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Optimizing the Euler-Sombor Index of (Molecular) Tricyclic Graphs

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Abstract

Let G be a graph with edge set $E(G)$. Denote by $d(u)$ the degree of a vertex u in G. The Euler-Sombor index of G is defined as $EU(G) = \sum_{uv\in E(G)} \sqrt{(d(u)+d(v))^2 - d(u)\,d(v)}$. A graph with a maximum degree not more than 4 is known as a molecular graph. By a tricyclic graph of order n, we mean a connected graph of order n and size $n+2$. This paper demonstrates that both the main results of the recent paper [G. O. Kızılırmak, MATCH Commun. Math. Comput. Chem. 94 (2025) 247–262] can be obtained by using the known results. The graphs attaining the optimal values of the Euler-Sombor index among all molecular tricyclic graphs of a given order are also reported.

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1 Introduction

This paper focuses exclusively on connected and simple graphs. For fundamental concepts in graph theory and chemical graph theory, we refer the reader to the standard references [4, 5, 7] and [24, 25], respectively.

In chemical graph theory, real-valued graph invariants are often referred to as topological indices. Using geometric principles, Gutman [9] introduced a novel approach to designing vertex-degree-based topological indices, leading to the definition of the so-called Sombor (SO) index. This index has been one of the most extensively studied topological indices in recent years (2021–2024). Given a graph G, its SO index is denoted by $SO(G)$ and 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 $d(u)$ represents the degree of vertex u (we use $d_G(u)$ to denote the degree of u in G if there is a confusion about the graph under consideration). Some chemical applications of the SO index can be found in [15,21], while its various mathematical properties are summarized in the survey articles [8, 17].

Recently, Gutman, Furtula, and Oz [11] proposed a new geometric technique for constructing vertex-degree-based topological indices and introduced the elliptic-Sombor (ESO) index. This index is defined as

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

The authors of [11] explored the chemical applications of the ESO index and derived several inequalities relating it to other topological indices. They also identified extremal graphs with respect to the ESO index among the classes of the following graphs with fixed orders: (i) trees and (ii) connected graphs. Additional known results about the ESO index can be found in [3, 6, 18–20, 23].

Another topological index developed using the methodology outlined in [11] is the Euler-Sombor index. This index is based on Euler's approximation formula for the perimeter of an ellipse. The Euler-Sombor index of a graph G is denoted by $EU(G)$ and is defined [10, 22] as

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

According to Ivan Gutman[†], among the topological indices that can be derived from perimeter approximation formulas of an ellipse, the Euler-Sombor index may be the most significant one. The existing mathematical findings on this index can be found in [3, 10, 12, 14, 22].

By a tricyclic graph of order n, we mean a connected graph of order n and size $n+2$. A graph of a maximum degree not larger than 4 is called a molecular graph. The present study is motivated by the recent paper [14], where the problem of characterizing graphs attaining the minimum and maximum values of the Euler-Sombor index among all tricyclic graphs of a given order was addressed. In this paper, we prove that both the main results of [14] can be obtained by using existing results. These existing results belong to the papers [2, 13, 16]. Since the obtained tricyclic graph attaining the minimum Euler-Sombor index has a maximum degree 3, this graph also minimizes the Euler-Sombor index among all tricyclic molecular graphs of a given order. For obtaining the maximum Euler-Sombor index of tricyclic molecular graphs of a given order, we utilize a result reported in [1].

2 Results

We start this section with the following lemma:

Lemma 1. *Define a function Ψ by $\Psi(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + x_1 x_2}$ for $x_1 \geq 0$ and $x_2 \geq 0$ such that $(x_1, x_2) \neq (0, 0)$. The function Ψ and its partial derivative function Ψ_{x_i} with respect to x_i are strictly increasing in x_i for $i = 1, 2$.*

[†] personal communication with Akbar Ali (on December 20, 2023)

Denote by $m_{i,j}$ the number of those edges of a graph G whose one endvertex has degree i and the other endvertex has degree j. By a k-cyclic graph, we mean a connected graph of order n and size $n+k-1$. Particularly, a 3-cyclic graph is also known as a tricyclic graph. The set of all different elements of the degree sequence of a graph G is called the degree set of G.

Now, we recall a known result established by Liu et al. [16].

Lemma 2. [16] *Let Ψ be a real-valued symmetric function defined on the Cartesian square of the set of all nonnegative real numbers such that the following three conditions hold:*

(i). *The function Ψ is increasing in either of its two variables.*

(ii). *The function f is strictly decreasing, where $f(x) = \Psi(a_1, x) - \Psi(a_2, x)$ with $x \geq 1$, and a_1, a_2, are fixed real numbers satisfying $a_1 > a_2 \geq 0$.*

(iii). *If $a > b + 1 \geq 2$, then the inequality*

$$a[\Psi(a, a) - \Psi(a - 1, a)] - b[\Psi(b + 1, b) - \Psi(b, b)] > 0$$

holds.

Then, in the class of all k-cyclic graphs of order n, only the graph(s) having the degree set $\{2, 3\}$ such that $m_{2,2} = n - 2k + 1$, $m_{2,3} = 2$ and $m_{3,3} = 3k - 4$, attain(s) the minimum value of the topological index $\sum_{uv \in E(G)} \Psi(d(u), d(v))$, where $n \geq 5(k - 1)$ and $k \geq 3$.

The following corollary (which covers the first main result of [14] for $n \geq 10$) follows from Lemma 2.

Corollary 1. *In the class of all k-cyclic graphs of order n, only the graph(s) having the degree set $\{2, 3\}$ such that $m_{2,2} = n - 2k + 1$, $m_{2,3} = 2$ and $m_{3,3} = 3k - 4$, attain(s) the minimum value of the Euler-Sombor index, where $n \geq 5(k - 1)$ and $k \geq 3$. Particularly, among all tricyclic graphs of order n, the graph $G^{\star}$ (depicted in Figure 1) uniquely attains the minimum value of the Euler-Sombor index for $n \geq 10$.*

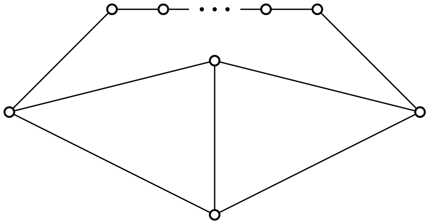

Figure 1. The tricyclic graph $G^\star$.

Proof. Let $\Psi(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + x_1x_2}$ with $x_1 \geq 0$ and $x_2 \geq 0$. We show that all three conditions of Lemma 2 hold for Ψ. Condition (i) follows from Lemma 1. To discuss condition (ii), for $x_1 > 0$ and $x_2 > 0$, we note that

$$\frac{\partial^2}{\partial x_1 \partial x_2}\Psi(x_1, x_2) = \frac{\partial^2}{\partial x_2 \partial x_1}\Psi(x_1, x_2) = -\frac{3x_1x_2}{4(x_1^2 + x_1x_2 + x_2^2)^{3/2}} < 0.$$

Thus, for $a_1 > a_2 > 0$, the derivative of the function f defined as $f(x) = \Psi(a_1, x) - \Psi(a_2, x)$ is strictly decreasing for $x \geq 1$. Also, if $a_1 > a_2 = 0$ and $x \geq 1$, then

$$f'(x) = \frac{2x + a_1}{2\sqrt{x^2 + a_1x + a_1^2}} - 1 < 0.$$

Next, we discuss condition (iii) of Lemma 2. For $a > b + 1 \geq 2$, we have

$$\begin{aligned} a[\Psi(a, a) - \Psi(a-1, a)] &> (b+1)[\Psi(b+1, b+1) - \Psi(b, b+1)] \\ &> b[\Psi(b+1, b) - \Psi(b, b)] \end{aligned}$$

and hence $a[\Psi(a, a) - \Psi(a-1, a)] - b[\Psi(b+1, b) - \Psi(b, b)] > 0$.

Consequently, the conclusion of the corollary follows from Lemma 2. ■

Remark. If we replace the text "graphs" with "molecular graphs" in the statement of Corollary 1, then the modified statement remains valid.

We note here that Corollary 1 does not provide graphs attaining the minimum Euler-Sombor index among all k-cyclic graphs of order n for

$n < 5(k-1)$. Next, we focus our attention on extending Corollary 1 by relaxing the condition $n \geq 5(k-1)$ to $n > 2(k-1)$. For this, we need some preparation first.

Lemma 3. [16] *Let Ψ be the function defined in Lemma 2 satisfying the three conditions listed there. Let G be a graph minimizing the topological index $\sum_{uv \in E(G)} \Psi(d(u), d(v))$ among all k-cyclic graphs of order n. Then, the difference between the maximum and minimum degrees of G is at most 1. If, in addition, $k \geq 1$ then the minimum degree of G is at least 2.*

In the proof of Corollary 1, we have verified all three conditions of Lemma 2 for $\Psi(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + x_1 x_2}$. Hence, we have the next result by Lemma 3.

Corollary 2. *Let G be a graph minimizing the Euler Sombor index among all k-cyclic graphs of order n. Then, the difference between the maximum and minimum degrees of G is at most 1. If, in addition, $k \geq 1$ then the minimum degree of G is at least 2.*

For a graph G, let $n_i = |\{v \in V(G) : d(v) = i\}|$.

Lemma 4. *For an integer k greater than 1, let G be a graph minimizing the Euler-Sombor index among all k-cyclic graphs of order n, where $n \geq 4$ if $k = 2$ and $n \geq 2(k-1)$ if $k \geq 3$. Then, the maximum degree of G is 3.*

Proof. Let δ and Δ be the minimum degree and maximum degree of G, respectively. From the assumption $k \geq 2$ and the fact that G is connected, it follows that $\Delta \geq 3$. Also, by Corollary 2, we have $\delta \geq 2$. Contrarily, assume that $\Delta \geq 4$. Since $k = |E(G)| - n + 1$, we have $n \geq 2(|E(G)| - n)$, which implies that

$$n_2 + \sum_{i=3}^{\Delta} n_i \geq 2\left(\frac{1}{2}\sum_{i=3}^{\Delta} i n_i - \sum_{i=3}^{\Delta} n_i\right)$$

which gives

$$n_2 \geq \sum_{i=4}^{\Delta} (i-3) n_i > 0.$$

Hence, $\delta = 2$, which gives $\Delta - \delta \geq 2$, a contradiction to Corollary 2. ■

Lemma 5. [16] *Let* Ψ *be the function defined in Lemma* 2 *satisfying the first two conditions listed there. Let* G *be a connected graph. Let* u, x, v, y *be distinct vertices of* G *such that* $ux, vy \in E(G)$ *and* $uy, vx \notin E(G)$*, provided that* $d_G(u) \geq d_G(v)$ *and* $d_G(y) \geq d_G(x)$*. If* G' *is the graph obtained from* G *by removing the edges* ux, vy *and adding the edges* uy, vx*, then*

$$\sum_{ab \in E(G)} \Psi(d_G(a), d_G(b)) \geq \sum_{ab \in E(G')} \Psi(d_{G'}(a), d_{G'}(b))$$

with equality if and only if either $d_G(u) = d_G(v)$ *or* $d_G(y) = d_G(x)$*.*

In the proof of Corollary 1, we have verified the first two conditions of Lemma 2 for $\Psi(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + x_1 x_2}$. Hence, we have the next result by Lemma 5.

Corollary 3. *For the graphs* G *and* G' *defined in Lemma* 5*, it holds that* $EU(G) \geq EU(G')$ *with equality if and only if either* $d_G(u) = d_G(v)$ *or* $d_G(y) = d_G(x)$*.*

Lemma 6. *For an integer* k *greater than* 1*, let* G *be a graph minimizing the Euler-Sombor index among all* k*-cyclic graphs of order* n*, where* $n \geq 4$ *if* $k = 2$ *and* $n > 2(k-1)$ *if* $k \geq 3$*. Then,* $m_{2,3} = 2$*.*

Proof. By Corollary 2 and Lemma 4, the minimum degree of G is at least 2 and its maximum degree is 3. Since $n_2+n_3 = n$ and $2n_2+3n_3 = 2(n+k-1)$, we have $n_2 = n - 2(k-1) > 0$, which implies that the minimum degree of G is 2. Hence, $m_{2,3} > 0$ because G is connected. Also, we note that $2m_{2,2}+m_{2,3} = 2n_2$, which confirms that $m_{2,3}$ is even, and hence $m_{2,3} \geq 2$. Contrarily, assume that $m_{2,3} \geq 4$. Then, G contains distinct vertices u, x, v, y such that $ux, vy \in E(G)$, $uy, vx \notin E(G)$, provided that $d_G(u) = 3, d_G(v) = 2$, $d_G(y) = 3$, $d_G(x) = 2$, and the graph G' obtained from G by removing the edges ux, vy and adding the edges uy, vx is connected. Then, by Corollary 3, we have $EU(G) > EU(G')$, a contradiction. ∎

Now, we are in a position to obtain an extended version of Corollary 1. Particularly, by Corollary 2, Lemma 4 and Lemma 6, we have the next result, which covers Theorem 1 of [14].

Theorem 1. *In the class of all k-cyclic graphs of order n, only the graph(s) having the degree set $\{2, 3\}$ such that $m_{2,2} = n - 2k + 1$, $m_{2,3} = 2$ and $m_{3,3} = 3k - 4$, attain(s) the minimum value of the Euler-Sombor index, where $n > 2(k - 1)$ for $k \geq 3$ and $n \geq 4$ for $k = 2$.*

Now, we focus on maximizing the Euler-Somber index of k-cyclic graphs of a given order. The next result is obtained by utilizing Lemma 2.1 of [2] and Lemma 1. This result also follows from Theorem 1.6 of [13] and Lemma 1.

Lemma 7. *If G is a graph maximizing the Euler-Sombor index among all k-cyclic graphs of order n, then the maximum degree of G is $n - 1$.*

Let $H_{n,i}$ be the graph of order n formed by inserting i edges in the star graph S_n of order n between a fixed vertex of degree one and i other vertices of degree one, where $n \geq 5$ and $i \in \{2, 3\}$. Denote by $H_{n,1}$ the unique 1-cyclic graph of order n and maximum degree $n - 1$, where $n \geq 4$. There are only two 2-cyclic graphs of order n and maximum degree $n - 1$; one of them is $H_{n,2}$ and the other, say J_n, is obtained from S_n by adding two non-adjacent edges. But, $EU(H_{n,2}) > EU(J_n)$. Hence, Lemma 7 provides the following:

Corollary 4. *The star graph uniquely maximizes the Euler-Sombor index among all trees of order n for $n \geq 4$. Also, $H_{n,k}$ uniquely maximizes the Euler-Sombor index among all k-cyclic graphs of order n, where $n \geq k + 3$ and $k \in \{1, 2\}$.*

Next, by using Lemma 7, we prove the second main result of [14].

Theorem 2. *The graph $H_{n,3}$ (depicted in Figure 2) uniquely maximizes the Euler-Sombor index among all tricyclic graphs of order n for $n \geq 5$.*

Proof. Because of Lemma 7, it is sufficient to consider all tricyclic graphs of order n with maximum degree $n - 1$. All such graphs, namely, G_1, G_2, G_3, G_4 and $H_{n,3}$, are shown in Figure 2. The Euler-Sombor indices of the graphs G_1, G_2, G_3, G_4, $H_{n,3}$, are given as follows, respectively:

$$(n-7)\sqrt{n^2-n+1} + 6\sqrt{n^2+3} + 6\sqrt{3},$$

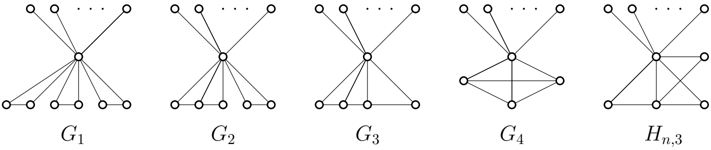

Figure 2. All tricyclic graphs of order n and maximum degree $n-1$.

$$(n-6)\sqrt{n^2-n+1}+4\sqrt{n^2+3}+\sqrt{n^2+n+7}+2\sqrt{19}+2\sqrt{3},$$

$$(n-5)\sqrt{n^2-n+1}+2\sqrt{n^2+3}+2\sqrt{n^2+n+7}+2\sqrt{19}+3\sqrt{3},$$

$$(n-4)\sqrt{n^2-n+1}+3\sqrt{n^2+n+7}+9\sqrt{3},$$

$$(n-5)\sqrt{n^2-n+1}+3\sqrt{n^2+3}+\sqrt{n^2+2n+13}+6\sqrt{7}.$$

After comparing each of the first four expressions with the last one, we conclude that $EU(G_i) < EU(H_{n,3})$ for every $i \in \{1,2,3,4\}$. ■

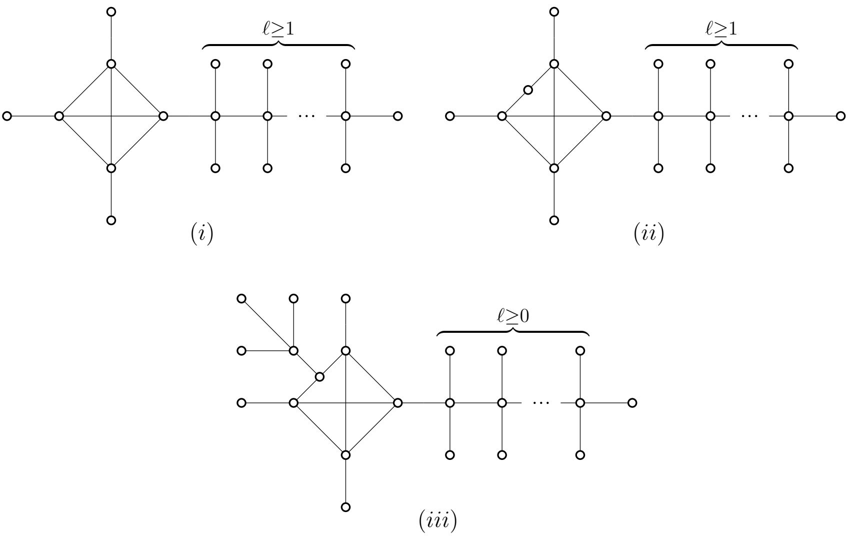

Figure 3. Examples of extremal graphs mentioned in Theorem 3.

We end this paper by reporting a result concerning the maximum Euler-Sombor index of tricyclic molecular graphs, which follows from Theorem 2 of [1].

Theorem 3. *Among all tricyclic molecular graphs of order n with $n \geq 11$,*

(i) only the graph(s) containing no vertices of degrees 2 and 3 maximize(s) the Euler-Sombor index, when $n \equiv 2 \pmod 3$;

(ii) only the graph(s) containing no vertex of degree 3 and possessing exactly one vertex of degree 2, which is adjacent to two vertices of degree 4, maximize(s) the Euler-Sombor index, when $n \equiv 0 \pmod 3$.

(iii) only the graph(s) containing no vertex of degree 2 and possessing exactly one vertex of degree 3, which is adjacent to three vertices of degree 4, maximize(s) the Euler-Sombor index, when $n \equiv 1 \pmod 3$.

An example of the extremal graphs mentioned in each of the three parts is given in Figure 3.

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