + 3^2}{3 + 3 - 2}}\\
&+ \sqrt{\frac{4^2 + (d_G(w_1'))^2}{4 + d_G(w_1') - 2}} - \sqrt{\frac{2^2 + (d_G(w_1'))^2}{2 + d_G(w_1') - 2}}\\
= &\sum_{w' \in N_G(w_1)\setminus\{w, w_1'\}} \left[\sqrt{\frac{16 + ((d_G(w'))^2}{2 + d_G(w')}} - \sqrt{\frac{9 + (d_G(w'))^2}{1 + d_G(w')}}\right] + 2\sqrt{5}\\
&- 2 - \sqrt{\frac{9}{2}} + \sqrt{\frac{16 + (d_G(w_1'))^2}{2 + d_G(w_1')}} - \sqrt{\frac{4 + (d_G(w_1'))^2}{d_G(w_1')}}\\
\geqslant &2\left(\sqrt{\frac{16}{3}} - \sqrt{5}\right) + \sqrt{\frac{17}{3}} - \sqrt{5} + 2\sqrt{5} - 2 - \sqrt{\frac{9}{2}}\\
> &0.64 > 0,
\end{aligned}$$

that is, $ASO(G) > ASO(G_3)$, a contradiction.

Subcase 3.2 Both w_1 and w_2 have three neighbors of degree 4.

Let G^* be the graph obtained from G by removing all vertices on the path P except w and their incident edges. Then, $d_{G^*}(w) = 2$ and $d_{G^*}(x) = d_G(x)$ for each $x \in V(G) \setminus V(P)$, where $V(P)$ is the set of all vertices belonging to the path P. To complete the proof, we first prove a claim.

Claim 1. There exists at least one vertex $y \in V(G^*) \setminus \{w\}$ such that $1 \leqslant d_G(y) \leqslant 3$.

Proof of Claim 1. This proof is by contradiction. Let each vertex $y \in V(G^*)\setminus\{w\}$ satisfy $d_G(y) = 4$, that is, $d_{G^*}(y) = 4$. Since both the graphs G and G^* have the same cyclomatic number ℓ, it follows from the Handshaking Lemma that

$$4(|V(G^*)| - 1) + 2 = 2|E(G^*)| = 2(|V(G^*)| + \ell - 1).$$

Therefore, $|V(G^*)| = \ell$.

If $\ell \leqslant 5$,then we have $|V(G^*)| \leqslant 5$. This contradicts the fact that $d_{G^*}(w) = 2$ because every $y \in V(G^*) \setminus \{w\}$ satisfies $d_{G^*}(y) = 4$, according to our assumption. We now consider the case where $\ell \geqslant 6$, i.e., $|V(G^*)| \geqslant 6$. Next, we first prove that for every ℓ ($\ell \geqslant 6$) ,there exists at least one connected graph of order ℓ and the degree sequence $(\underbrace{4, 4, \cdots, 4}_{\ell-1}, 2)$.

The circulant graph $C(\ell-1; 1, 2)$ is a 4-regular graph for $\ell \geqslant 6$. By Lemma 1, $C(\ell-1; 1, 2)$ is a connected graph. Let $C^*(\ell-1; 1, 2) = C(\ell-1; 1, 2) - \{v_0v_1\} + \{v'v_0, v'v_1\}$, where v' is the newly added vertex. Clearly, the order and the degree sequence of the graph $C^*(\ell-1; 1, 2)$ are ℓ and $(\underbrace{4, 4, \cdots, 4}_{\ell-1}, 2)$,respectively. Therefore, we have

$$m_{1,2}(G) = 1 = m_{2,3}(G), m_{3,4}(G) = 2, m_{4,4}(G) = 2\ell - 3, m_{2,2}(G) = n - \ell - 2,$$

where $m_{i,j}(G)$ denotes the number of edges with end vertices of degrees i and j in G. Then, we have

$$\begin{aligned} ASO(G) =&(n-\ell-2)\sqrt{\frac{2^2+2^2}{2+2-2}} + (2\ell-3)\sqrt{\frac{4^2+4^2}{4+4-2}} + \sqrt{\frac{1^2+2^2}{1+2-2}} \\ &+ \sqrt{\frac{2^2+3^2}{2+3-2}} + 2\sqrt{\frac{3^2+4^2}{3+4-2}} \\ =&2(n-\ell-2) + (2\ell-3)\sqrt{\frac{16}{3}} + 3\sqrt{5} + \sqrt{\frac{13}{3}}. \end{aligned}$$

Let G' be the n-order molecular graph with cyclomatic number ℓ such that $4 \leqslant 2(\ell-1) \leqslant n$ and

$$m_{2,3}(G') = 2, m_{3,3}(G') = 3\ell - 4, m_{2,2}(G') = n - 2\ell + 1.$$

Then, we have

$$\begin{aligned} ASO(G') =&(n-2\ell+1)\sqrt{\frac{2^2+2^2}{2+2-2}} + (3\ell-4)\sqrt{\frac{3^2+3^2}{3+3-2}} + 2\sqrt{\frac{2^2+3^2}{2+3-2}} \\ =&2(n-2\ell+1) + (3\ell-4)\sqrt{\frac{9}{2}} + 2\sqrt{\frac{13}{3}}. \end{aligned}$$

Therefore,

$$ASO(G) - ASO(G') = \left(2 + \frac{8\sqrt{3}}{3} - \frac{9\sqrt{2}}{2}\right)\ell - 6 - 4\sqrt{3} + 6\sqrt{2} + 3\sqrt{5} - \frac{\sqrt{39}}{3}.$$

Since $2 + \frac{8\sqrt{3}}{3} - \frac{9\sqrt{2}}{2} > 0.25 > 0$ and $-6 - 4\sqrt{3} + 6\sqrt{2} + 3\sqrt{5} - \frac{\sqrt{39}}{3} > 0.18 > 0$, we have $ASO(G) - ASO(G') > 0$. Namely, $ASO(G) > ASO(G')$, a contradiction. This completes the proof of Claim 1.

Next, using Claim 1, we proceed with the following three cases based on the minimum vertex degree in $V(G^*) \setminus \{w\}$.

Subcase 3.2.1 There exists a vertex $p \in V(G^*) \setminus \{w\}$ such that $d_G(p) = 1$.

Let p_1 be the unique neighbor of p in G and $G_4 = G - \{w_1w, w_2w\} + \{w_1w_2, wp\}$. By a direct computation, we have

$$\sqrt{\frac{17}{3}} - \sqrt{5} < \sqrt{5} - \sqrt{\frac{13}{3}} < \sqrt{5} - 2.$$

Therefore,

$$\begin{aligned}
ASO(G) - ASO(G_4) =& \sqrt{\frac{1^2 + (d_G(p_1))^2}{1 + d_G(p_1) - 2}} - \sqrt{\frac{2^2 + (d_G(p_1))^2}{2 + d_G(p_1) - 2}} + \sqrt{\frac{2^2 + 3^2}{2 + 3 - 2}} \\
& + 2\sqrt{\frac{3^2 + 4^2}{3 + 4 - 2}} - 2\sqrt{\frac{2^2 + 2^2}{2 + 2 - 2}} - \sqrt{\frac{4^2 + 4^2}{4 + 4 - 2}} \\
=& \sqrt{\frac{1 + (d_G(p_1))^2}{d_G(p_1) - 1}} - \sqrt{\frac{4 + (d_G(p_1))^2}{d_G(p_1)}} + \sqrt{\frac{13}{3}} + 2\sqrt{5} \\
& - 4 - \sqrt{\frac{16}{3}} \\
\geqslant& \sqrt{\frac{17}{3}} - \sqrt{5} + \sqrt{\frac{13}{3}} + 2\sqrt{5} - 4 - \sqrt{\frac{16}{3}} \\
>& 0.38 > 0,
\end{aligned}$$

that is, $ASO(G) > ASO(G_4)$, a contradiction.

Subcase 3.2.2 There does not exist any vertex $p \in V(G^*) \setminus \{w\}$ such that $d_G(p) = 1$, but there is a vertex $q \in V(G^*) \setminus \{w\}$ such that $d_G(q) = 2$.

Since G is connected, we choose a vertex q such that at least one of its neighbors has degree at least 3 in G. Let q_1 and q_2 be the neighbors of q such that $d_G(q_1) \geqslant 3$ and $d_G(q_2) \geqslant 2$. Let $G_5 = G - \{w_1w, w_2w\} + \{w_1w_2, wq\}$. By a direct computation, we have

$$2 - \sqrt{\frac{13}{3}} < \sqrt{\frac{13}{3}} - \sqrt{\frac{9}{2}} < \sqrt{5} - \sqrt{5} = 0$$

Then, we have

$$
\begin{aligned}
&ASO(G) - ASO(G_5)\\
&= \sum_{i=1}^{2}\left[\sqrt{\frac{2^2+(d_G(q_i))^2}{2+d_G(q_i)-2}} - \sqrt{\frac{3^2+(d_G(q_i))^2}{3+d_G(q_i)-2}}\right] + 2\sqrt{\frac{3^2+4^2}{3+4-2}} - \sqrt{\frac{2^2+2^2}{2+2-2}}\\
&\quad - \sqrt{\frac{4^2+4^2}{4+4-2}} + \sqrt{\frac{2^2+3^2}{2+3-2}} - \sqrt{\frac{2^2+3^2}{2+3-2}}\\
&= \sum_{i=1}^{2}\left[\sqrt{\frac{4+(d_G(q_i))^2}{d_G(q_i)}} - \sqrt{\frac{9+(d_G(q_i))^2}{1+d_G(q_i)}}\right] + 2\sqrt{5} - 2 - \sqrt{\frac{16}{3}}\\
&\geqslant 2 - \sqrt{\frac{13}{3}} + \sqrt{\frac{13}{3}} - \sqrt{\frac{9}{2}} + 2\sqrt{5} - 2 - \sqrt{\frac{16}{3}}\\
&> 0.04 > 0,
\end{aligned}
$$

that is, $ASO(G) > ASO(G_5)$, a contradiction.

Subcase 3.2.3 There does not exist any vertex $p \in V(G^*) \setminus \{w\}$ such that $d_G(p) = 1$ or $d_G(p) = 2$, but there is a vertex $z \in V(G^*) \setminus \{w\}$ such that $d_G(z) = 3$.

Since G is connected, we choose a vertex z such that at least one of its neighbors has degree at least 4 in G. Let z_i for $i \in \{1, 2, 3\}$ be the neighbors of z such that $d_G(z_1) = 4$, $d_G(z_2) \geqslant 3$ and $d_G(z_3) \geqslant 3$.

Subcase 3.2.3.1 $d_G(z_2) = d_G(z_3) = 4$.

Let $G_6 = G - \{w_1w, w_2w, z_2z\} + \{w_1w_2, wz, z_2u\}$. Then, we have

$$
\begin{aligned}
ASO(G) - ASO(G_6) =& \sqrt{\frac{1^2+2^2}{1+2-2}} - 2\sqrt{\frac{2^2+2^2}{2+2-2}} + 3\sqrt{\frac{4^2+3^2}{4+3-2}} - \sqrt{\frac{4^2+4^2}{4+4-2}}\\
&- \sqrt{\frac{2^2+4^2}{2+4-2}} + \sqrt{\frac{2^2+3^2}{2+3-2}} - \sqrt{\frac{2^2+3^2}{2+3-2}}\\
=& 3\sqrt{5} - 4 - \sqrt{\frac{16}{3}}\\
>& 0.39 > 0,
\end{aligned}
$$

that is, $ASO(G) > ASO(G_6)$, a contradiction.

Subcase 3.2.3.2 $\min\{d_G(z_2), d_G(z_3)\} = 3$.

Without loss of generality, we assume that $d_G(z_2) = 3$. Then, either $d_G(z_3) = 3$ or

$d_G(z_3) = 4$.Let $G_7 = G - \{w_1w, w_2w, z_2z\} + \{w_1w_2, wz, z_2u\}$. Then, we have

$$\begin{aligned}ASO(G) - ASO(G_7) =&\sqrt{\frac{1^2+2^2}{1+2-2}} + 2\sqrt{\frac{3^2+4^2}{3+4-2}} + \sqrt{\frac{3^2+3^2}{3+3-2}} - 2\sqrt{\frac{2^2+2^2}{2+2-2}} \\ &- \sqrt{\frac{4^2+4^2}{4+4-2}} - \sqrt{\frac{2^2+3^2}{2+3-2}} + \sqrt{\frac{2^2+3^2}{2+3-2}} - \sqrt{\frac{2^2+3^2}{2+3-2}} \\ =&3\sqrt{5} + \sqrt{\frac{9}{2}} - 4 - \sqrt{\frac{16}{3}} - \sqrt{\frac{13}{3}} \\ >&0.43 > 0,\end{aligned}$$

that is, $ASO(G) > ASO(G_7)$, a contradiction.

Therefore, G contains no pendant edge incident to a vertex of degree 2. $\square$

Theorem 3.3 *Let G be a molecular n-order graph with cyclomatic number ℓ such that $4 \leqslant 2(\ell-1) \leqslant n$.*

(1) *If $n = 2(\ell-1)$, then*

$$ASO(G) \geqslant \frac{9\sqrt{2}}{2}(\ell-1)$$

with equality if and only if G is a 3-regular graph;

(2) *If $n > 2(\ell-1)$, then*

$$ASO(G) \geqslant 2n + \left(\frac{9\sqrt{2}}{2} - 4\right)\ell + 2 - 6\sqrt{2} + \frac{2\sqrt{39}}{3}$$

with equality if and only if

$$\delta(G) = 2, \quad \Delta(G) = 3$$

and

$$m_{3,3}(G) = 3\ell - 4, \quad m_{2,3}(G) = 2, \quad m_{2,2}(G) = n - 2\ell + 1.$$

Proof Let G^* be a graph minimizing the augmented Sombor index among all molecular n-order graphs with cyclomatic number ℓ such that $4 \leqslant 2(\ell-1) \leqslant n$. Then, we have

$$ASO(G) \;\geqslant\; ASO(G^*).$$

By Lemma 3.2, graph G^* contains no pendant edge incident to a vertex of degree 2. Namely, $m_{1,2}(G^*) = 0$. Let $m_{i,j}(G) = m_{i,j}(G^*)$ and

$$A := \{(i,j) : 1 \leqslant i \leqslant j \leqslant 4 \text{ and } i,j \in \mathbb{Z}_+\} \setminus \{(1,1),(1,2)\},$$

where $\mathbb{Z}_+$ denotes the set of positive integers. Since

$$\sum_{(i,j)\in A}\left(\frac{1}{i}+\frac{1}{j}\right)m_{i,j} = |V(G^*)| = n,$$

we have

$$\sum_{(i,j)\in A^*}\left(\frac{1}{i}+\frac{1}{j}\right)m_{i,j}=n-m_{2,2}-\frac{5}{6}m_{2,3}-\frac{2}{3}m_{3,3}, \tag{1}$$

where $A^*:=A\setminus\{(2,2),(2,3),(3,3)\}$.

Moreover, since $\sum_{(i,j)\in A}m_{i,j}=n+\ell-1$, we have

$$\sum_{(i,j)\in A^*}m_{i,j}=n+\ell-1-m_{2,2}-m_{2,3}-m_{3,3}. \tag{2}$$

By solving (1) and (2), we have

$$m_{2,3}=2(n-2\ell-m_{2,2}+2)+\sum_{(i,j)\in A^*}\left(4-6\left(\frac{1}{i}+\frac{1}{j}\right)\right)m_{i,j}$$

and

$$m_{3,3}=5(\ell-1)+m_{2,2}-n+\sum_{(i,j)\in A^*}\left(6\left(\frac{1}{i}+\frac{1}{j}\right)-5\right)m_{i,j}.$$

By substituting $m_{2,3}$ and $m_{3,3}$, we obtain

$$\begin{aligned}ASO(G^*)=&\sum_{(i,j)\in A}\sqrt{\frac{i^2+j^2}{i+j-2}}m_{i,j}\\ =&\sqrt{\frac{2^2+2^2}{2+2-2}}m_{2,2}+\sqrt{\frac{2^2+3^2}{2+3-2}}m_{2,3}+\sqrt{\frac{3^2+3^2}{3+3-2}}m_{3,3}+\sum_{(i,j)\in A^*}\sqrt{\frac{i^2+j^2}{i+j-2}}m_{i,j}\\ =&2m_{2,2}+\sqrt{\frac{13}{3}}m_{2,3}+\sqrt{\frac{9}{2}}m_{3,3}+\sum_{(i,j)\in A^*}\sqrt{\frac{i^2+j^2}{i+j-2}}m_{i,j}\\ =&\left(\frac{2\sqrt{39}}{3}-\frac{3\sqrt{2}}{2}\right)n+\left(\frac{15\sqrt{2}}{2}-\frac{4\sqrt{39}}{3}\right)\ell+\left(2+\frac{3\sqrt{2}}{2}-\frac{2\sqrt{39}}{3}\right)m_{2,2}+\frac{4\sqrt{39}}{3}\\ &-\frac{15\sqrt{2}}{2}+\sum_{(i,j)\in A^*}\left[(9\sqrt{2}-2\sqrt{39})\left(\frac{1}{i}+\frac{1}{j}\right)+\sqrt{\frac{i^2+j^2}{i+j-2}}+\frac{4\sqrt{39}}{3}-\frac{15\sqrt{2}}{2}\right]m_{i,j}.\end{aligned}$$

Let

$$f(i,j)=(9\sqrt{2}-2\sqrt{39})\left(\frac{1}{i}+\frac{1}{j}\right)+\sqrt{\frac{i^2+j^2}{i+j-2}}+\frac{4\sqrt{39}}{3}-\frac{15\sqrt{2}}{2}.$$

By a direct computation, we have

$$\begin{aligned}&f(1,3)>0.27,\quad f(1,4)>0.39,\quad f(2,4)>0.13,\\ &f(3,4)>0.09,\quad f(4,4)>0.14.\end{aligned}$$

Hence,

$$\begin{aligned} ASO(G^*) \quad \geqslant \quad & \left(\frac{2\sqrt{39}}{3}-\frac{3\sqrt{2}}{2}\right)n+\left(\frac{15\sqrt{2}}{2}-\frac{4\sqrt{39}}{3}\right)\ell \\ & +\left(2+\frac{3\sqrt{2}}{2}-\frac{2\sqrt{39}}{3}\right)m_{2,2}+\frac{4\sqrt{39}}{3}-\frac{15\sqrt{2}}{2}. \end{aligned}$$

By the definition of G^*, the inequality above must hold with equality. This implies that $m_{i,j}=0$ for every $(i,j)\in A^*$, which means G^* contains neither vertices of degree 4 nor pendant edges incident to vertices of degree 3. Therefore, we have either $\delta(G^*)=\Delta(G^*)=3$ or $(\delta(G^*),\Delta(G^*))=(2,3)$.

Case 1. If $n=2(\ell-1)$, we can not have $(\delta(G^*),\Delta(G^*))=(2,3)$. Otherwise, we would have $n_2(G^*)=n-2(\ell-1)=0$, a contradiction. Therefore, if $n=2(\ell-1)$, we have $\delta(G^*)=\Delta(G^*)=3$, that is, G^* is a 3-regular graph. Consequently, we have

$$ASO(G^*)=\frac{9\sqrt{2}}{2}(\ell-1).$$

Case 2. If $n>2(\ell-1)$, we can not have $\delta(G^*)=\Delta(G^*)=3$. Otherwise, we would have $3n=2(n+\ell-1)$ by the Handshaking Lemma, a contradiction. Therefore, if $n>2(\ell-1)$, we have $(\delta(G^*),\Delta(G^*))=(2,3)$. Since G^* is a connected graph, it holds that $m_{2,3}>0$. Moreover, since $2m_{2,2}+m_{2,3}=2n_2$, it follows that $m_{2,3}$ must be a positive even integer. Hence,

$$2m_{2,2}+2\leqslant 2m_{2,2}+m_{2,3}=2n_2=2(n-2(\ell-1)),$$

which yields $m_{2,2}\leqslant n-2\ell+1$ with equality if and only if $m_{2,3}=2$. Therefore, from the definition of G^*, we obtain $m_{2,2}=n-2\ell+1$, $m_{2,3}=2$, $m_{3,3}=3\ell-4$. Consequently, we have

$$\begin{aligned} ASO(G^*)=& \left(\frac{2\sqrt{39}}{3}-\frac{3\sqrt{2}}{2}\right)n+\left(\frac{15\sqrt{2}}{2}-\frac{4\sqrt{39}}{3}\right)\ell \\ & +\left(2+\frac{3\sqrt{2}}{2}-\frac{2\sqrt{39}}{3}\right)(n-2\ell+1)+\frac{4\sqrt{39}}{3}-\frac{15\sqrt{2}}{2} \\ =& 2n+\left(\frac{9\sqrt{2}}{2}-4\right)\ell+2-6\sqrt{2}+\frac{2\sqrt{39}}{3}. \end{aligned}$$

This completes the proof. □

References

[1] A.M. Alotaibi, A.M. Alanazi, T.S. Hassan and A. Ali, On the diminished Sombor index of fixed-order molecular graphs with cyclomatic number at least 3, *MATCH Commun. Math. Comput. Chem.*, 95 (2026) 813-828.

[2] J. Barman and S. Das, Geometric approach to degree-based topological index: Hyperbolic

Sombor index, *MATCH Commun. Math. Comput. Chem.*, 95 (2026) 63-94.

[3] J. Barman and S. Das, Chemical applicability of the hyperbolic Sombor index, *Chem. Phys. Lett.*, 878 (2025) 142340.

[4] F. Boesch and R. Tindell, Circulants and their connectivities, *J. Graph Theory*, 8 (1984) 487-499.

[5] K.C. Das, I. Gutman and A. Ali, Augmented Sombor index, *MATCH Commun. Math. Comput. Chem.*, 95 (2026) 523-547.

[6] H. Deng, Z. Tang and R. Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum Chem.*, 121 (2021) e26622.

[7] B. Furtula, I. Gutman and M. Dehmer, On structure-sensitivity of degree-based topological indices, *Appl. Math. Comput.* 219 (2013) 8973-8978.

[8] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.*, 86 (2021) 11-16.

[9] I. Gutman, Sombor indices-back to geometry, *Open J. Discret. Appl. Math.*, 5 (2022) 1-5.

[10] I. Gutman, B. Furtula and M.S. Oz, Geometric approach to vertex-degree-based topological indices-Elliptic Sombor index, theory and application, it Int. J. Quantum Chem., 124 (2024) e27346.

[11] S. Hayat and S. Khan, Quality testing of spectrum-based valency descriptors for polycyclic aromatic hydrocarbons with applications, *J. Mol. Struct.*, 1228 (2021) 129789.

[12] Z. Lin, Sombor-type indices for certain interconnection networks, *MATCH Commun. Math. Comput. Chem.*, 94 (2025) 701-724.

[13] H. Liu, H. Chen, Q. Xiao, X. Fang and Z. Tang, More on Sombor indices of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons, *Int. J. Quantum Chem.*, 121 (2021) e26689.

[14] H. Liu, I. Gutman, L. You and Y. Huang, Sombor index: review of extremal results and bounds, *J. Math. Chem.*, 60 (2022) 771-798.

[15] F. Movahedi, I. Gutman, I. Redžepović and B. Furtula, Diminished Sombor index, *MATCH Commun. Math. Comput. Chem.*, 95 (2026) 141-162.

[16] S. Nikolić, N. Trinajstić and I. Baucčić, Comparison between the vertex- and edge-connectivity indices for benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.*, 38 (1998) 42-46.

[17] B. A. Ravindran, Sombor index on trees-A review, *MATCH Commun. Math. Comput. Chem.*, 94 (2025) 291-305.

[18] A. Rauf and S. Ahmad, On sombor indices of tetraphenylethylene, terpyridine rosettes and QSPR analysis on fluorescence properties of several aromatic hetero-cyclic species, *Int. J. Quantum Chem.*, 123 (2023) e27261.

[19] M.C. Shanmukha, A. Usha, V. R. Kulli and K.C. Shilpa, Chemical applicability and curvilinear regression models of vertex-degree-based topological index: Elliptic Sombor index, *Int. J. Quantum Chem.*, 124 (2024) e27376.

[20] Z. Tang, Y. Li and H. Deng, The Euler Sombor index of a graph, *Int. J. Quantum Chem.*, 124 (2024) e27387.