

On the Diminished Sombor Index of Fixed-Order Molecular Graphs With Cyclomatic Number at Least 3

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Abstract

For a graph G with edge set E , let $d(u)$ denote the degree of a vertex u in G . The diminished Sombor (DSO) index of G is defined as $DSO(G) = \sum_{uv \in E} \sqrt{(d(u))^2 + (d(v))^2} (d(u) + d(v))^{-1}$. The cyclomatic number of a graph is the smallest number of edges whose removal makes the graph acyclic. A connected graph of maximum

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degree at most 4 is known as a molecular graph. The primary motivation of the present study comes from a conjecture, concerning the minimum DSO index of fixed-order connected graphs with cyclomatic number 3, posed in the recent paper [F. Movahedi, I. Gutman, I. Redžepović, B. Furtula, Diminished Sombor index, *MATCH Commun. Comput. Chem.* **95** (2026) 141–162]. The present paper gives all graphs minimizing the DSO index among all molecular graphs of order n with cyclomatic number ℓ , provided that $n \geq 2(\ell - 1) \geq 4$.

1 Introduction

Chemical graph theory [27], a branch of mathematical chemistry, employs graph-theoretical concepts and techniques to model and analyze molecular structures. (The graph-theoretical and chemical graph-theoretical terminology, used in this study, but not defined here, can be found in [12, 15] and [37, 39], respectively.) In this framework, molecules are represented by graphs in which atoms correspond to vertices and chemical bonds to edges, providing a rigorous mathematical basis for investigating molecular properties. In graph-theoretical language, a connected graph of maximum degree at most 4 is known as a molecular graph. (Sometimes, molecular graphs are defined as the connected graphs of maximum degree at most 3; e.g., see [13].)

Molecular descriptors are fundamental tools for virtual screening of molecular libraries and for predicting the physicochemical properties of molecules [10]. According to Todeschini and Consonni [36], a molecular descriptor is “the final result of a logical and mathematical procedure that transforms chemical information encoded in a symbolic representation of a molecule into a useful number or the result of some standardized experiment.” When such descriptors are defined using molecular graphs, they are commonly referred to as topological indices in chemical graph theory. For details on the chemical applications of topological indices, readers may consult the recent works [21, 27].

Among these indices, degree-based topological indices [1, 2, 8, 9, 14, 19, 22, 25, 32] play a particularly prominent role. Owing to their computational efficiency and predictive power, degree-based indices are fundamental tools in quantitative structure-property relationship (QSPR) studies, which fa-

cilitate the design and analysis of new chemical compounds.

Among the many degree-based topological indices, one of the widely studied is the Sombor index, introduced by Gutman [23]. For a graph G , it is defined as

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

where $E(G)$ denotes the edge set of G , and $d(u)$ and $d(v)$ represent the degrees of the vertices u and v , respectively. (When more than one graph is under discussion simultaneously, we write $d_G(u)$ to specify the degree of vertex u in the graph G .) The Sombor index has attracted considerable research attention; e.g., see the survey [28] and some recent publications [16, 18, 29, 30, 33].

In [23], two variants of the Sombor index were considered, namely the reduced and average Sombor indices. Since then, numerous further modifications have been proposed, including the elliptic Sombor [24, 26], Euler–Sombor [7, 35], Zagreb–Sombor [5, 6], diminished Sombor [31], and augmented Sombor [20] indices. The present paper is concerned with the diminished Sombor (DSO) index. For a graph G , the DSO index is defined by

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

The cyclomatic number of a graph is the smallest number of edges whose removal makes the graph acyclic. The primary motivation of the present study comes from a conjecture, concerning the graphs minimizing the DSO index among all fixed-order connected graphs with cyclomatic number 3, posed in the recent paper [31]. According to this conjecture, the aforementioned extremal graphs minimizing the DSO index “are those obtained by connecting two disjoint cycles by two edges, so that a quadrangle is formed.” In this paper, it is shown that the graphs minimizing the DSO index among all molecular graphs of order n with cyclomatic number ℓ are either 3-regular graphs, or graphs with maximum degree 3 and minimum degree 2 in which the number of edges connecting the vertices of degrees 2 and 3 is 2, provided that $n \geq 2(\ell - 1) \geq 4$. Consequently, the structures of the extremal graphs conjectured in [31] differ slightly from

the actual ones.

We end this introductory section with the remark that the literature contains many general results about degree-based topological indices, in which the extremal graphs are similar to the ones obtained in the present paper; e.g., see the recent papers [3, 34] as well as Theorem 5.5, Theorems 5.9–5.17, and Theorem 5.23 in the recent survey paper [4]. However, none of these general results is applicable to the DSO index.

2 Results

We start this section by recalling some definitions. Let G be a graph with vertex set $V(G)$ such that $|V(G)| = n$. The graph G is known as an n -order graph. For a vertex $u \in V(G)$, define $N_G(u) = \{v \in V(G) : uv \in E(G)\}$. The elements of $N_G(u)$ are called neighbors of u in G . 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.

Now, we recall the definition of circulant graphs (see, e.g., [17, 38]). Let r , k and $a_1, a_2, \dots, a_k$ be positive integers such that

$$1 \leq a_1 < a_2 < \dots < a_k \leq \lfloor r/2 \rfloor.$$

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

$$\{v_i v_{i+a_j} : 0 \leq i \leq r-1 \text{ and } 1 \leq j \leq k, \text{ where } i+a_j \text{ is taken modulo } r\}.$$

Observation 1 (e.g., see [11, 38]). *If $a_k < r/2$, then $C(r; a_1, a_2, \dots, a_k)$ is $2k$ -regular.*

Lemma 1. [11] *The circulant graph $C(r; a_1, a_2, \dots, a_k)$ is connected if and only if $\gcd(a_1, a_2, \dots, a_k, r) = 1$.*

Lemma 2. *Let G be a graph minimizing the DSO index among all molecular n -order graphs with cyclomatic number ℓ such that $n \geq 2(\ell - 1) \geq 4$.*

Then, G contains no pendent edge incident with a vertex of degree 2.

Proof. We suppose to the contrary that G contains at least one pendent edge incident with a vertex of degree 2, say $uv \in E(G)$, where $d_G(u) = 1$ and $d_G(v) = 2$. We consider a branching vertex $w \in V(G)$ in such a way that the distance between w and u is the least. Then, every vertex different from u and w on the unique $u - w$ path, say P , has degree 2 in G . Since $\ell \geq 3$, w has at least two non-pendent neighbors. Let $N_G(w) = \{w_1, w_2, \dots, w_s\}$, where w_s lies on P and $s \in \{3, 4\}$. We may assume that $d_G(w_1) = \max\{d_G(w_i) : 1 \leq i \leq s-1\}$. Here, we define $f(i, j) := \sqrt{i^2 + j^2}/(i + j)$.

Case 1. Either $d_G(w) = 4$, or $d_G(w) = 3$ and $(d_G(w_1), d_G(w_2)) \neq (4, 4)$. We form a new graph G_1 using G by removing the edge w_1w and inserting the edge w_1u . Then

$$\begin{aligned} \mathcal{DSO}(G) - \mathcal{DSO}(G_1) &= \sum_{i=2}^{s-1} [f(d_G(w), d_G(w_i)) - f(d_G(w) - 1, d_G(w_i))] \\ &\quad + f(d_G(w), 2) - f(d_G(w) - 1, 2) + f(1, 2) \\ &\quad - f(2, 2) + f(d_G(w), d_G(w_1)) - f(2, d_G(w_1)). \quad (1) \end{aligned}$$

If $d_G(w) = 4$ (that is, $s = 4$), then using the facts that $d_G(w_1) \geq 2$ and $1 \leq d_G(w_i) \leq d_G(w_1) \leq 4$ for each $i \in \{2, 3\}$, we obtain from (1), $\mathcal{DSO}(G) - \mathcal{DSO}(G_1) > 0$, a contradiction to the definition of G .

If $d_G(w) = 3$ (that is, $s = 3$) and $(d_G(w_1), d_G(w_2)) \neq (4, 4)$, then using the facts that $d_G(w_1) \geq 2$ and $1 \leq d_G(w_2) \leq d_G(w_1) \leq 4$, we again obtain from (1), $\mathcal{DSO}(G) - \mathcal{DSO}(G_1) > 0$, a contradiction.

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

Case 2.1. Either w_1 or w_2 does not have three neighbors of degree 4. Without loss of generality, we assume that w_1 does not have three neighbors of degree 4. We choose a vertex $w'_1 \in N_G(w_1) \setminus \{w\}$ in such a way that it satisfies the equation $d_G(w'_1) = \min\{d_G(w') : w' \in N_G(w_1) \setminus \{w\}\}$. Then, $d_G(w'_1) \leq 3$. Now, we form a new graph G_2 using G by deleting the

edge $w'_1 w_1$ and inserting the edge $w'_1 u$. Then, we have

$$\begin{aligned} \mathcal{DSO}(G) - \mathcal{DSO}(G_2) &= \sum_{w' \in N_G(w_1) \setminus \{w, w'_1\}} [f(d_G(w'), 4) - f(d_G(w'), 3)] \\ &\quad + f(d_G(w'_1), 4) - f(d_G(w'_1), 2) + f(1, 2) - f(2, 2) \\ &\quad + f(3, 4) - f(3, 3) > 0, \end{aligned}$$

a contradiction.

Case 2.2. Both w_1 and w_2 have three neighbors of degree 4.

We consider the graph G^* obtained from G by removing all the vertices of P except w and the edges incident with them. Then, $d_{G^*}(w) = 2$ and $d_{G^*}(x) = d_G(x)$ for every $x \in V(G) \setminus V(P)$, where $V(P)$ is the set of all vertices belonging to the path P . In order to complete the discussion of Case 2.2 (and the proof of the lemma), we first prove a claim.

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

Proof of Claim 1. Contrarily, assume that every $y \in V(G^*) \setminus \{w\}$ satisfies $d_G(y) = 4$, that is, $d_{G^*}(y) = 4$. We note that both the graphs G and G^* have the same cyclomatic number, namely, ℓ . Hence, by the Handshaking Lemma, we have

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

If $\ell \leq 5$, then by Equation (2), we have $|V(G^*)| \leq 5$, which 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. Next, we consider the case where $\ell \geq 6$. Then, by Equation (2), we have $|V(G^*)| \geq 6$. Now, we show that for every $\ell (\geq 6)$, there exists at least one connected graph with order ℓ and degree sequence $(\underbrace{4, 4, \dots, 4}_{\ell-1}, 2)$. By Observation 1, the circulant graph $C(\ell - 1; 1, 2)$, with $\ell \geq 6$, is 4-regular. Also, by Lemma 1, $C(\ell - 1; 1, 2)$ is connected. Let $C^*(\ell - 1; 1, 2)$ denote the graph formed from $C(\ell - 1; 1, 2)$ by removing an edge $v_0 v_1$ and adding a new vertex v' together with the edges

$v'v_0$ and $v'v_1$. Certainly, the order and the degree sequence of the graph $C^*(\ell - 1; 1, 2)$ are ℓ and $(\underbrace{4, 4, \dots, 4}_{\ell-1}, 2)$, respectively. Thus, by keeping in mind the above discussion, we have

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

and $m_{2,2}(G) = n - \ell - 2$, where $m_{i,j}(G)$ represents the number of edges of G with end vertices of degrees i and j . Consequently, we have

$$\mathcal{DSO}(G) = (n - \ell - 2)f(2, 2) + (2\ell - 3)f(4, 4) + f(1, 2) + f(2, 3) + 2f(3, 4).$$

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

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

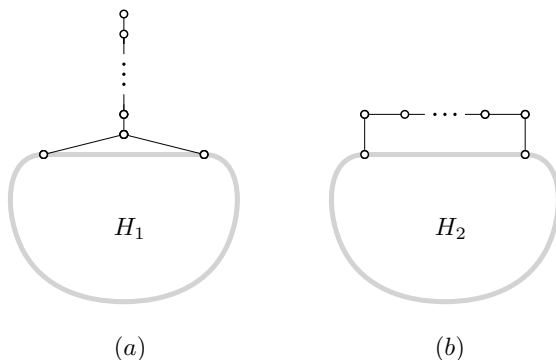


Figure 1. Two graphs used in the proof of Claim 1 of Lemma 2.

Figure 1(a) depicts G (where every vertex in its subgraph H_1 has a degree 4 in G), whereas Figure 1(b) shows the graph $G^\dagger$ (where every vertex in its subgraph H_2 has a degree 3 in $G^\dagger$). Here, we have

$$\mathcal{DSO}(G^\dagger) = (n - 2\ell + 1)f(2, 2) + (3\ell - 4)f(3, 3) + 2f(2, 3).$$

Hence, the difference $\mathcal{DSO}(G) - \mathcal{DSO}(G^\dagger)$ is equal to

$$(\ell - 3)f(2, 2) + (2\ell - 3)f(4, 4) + f(1, 2) - f(2, 3) + 2f(3, 4) - (3\ell - 4)f(3, 3),$$

which (is independent of ℓ because $f(2, 2) = f(3, 3) = f(4, 4)$ and) is positive. This contradicts the definition of G . This completes the proof of Claim 1.

Next, using Claim 1, we discuss several possibilities.

Case 2.2.1. 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 . We form a new graph G_3 using G by deleting the edges w_1w, w_2w , and inserting the edges w_1w_2, wp . Then, we have

$$\begin{aligned} \mathcal{DSO}(G) - \mathcal{DSO}(G_3) &= f(d_G(p_1), 1) - f(d_G(p_1), 2) \\ &\quad + f(2, 3) + 2f(3, 4) - f(2, 2) \\ &\quad - f(2, 2) - f(4, 4) > 0, \end{aligned}$$

a contradiction.

Case 2.2.2. There does not exist any vertex $p \in V(G^*) \setminus \{w\}$ satisfying $d_G(p) = 1$, but there is a vertex $q \in V(G^*) \setminus \{w\}$ such that $d_G(q) = 2$. Since G is connected, we choose q in such a way 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 $d_G(q_1) \geq 3$ and $d_G(q_2) \geq 2$. We form a new graph G_4 using G by deleting the edges w_1w, w_2w , and inserting the edges w_1w_2, wq . Then, we have

$$\begin{aligned} \mathcal{DSO}(G) - \mathcal{DSO}(G_4) &= \sum_{i=1}^2 [f(d_G(q_i), 2) - f(d_G(q_i), 3)] \\ &\quad + 2f(3, 4) - f(2, 2) - f(4, 4) > 0, \end{aligned}$$

a contradiction.

Case 2.2.3. 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 z in such a way that at least one of its neighbors has degree 4 in G . Let z_1, z_2 and z_3 be the neighbors of z such that $d_G(z_1) = 4$, $d_G(z_2) \geq 3$ and $d_G(z_3) \geq 3$.

Case 2.2.3.1. $d_G(z_2) = d_G(z_3) = 4$.

We form a new graph G_5 using G by deleting the edges w_1w, w_2w , and inserting the edges w_1w_2, wz . Then, we have

$$\begin{aligned} \mathcal{DSO}(G) - \mathcal{DSO}(G_5) &= 5f(4, 3) - 4f(4, 4) + f(2, 3) \\ &\quad - f(2, 4) - f(2, 2) > 0, \end{aligned}$$

a contradiction.

Case 2.2.3.2. $\min\{d_G(z_2), d_G(z_3)\} = 3$.

Without loss of generality, we assume that $d_G(z_2) = 3$. Then, either $d_G(z_3) = 3$ or $d_G(z_3) = 4$. Now, we form a new graph G_6 using G by deleting the edges w_1w, w_2w, z_2z , and inserting the edges w_1w_2, wz, z_2u . Then, we have

$$\begin{aligned} \mathcal{DSO}(G) - \mathcal{DSO}(G_6) &= f(1, 2) + 2f(3, 4) + f(3, 3) \\ &\quad - 2f(2, 2) - f(4, 4) - f(2, 3) > 0, \end{aligned}$$

a contradiction. ■

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

$$\mathcal{DSO}(G) \geq \frac{n + \ell - 3}{\sqrt{2}} + \frac{2\sqrt{13}}{5}. \quad (3)$$

If $n = 2(\ell - 1)$, then the equality in (3) holds if and only if G is 3-regular. If $n > 2(\ell - 1)$, then the equality in (3) holds if and only if $\delta(G) = 2$, $\Delta(G) = 3$, $m_{3,3}(G) = 3\ell - 4$, $m_{2,3}(G) = 2$ and $m_{2,2}(G) = n - 2\ell + 1$.

Examples of graphs satisfying the equality in (3) are given in Figure 2.

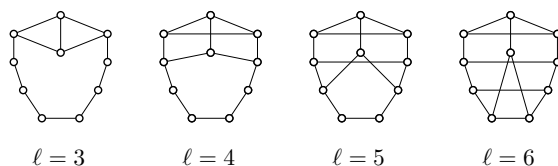


Figure 2. Examples of 10-order graphs satisfying the equality in (3).

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

$$\mathcal{DSO}(G) \geq \mathcal{DSO}(G^*). \quad (4)$$

Also, by Lemma 2, G^* contains no pendent edge incident with a vertex of degree 2; that is, $m_{1,2}(G^*) = 0$. In the rest of the proof, we use the notations $m_{i,j} := m_{i,j}(G^*)$ and

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

where $\mathbb{Z}_+$ represents the set of positive integers. Here, we have

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

which yields

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

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

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

gives

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

By solving (5) and (6) for $m_{2,3}$ and $m_{3,3}$, we obtain

$$m_{2,3} = 2(n - 2\ell - m_{2,2} + 2) + \sum_{(i,j) \in A^*} \left(4 - 6 \left(\frac{1}{i} + \frac{1}{j}\right)\right) m_{i,j} \quad (7)$$

and

$$m_{3,3} = 5(\ell - 1) + m_{2,2} - n + \sum_{(i,j) \in A^*} \left(6 \left(\frac{1}{i} + \frac{1}{j}\right) - 5\right) m_{i,j} \quad (8)$$

Now, using (7) and (8) in the formula of $\mathcal{DSO}(G^*)$, we obtain

$$\begin{aligned} \mathcal{DSO}(G^*) &= \sum_{(i,j) \in A} \frac{\sqrt{i^2 + j^2}}{i + j} m_{i,j} \\ &= \frac{1}{\sqrt{2}}(m_{2,2} + m_{3,3}) + \frac{\sqrt{13}}{5} m_{2,3} + \sum_{(i,j) \in A^*} \frac{\sqrt{i^2 + j^2}}{i + j} m_{i,j} \\ &= \left(\sqrt{2} - \frac{2\sqrt{13}}{5}\right) m_{2,2} + \left(\frac{2\sqrt{13}}{5} - \frac{1}{\sqrt{2}}\right) n + \left(\frac{5}{\sqrt{2}} - \frac{4\sqrt{13}}{5}\right) (\ell - 1) \\ &\quad + \sum_{(i,j) \in A^*} \underbrace{\left[\left(3\sqrt{2} - \frac{6\sqrt{13}}{5}\right) \left(\frac{1}{i} + \frac{1}{j}\right) + \frac{\sqrt{i^2 + j^2}}{i + j} + \frac{4\sqrt{13}}{5} - \frac{5}{\sqrt{2}} \right]}_{h(i,j)} m_{i,j} \\ &\geq \underbrace{\left(\sqrt{2} - \frac{2\sqrt{13}}{5}\right)}_{\text{negative}} m_{2,2} + \left(\frac{2\sqrt{13}}{5} - \frac{1}{\sqrt{2}}\right) n + \left(\frac{5}{\sqrt{2}} - \frac{4\sqrt{13}}{5}\right) (\ell - 1), \end{aligned} \quad (9)$$

where the inequality in (9) follows from Table 1.

Table 1. Approximate values of $h(i, j)$ used in the inequality (9).

(i, j)	(1, 3)	(1, 4)	(2, 4)	(3, 4)	(4, 4)
$h(i, j)$	0.0274	0.0685	0.0312	0.0142	0.0140

Because of the definition of G^* , the inequality in (9) must be equality, which implies that $m_{i,j} = 0$ for every $(i, j) \in A^*$. Hence, we have either $\delta(G^*) = \Delta(G^*) = 3$ or $(\delta(G^*), \Delta(G^*)) = (2, 3)$.

If $n = 2(\ell - 1)$, then we can not have $(\delta(G^*), \Delta(G^*)) = (2, 3)$; for otherwise, we have $n_2(G^*) = n - 2(\ell - 1) = 0$, a contradiction. Hence, if $n = 2(\ell - 1)$, then G^* is a 3-regular graph.

In the rest of the proof, we assume that $n > 2(\ell - 1)$. Then, we can not have $\delta(G^*) = \Delta(G^*) = 3$; for otherwise, we have $3n = 2(n + \ell - 1)$ (by the Handshaking Lemma), a contradiction. Hence, $(\delta(G^*), \Delta(G^*)) = (2, 3)$. Since G^* is connected, it holds that $m_{2,3} > 0$. Hence, from the relation $2m_{2,2} + m_{2,3} = 2n_2$, we conclude that $m_{2,3}$ is a positive even integer. So, $2m_{2,2} + 2 \leq 2m_{2,2} + m_{2,3} = 2n_2 = 2(n - 2(\ell - 1))$, which yields $m_{2,2} \leq n - 2\ell + 1$ with equality if and only if $m_{2,3} = 2$. Consequently, by keeping in mind the definition of G^* , from (9), we have $m_{2,2} = n - 2\ell + 1$, which implies $m_{2,3} = 2$, and hence, $m_{3,3} = 3\ell - 4$. Thus,

$$\begin{aligned} \mathcal{DSO}(G^*) &= \left(\sqrt{2} - \frac{2\sqrt{13}}{5} \right) (n - 2\ell + 1) + \left(\frac{2\sqrt{13}}{5} - \frac{1}{\sqrt{2}} \right) n \\ &\quad + \left(\frac{5}{\sqrt{2}} - \frac{4\sqrt{13}}{5} \right) (\ell - 1), \end{aligned}$$

that is,

$$\mathcal{DSO}(G^*) = \frac{1}{\sqrt{2}}(n + \ell - 3) + \frac{2\sqrt{13}}{5}.$$

Therefore, by (4), the theorem follows. ■

3 Concluding remarks

One of the natural extensions of the present study is to extend Theorem 2 for all fixed-order connected graphs with a given cyclomatic number $\ell \geq 3$. Particularly, if the text “molecular” is replaced with “connected” in Theorem 2, then it is expected that the resulting statement remains valid. To prove this modified statement of Theorem 2, it is enough to prove the corresponding modified statement of Lemma 2 (which is obtained by

replacing the text “molecular” with “connected” there) because we observe that the function $h(i, j)$ used in the inequality (9) remains positive for every $(i, j) \in A^{**}$, where A^{**} is the set obtained from A^* by replacing the constraint $1 \leq i \leq j \leq 4$ with $1 \leq i \leq j$.

Establishing the maximal version of Theorem 2 (for molecular graphs as well as for all connected graphs) is another natural open problem concerning the present study.

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