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Extremal Unicyclic Graphs for the Euler Sombor Index

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Abstract

The Euler Sombor index of a graph G is a recently introduced topological index, defined as

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

where $d(u)$, $d(v)$ are the degrees of the vertices u, respectively v of G. The purpose of this paper is to determine the first, second and third minimal and maximal unicyclic graphs of order n with respect to the Euler Sombor index for all $n \geq 5$.

1 Introduction

Following standard notations in graph theory [1], let $G = (V(G), E(G))$ be a simple, undirected, and connected graph with $V(G)$ the set of its vertices

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and $E(G)$ the set of its edges. Let $u \in V(G)$ be a vertex and denote by $N_G(u)$ the set of its neighbors and by $d(u)$ its degree. If a vertex has degree equal to one, we say that it is pendent. We use the notation C_r for a cycle with r edges. The path $[x_1, x_2, ..., x_k]$ with $d(x_1) \geq 2$ and $d(x_i) = 2$ for all $1 < i < k$ is called pendent if $d(x_k) = 1$ and internal if $d(x_k) \geq 2$. Moreover, where there is no danger of confusion, the notation $P_{x_1 x_k}$ is used.

The Euler Sombor index given by

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

first alluded to in [5], and fully introduced in [4], is the most recently defined topological index based on a novel geometric approach proposed by I. Gutman [3] and intensely studied in recent years [9]. This approach produces an increasing set of graph invariants, collectively known as the Sombor topological indices, which includes the Sombor index, the reduced Sombor index and the average Sombor index, the elliptic Sombor index and the newly introduced Euler Sombor index, with great applicability in mathematical chemistry [3–5].

Recent research established several properties of the elliptic Sombor index and its generalization [2, 10–12], and of the Euler Sombor index [4, 6, 8, 13]. Due to the high correlation with previous well-known indices, the Euler Sombor index was shown to be useful for predicting physicochemical properties of substances [13].

In this paper, we extend the study of the Euler Sombor index by determining the top three minimal and maximal unicyclic graphs of order n for all $n \geq 5$.

2 Maximal unicyclic graphs with respect to the Euler Sombor index

In what follows, we denote by $\mathcal{U}_n$ the set of unicyclic graphs of order n, by $\mathcal{U}_{n,p}$ the set of unicyclic graphs of order n with a cycle of length p and by

$\tilde{\mathcal{U}}_{n,p}$ the subset of $\mathcal{U}_{n,p}$ that contains unicyclic graphs in which any edge that does not belong to the cycle is pendent.

First, we introduce the next result, given in a particular form in [8]:

Lemma 1. *[13] Let G be a simple, connected graph and a path $P_{x_1x_k} = [x_1, x_2, ..., x_k]$ with $k \geq 2$, $d(x_1) \geq 2$, $d(x_k) \geq 2$, $d(x_i) = 2$ for $1 < i < k$. Let G' the graph obtained by transforming the internal path $P_{x_1x_k}$ into a pendent path: $G' = G - \{x_k y \mid y \neq x_{k-1}\} + \{x_1 y \mid y \in N_G(x_k) - \{x_{k-1}\}\}$ (Fig. 1). Then $EU(G') > EU(G)$.*

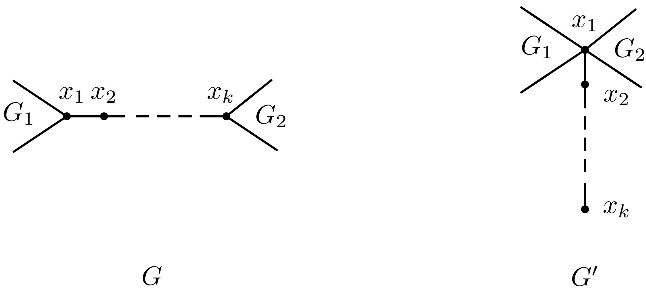


Figure 1. Transforming an internal path into a pendent path

Remark. Let $U \in \mathcal{U}_{n,p}$ be a unicyclic graph. By applying $p-3$ times the transformation from Lemma 1 for any edge situated on the graph's cycle, we obtain a graph $U' \in \mathcal{U}_{n,3}$, where every cycle's vertex is incident to a (possibly empty) tree. Furthermore, by applying the same transformation to every internal edge of these trees, we obtain a new graph $U'' \in \tilde{\mathcal{U}}_{n,3}$ where every cycle's vertex is the center of a (possibly empty) star tree. According to Lemma 1, $EU(U'') \geq EU(U)$ with equality if and only if $U \in \tilde{\mathcal{U}}_{n,3}$ (meaning that no transformation was applied to U).

The next lemma gathers some technical results that will be used repeatedly throughout this section.

Lemma 2. *(i) $x < \sqrt{x^2 + a} < x + \frac{a}{2x}$ for all $x > 0$, $a > 0$.*

(ii) Let $N > 0$, $D_1 = D_2 = [0, N]$, $D_3 = (0, N)$ and $f_i : D_i \to \mathbb{R}$ for $1 \leq i \leq 3$ given by $f_1(x) = N^2 - x(N-x)$, $f_2(x) = x^2 + (N-x)^2$,

$f_3(x) = \frac{1}{x(N-x)}$. *Then, for* $1 \le i \le 3$, f_i *strictly decreases in* $D_i \cap [0, \frac{N}{2}]$, *strictly increases in* $D_i \cap [\frac{N}{2}, N]$ *and is symmetric around* $N/2$ *in the sense that* $f_i(x) = f_i(N-x)$ *for all* $x \in D_i$.

(*iii*) *Let* $\alpha \ge 0$ *and* $x_i \ge \alpha$ *for* $1 \le i \le 3$. *Then* $\sum_{i=1}^{3} x_i^2 \le (x_1 + x_2 + x_3 - \alpha)^2 - \alpha^2$ *with equality if and only if* $x_i = \alpha$ *for* $1 \le i \le 3$.

Proof. (i) Obvious by squaring. For (ii) the monotonicity follows by establishing the sign of the derivative of f_1, f_2, and $x \to x(N-x)$, respectively, and the symmetry follows by direct checking. For (iii) observe that $(x_1+x_2+x_3-\alpha)^2-\alpha^2 = \sum_{i=1}^{3} x_i^2+2\big[x_1(x_2-\alpha)+x_2(x_3-\alpha)+x_3(x_1-\alpha)\big]$. ■

Before we give the following lemma, we note that any graph U in $\tilde{\mathcal{U}}_{n,3}$ is completely characterized by a triplet of whole numbers (p_1, p_2, p_3) with $0 \le p_1 \le p_2 \le p_3$ and $p_1 + p_2 + p_3 = n - 3$ representing the number of pendents at each vertex of the length three cycle of U. We denote such a graph by U_{p_1,p_2,p_3}.

Lemma 3. *If* $n \ge 7$, *then the first, second and third greatest graphs in* $\tilde{\mathcal{U}}_{n,3}$ *with respect to the EU index are* $U_{0,0,n-3}$, $U_{0,1,n-4}$, *and respectively* $U_{0,2,n-5}$.

Proof. A direct computation gives
$EU(U_{0,0,n-3}) = (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + 2\sqrt{3}$,
$EU(U_{0,1,n-4}) = (n-4)\sqrt{n^2-3n+3} + \sqrt{n^2-n+7} + \sqrt{n^2-2n+4} + \sqrt{13} + \sqrt{19}$, and
$EU(U_{0,2,n-5}) = (n-5)\sqrt{n^2-5n+7} + \sqrt{n^2-2n+13} + \sqrt{n^2-4n+7} + 2\sqrt{7} + 2\sqrt{21}$.

Applying Lemma 2 (i) to each non-constant square root term of each equality we have

$$EU(U_{0,0,n-3}) > (n-3)(n-\frac{1}{2}) + 2n + 2\sqrt{3} > n^2 - \frac{3}{2}n + 4.96, \tag{1}$$

$$EU(U_{0,1,n-4}) > (n-4)(n-\frac{3}{2}) + 2n - \frac{3}{2} + \sqrt{13} + \sqrt{19} > n^2 - \frac{7}{2}n + 12.46, \tag{2}$$

$$EU(U_{0,2,n-5}) > (n-5)(n-\frac{5}{2}) + 2n - 3 + \sqrt{28} + \sqrt{84} > n^2 - \frac{11}{2}n + 23.95, \tag{3}$$

and

$$
\begin{aligned}
EU(U_{0,1,n-4}) <&(n-4)\Big(n-\frac{3}{2}+\frac{3}{4(2n-3)}\Big)+\Big(n-\frac{1}{2}+\frac{27}{4(2n-1)}\Big)+\\
&\Big(n-1+\frac{3}{2(n-1)}\Big)+\sqrt{13}+\sqrt{19}\\
&\approx n^2-\frac{7}{2}n+\frac{3(n-4)}{8(n-\frac{3}{2})}+\frac{27}{4(2n-1)}+\frac{3}{2(n-1)}+12.464\\
&< n^2-\frac{7}{2}n+13.62,
\end{aligned}
\tag{4}
$$

$$
\begin{aligned}
EU(U_{0,2,n-5}) <&(n-5)\Big(n-\frac{5}{2}+\frac{3}{4(2n-5)}\Big)+\Big(n-1+\frac{12}{2(n-1)}\Big)+\\
&\Big(n-2+\frac{3}{2(n-2)}\Big)+\sqrt{28}+\sqrt{84}\\
&< n^2-\frac{11}{2}n+\frac{3(n-5)}{8(n-\frac{5}{2})}+\frac{6}{n-1}+\frac{3}{2(n-2)}+23.956\\
&< n^2-\frac{11}{2}n+25.64
\end{aligned}
\tag{5}
$$

for all $n \geq 7$.

Since $n^2-\frac{7}{2}n+13.62 < n^2-\frac{3}{2}n+4.96$ for all $n \geq 7$, by using inequalities (1) and (4) we have that $EU(U_{0,0,n-3}) > EU(U_{0,1,n-4})$. Similarly, since $n^2-\frac{11}{2}n+25.64 < n^2-\frac{7}{2}n+12.46$ for all $n \geq 7$, by using inequalities (2) and (5) we have that $EU(U_{0,1,n-4}) > EU(U_{0,2,n-5})$. It remains to be proven that $EU(U_{0,p_2,p_3}) < EU(U_{0,2,n-5})$ for all $3 \leq p_2 \leq p_3$ with $p_2+p_3 = n-3$ and $EU(U_{p_1,p_2,p_3}) < EU(U_{0,2,n-5})$ for all $1 \leq p_1 \leq p_2 \leq p_3$ with $p_1+p_2+p_3 = n-3$.

We first proceed with the former inequality. By a direct computation

$$
\begin{aligned}
EU(U_{0,p_2,p_3}) =& \sum_{i=2}^{3} p_i\sqrt{p_i^2+5p_i+7}+\sum_{i=2}^{3}\sqrt{p_i^2+6p_i+12}\ +\\
&\sqrt{(n+1)^2-(p_2+2)\big[(n+1)-(p_2+2)\big]}
\end{aligned}
$$

Observe that $3 \leq p_2 \leq p_3$ and $p_2+p_3 = n-3$ imply $3 \leq p_2 \leq \frac{n-3}{2}$, $\frac{n-3}{2} \leq p_3 \leq n-6$ and $n \geq 9$. We apply Lemma 2 (i) to each term in each sum. For the last term we need Lemma 2 (ii) for f_1 with $N = n+1$ and

$x = p_2 + 2$. Noting that $5 \le p_2 + 2 \le \frac{n-3}{2} + 2 = \frac{N}{2}$ we have

$$\begin{aligned} EU(U_{0,p_2,p_3}) <& \sum_{i=2}^{3} p_i\Big(p_i + \frac{5}{2} + \frac{3}{4(2p_i+5)}\Big) + \sum_{i=2}^{3}\Big(p_i + 3 + \frac{3}{2(p_i+3)}\Big) + \\ & \sqrt{n^2 - 3n + 21} \\ &= p_2^2 + \big[(n-3) - p_2\big]^2 + \frac{7}{2}n - \frac{9}{2} + \sqrt{n^2 - 3n + 21} + \\ & \frac{3}{8}\sum_{i=2}^{3}\frac{p_i}{p_i + \frac{5}{2}} + \frac{3}{2}\cdot\frac{n+3}{(p_2+3)\big[(n+3)-(p_2+3)\big]} \end{aligned}$$

Next, we apply Lemma 2 (ii) for f_2 with $N = n-3$ and $x = p_2$ to the first two terms, for f_3 with $N = n+3$ and $x = p_2 + 3$ to the last term, and Lemma 2 (i) to the square root term. Keeping into account that $p_2 \ge 3$ we get

$$\begin{aligned} EU(U_{0,p_2,p_3}) <&(n-6)^2 + \frac{9}{2}n + 3 + \frac{75}{4(2n-3)} + 2\cdot\frac{3}{8} + \frac{n+3}{4(n-3)} \\ &= n^2 - \frac{15}{2}n + 40 + \frac{75}{4(2n-3)} + \frac{6}{4(n-3)} \\ &< n^2 - \frac{15}{2}n + 41.51, \end{aligned}$$

knowing that $n \ge 9$.

Since $n^2 - \frac{15}{2}n + 41.51 < n^2 - \frac{11}{2}n + 23.95$ for all $n \ge 9$, by using (3) the inequality follows.

Finally, we prove that for all $1 \le p_1 \le p_2 \le p_3$ with $p_1 + p_2 + p_3 = n-3$ $EU(U_{p_1,p_2,p_3}) < EU(U_{0,2,n-5})$. We distinguish two cases.

Case 1. $p_1 = 1$. A direct computation gives

$$\begin{aligned} EU(U_{1,p_2,p_3}) =& \sum_{i=2}^{3} p_i\sqrt{p_i^2 + 5p_i + 7} + \sum_{i=2}^{3}\sqrt{p_i^2 + 7p_i + 19} + \\ & \sqrt{n^2 - (p_2+2)\big[n - (p_2+2)\big]} + \sqrt{13}\,. \end{aligned}$$

By applying Lemma 2 (i) to each square root term in each sum and Lemma 2 (ii) for f_1 to the second to last term, and remembering that $p_2 \ge 2$ we have

$$
\begin{aligned}
EU(U_{1,p_2,p_3}) <& \sum_{i=2}^{3} p_i\Big(p_i+\frac{5}{2}+\frac{3}{4(2p_i+5)}\Big)+\sum_{i=2}^{3}\Big(p_i+\frac{7}{2}+\frac{27}{4(2p_i+7)}\Big)\\
&+\sqrt{n^2-3n+9}+\sqrt{13}\\
&=p_2^2+\big[(n-4)-p_2\big]^2+\frac{7}{2}n-7+\sqrt{\Big(n-\frac{3}{2}\Big)^2+\frac{27}{4}}+\\
&\frac{3}{8}\sum_{i=2}^{3}\frac{p_i}{p_i+\frac{5}{2}}+\frac{27}{4}\cdot\frac{2n+6}{(2p_2+7)\big[(2n+6)-(2p_2+7)\big]}+\sqrt{13}
\end{aligned}
$$

Next, we apply Lemma 2 (ii) for f_2 to the first two terms and for f_3 with $N=2n+6$ and $x=2p_2+7$ to the second to last term. Using Lemma 2 (i) for the non-constant square root term, and keeping into account that $p_2 \geq 1$ we get

$$
\begin{aligned}
EU(U_{1,p_2,p_3}) <&(n-5)^2+\frac{9}{2}n-\frac{15}{2}+\frac{27}{4(2n-3)}+2\cdot\frac{3}{8}+\frac{3(n+3)}{2(2n-3)}+\sqrt{13}\\
&=n^2-\frac{11}{2}n+19+\sqrt{13}+2\cdot\frac{27}{4(2n-3)}\\
&<n^2-\frac{11}{2}n+23.84,
\end{aligned}
$$

for all $n \geq 7$. By using (3) the inequality follows.

Case 2. $2 \leq p_1 \leq p_2 \leq p_3$.

Since $p_1+p_2+p_3=n-3$, $p_i \leq n-7$ for $1 \leq i \leq 3$ and $n \geq 9$. By direct computation

$$
\begin{aligned}
EU(U_{p_1,p_2,p_3}) =& \sum_{1\leq i<j\leq 3}\sqrt{(p_i+p_j+4)^2-(p_i+2)(p_j+2)}+\\
&\sum_{i=1}^{3} p_i\sqrt{p_i^2+5p_i+7}\,.
\end{aligned}
$$

Observe that in the first sum the term under the square root can be written as $(n+1-p_k)^2-(p_i+2)\big[(n+1-p_k)-(p_i+2)\big]$ where k is such that $\{i,j,k\}=\{1,2,3\}$. By applying Lemma 2 (ii) for f_1 with $N=n+1-p_k$ and $x=p_i+2$ to this expression together with Lemma 2 (i) to the term of the second sum we have

$$EU(U_{p_1,p_2,p_3}) < \sum_{k=1}^{3} \sqrt{(n+1-p_k)^2 - 4(n+1-p_k) + 16} + \sum_{i=1}^{3} p_i\Big(p_i + \frac{5}{2} + \frac{3}{4(2p_i+5)}\Big) \tag{6}$$

Denoting by S_1 the first sum of (6) and applying Lemma 2 (i) to each of its terms we get

$$S_1 < \sum_{k=1}^{3} \Big(n - 1 - p_k + \frac{6}{n-1-p_k}\Big) = 2n + \sum_{k=1}^{3} \frac{6}{n-1-p_k} \leq 2n+3, \tag{7}$$

since $p_k \leq n-7$ for $1 \leq k \leq 3$. Denoting by S_2 the second sum of (6), applying Lemma 2 (iii) and using $p_i \geq 2$ for $1 \leq i \leq 3$ we have

$$S_2 \leq (n-5)^2 - 2^2 + \frac{5}{2}(n-3) + \frac{9}{4} = n^2 - \frac{15}{2}n + 14.625 \tag{8}$$

Combining (6)–(8) gives $EU(U_{p_1,p_2,p_3}) < n^2 - \frac{11}{2}n + 17.625$. This, together with (3) concludes the proof. ∎

The next notion is useful in what follows.

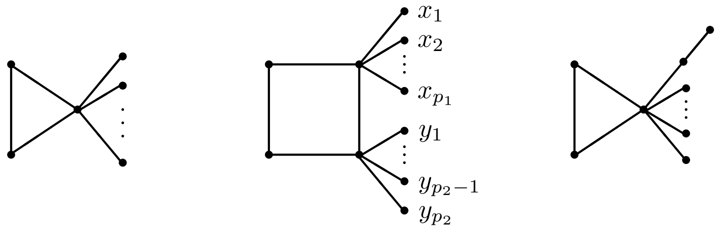
Definition 1. Let G and G' be two graphs of order n. If G' can be obtained by applying the transform given in Lemma 1 once to G, we say that G is a direct ascendant of G'. If the minimum number of times needed to apply the transform to G in order to obtain G' is greater than 1, we say that G is an indirect ascendant of G'.

Before we give the next lemmas, we need the following examples.

Example 1. $U_{0,0,n-3}$ has two (families of) direct ascendants:

1. the family of graphs obtained by choosing an edge uv of C_4 and attaching p_1 pendents to u and p_2 pendents to v such that $0 \leq p_1 \leq p_2$ and $p_1 + p_2 = n-4$; since p_2 is completely determined by p_1, we denote it $U^{\mathrm{I}}_{0,0,n-3}(p_1)$

2. the single graph obtained by attaching $n-5$ pendents and a path of length 2 to one vertex of C_3; denote it $U^{\mathrm{II}}_{0,0,n-3}$.

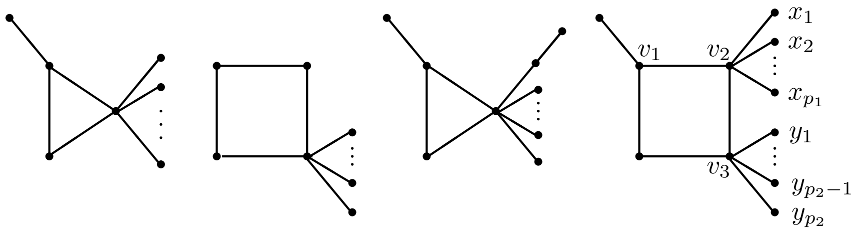


$U_{0,0,n-3}$ $\quad$ $U^{\mathrm{I}}_{0,0,n-3}(p_1)$ $\quad$ $U^{\mathrm{II}}_{0,0,n-3}$

Figure 2. The graphs from Example 1

Example 2. $U_{0,1,n-4}$ has three (families of) direct ascendants:

1. the single graph $U^{\mathrm{I}}_{0,0,n-3}(0)$
2. the single graph obtained by choosing and edge uv of C_3 and attaching one pendent to u and to v a path of length 2 and $n-6$ pendents; denote it $U^{\mathrm{II}}_{0,1,n-4}$
3. the family of graphs obtained by choosing a path (v_1, v_2, v_3) of C_4 and attaching one pendent to v_1, $p_1 \geq 0$ pendents to v_2 and $p_2 \geq 0$ pendents to v_3 such that $p_1 + p_2 = n - 5$; denote it $U^{\mathrm{III}}_{0,1,n-4}(p_1, p_2)$.



$U_{0,1,n-4}$ $\quad$ $U^{\mathrm{I}}_{0,0,n-3}(0)$ $\quad$ $U^{\mathrm{II}}_{0,1,n-4}$ $\quad$ $U^{\mathrm{III}}_{0,0,n-4}(p_1, p_2)$

Figure 3. The graphs from Example 2

Lemma 4. *Denote by* $M_n = \max\left\{EU\left(U^{\mathrm{II}}_{0,0,n-3}\right), EU\left(U_{0,2,n-5}\right)\right\}$. *If* $n \geq 7$ *then* $M_n < EU\left(U^{\mathrm{I}}_{0,0,n-3}(0)\right) < EU\left(U_{0,1,n-4}\right)$.

Proof. By direct computation

$$EU\left(U^{\mathrm{I}}_{0,0,n-3}(0)\right) = (n-4)\sqrt{n^2-3n+3} + 2\sqrt{n^2-2n+4} + 2\sqrt{12},$$

$$EU\left(U^{\mathrm{II}}_{0,0,n-3}\right) = (n-5)\sqrt{n^2-3n+3} + 3\sqrt{n^2-2n+4} + \sqrt{7} + \sqrt{12}$$

and

$$\begin{aligned} EU\left(U^{\mathrm{I}}_{0,0,n-3}(0)\right) - EU\left(U^{\mathrm{II}}_{0,0,n-3}\right) =& \sqrt{n^2-3n+3} - \sqrt{n^2-2n+4} + \\ & \sqrt{12} - \sqrt{7}. \end{aligned}$$

Since

$$\begin{aligned} \sqrt{n^2-3n+3} - \sqrt{n^2-2n+4} &= -\frac{n+1}{\sqrt{n^2-3n+3} + \sqrt{n^2-2n+4}} \\ &> -\frac{n+1}{(n-\frac{3}{2}) + (n-1)} = -\frac{1}{2} - \frac{9}{8n-10} \\ &\geq -\frac{1}{2} - \frac{9}{46} > -0.7 > \sqrt{7} - \sqrt{12} \end{aligned}$$

for all $n \geq 7$, we have $EU\left(U^{\mathrm{I}}_{0,0,n-3}(0)\right) > EU\left(U^{\mathrm{II}}_{0,0,n-3}\right)$. By applying Lemma 2 (i) again

$$\begin{aligned} EU\left(U^{\mathrm{I}}_{0,0,n-3}(0)\right) &> (n-4)(n-\frac{3}{2}) + 2(n-1) + 2\sqrt{12} = n^2 - \frac{7}{2}n + 4 + \sqrt{48} \\ &> n^2 - \frac{7}{2}n + 10.92 > n^2 - \frac{11}{2}n + 25.64 > EU\left(U_{0,2,n-5}\right) \end{aligned}$$

for all $n \geq 8$, where in the last inequality we used (5). For $n = 7$ a direct computation gives $EU\left(U^{\mathrm{I}}_{0,0,4}(0)\right) = 3\sqrt{31} + 2\sqrt{39} + 2\sqrt{12} \approx 36.12$ and $EU\left(U_{0,2,2}\right) = 4(\sqrt{3} + \sqrt{7} + \sqrt{21}) \approx 35.84$, which completes the proof of the left inequality. Using Lemma 2 (i) one more time we have

$$\begin{aligned} EU\left(U^{\mathrm{I}}_{0,0,n-3}(0)\right) <& (n-4)\left(n - \frac{3}{2} + \frac{3}{4(2n-3)}\right) + 2\left(n - 1 + \frac{3}{2(n-1)}\right) + \\ & 2\sqrt{12} < n^2 - \frac{7}{2}n + \frac{3(n-4)}{8(n-\frac{3}{2})} + \frac{3}{n-1} + 10.93 \\ &< n^2 - \frac{7}{2}n + 11.81, \end{aligned}$$

for all $n \geq 7$. This, together with (2) establishes the right inequality. ■

Lemma 5. *Using the notation of Lemma 4, if $n \geq 7$ and U is one of the graphs $U^{\mathrm{I}}_{0,0,n-3}(p_1)$ with $p_1 \geq 1$, $U^{\mathrm{II}}_{0,1,n-4}$ or $U^{\mathrm{III}}_{0,1,n-4}(p_1,p_2)$ with $p_1 \geq 0$ and $p_2 \geq 0$, then $EU(U) < M_n$.*

Proof. By (3) it is sufficient to show that $EU(U) < n^2 - \frac{11}{2}n + 23$.

Case 1. $U = U^{\mathrm{I}}_{0,0,n-3}(p_1)$ with $p_1 \geq 1$. A direct computation gives

$$\begin{aligned}EU(U) = &\sum_{i=1}^{2} p_i\sqrt{p_i^2+5p_i+7} + \sum_{i=1}^{2}\sqrt{p_i^2+6p_i+12}+\\ &\sqrt{n^2-(p_1+2)\big[n-(p_1+2)\big]}+\sqrt{12}.\end{aligned}$$

By using Lemma 2 (i) to each term in each sum and Lemma 2 (ii) for f_1 to the third term, we have

$$\begin{aligned}EU(U) < &\sum_{i=1}^{2} p_i\Big(p_i+\frac{5}{2}+\frac{3}{4(2p_i+5)}\Big)+\sum_{i=1}^{2}\Big(p_i+3+\frac{3}{2(p_i+3)}\Big)+\\ &\sqrt{n^2-3n+9}+\sqrt{12}\\ = &\,p_1^2+\big[(n-4)-p_1\big]^2+\frac{7}{2}n-8+\sqrt{\Big(n-\frac{3}{2}\Big)^2+\frac{27}{4}}+\\ &\frac{3}{8}\sum_{i=1}^{2}\frac{p_i}{p_i+\frac{5}{2}}+\frac{3}{2}\cdot\frac{n+2}{(p_1+3)\big[(n+2)-(p_1+3)\big]}+\sqrt{12}\end{aligned}$$

We apply Lemma 2 (ii) for f_2 to the first two terms, for f_3 to the second to last term and Lemma 2 (i) to the non-constant square root term. Remembering that $p_1 \geq 1$ we get

$$\begin{aligned}EU(U) < &(n-5)^2+\frac{9}{2}n-\frac{17}{2}+\frac{27}{4(2n-3)}+2\cdot\frac{3}{8}+\frac{3(n+2)}{8(n-2)}+\sqrt{12}\\ = &\,n^2-\frac{11}{2}n+17.625+\sqrt{13}+\frac{27}{4(2n-3)}+\frac{3}{2(n-2)}\\ < &\,n^2-\frac{11}{2}n+23,\end{aligned}$$

for all $n \geq 7$.

Case 2. $U = U^{\mathrm{II}}_{0,1,n-4}$. A direct computation gives

$$\begin{aligned}EU(U) =&(n-6)\sqrt{n^2-5n+7}+2\sqrt{n^2-4n+7}+\sqrt{n^2-3n+9}+\\&\sqrt{7}+\sqrt{13}+\sqrt{19}.\end{aligned}$$

By using Lemma (2) (i) to all non-constant square root terms we have

$$\begin{aligned}EU(U) <&(n-6)\Big(n-\frac{5}{2}+\frac{3}{(2n-5)}\Big)+2\Big(n-2+\frac{3}{2(n-2)}\Big)+\\&\Big(n-\frac{3}{2}+\frac{27}{4(2n-3)}\Big)+\sqrt{7}+\sqrt{13}+\sqrt{19}\\&\approx n^2-\frac{11}{2}n+\frac{3(n-6)}{8(n-\frac{5}{2})}+\frac{3}{n-2}+\frac{27}{4(2n-3)}+20.11\\&< n^2-\frac{11}{2}n+23,\end{aligned}$$

for all $n \geq 7$.

Case 3. $U = U^{\mathrm{III}}_{0,1,n-4}(p_1, p_2)$ with $p_1 \geq 0$ and $p_2 \geq 0$. A direct computation gives

$$\begin{aligned}EU(U) =&\sum_{i=1}^{2} p_i\sqrt{p_i^2+5p_i+7}+\sqrt{p_1^2+7p_1+19}+\sqrt{p_2^2+6p_2+12}+\\&\sqrt{(n-1)^2-(p_1+2)\big[(n-1)-(p_1+2)\big]}+\sqrt{13}+\sqrt{19}.\end{aligned}$$

By applying Lemma 2 (i) to the first three terms and (ii) for f_1 to the fourth term we get

$$\begin{aligned}EU(U) <&\sum_{i=1}^{2} p_i\Big(p_i+\frac{5}{2}+\frac{3}{4(2p_i+5)}\Big)+\Big(p_1+\frac{7}{2}+\frac{27}{4(2p_1+7)}\Big)+\\&\Big(p_2+3+\frac{3}{2(p_2+3)}\Big)+\sqrt{n^2-4n+7}+\sqrt{13}+\sqrt{19}\\&=p_1^2+(n-5-p_1)^2+\frac{7}{2}(n-5)+\sqrt{(n-2)^2+3}+\frac{3}{8}\sum_{i=1}^{2}\frac{p_i}{p_i+\frac{5}{2}}+\\&\frac{27}{8p_1+28}+\frac{3}{2p_2+6}+\frac{13}{2}+\sqrt{13}+\sqrt{19}\end{aligned}$$

Using Lemma 2 (i) and (ii) for f_2 and knowing that $p_i \geq 0$ for $1 \leq i \leq 2$

gives

$$EU(U) < (n-5)^2 + \frac{7}{2}(n-5) + \left(n - 2 + \frac{3}{2(n-2)}\right) + 2 \cdot \frac{3}{8} + \frac{41}{28} + \frac{13}{2} + \sqrt{13} + \sqrt{19}$$
$$\approx n^2 - \frac{11}{2}n + \frac{3}{2(n-2)} + 22.17 < n^2 - \frac{11}{2}n + 23,$$

for all $n \geq 7$. ■

Theorem 1. *If $n \geq 7$, then the first, second and third greatest graphs with respect to the Euler Sombor index in the class of unicyclic graphs of order n are $U_{0,0,n-3}$, $U_{0,1,n-4}$ and $U^{\mathrm{I}}_{0,0,n-3}(0)$, respectively.*

Proof. Denote by $A = \{U_{0,0,n-3}, U_{0,1,n-4}\}$ and let U be a unicyclic graph of order n. By Lemma 3, if $U \in \tilde{\mathcal{U}}_{n,3} \setminus A$ then $EU(U) \leq M_n$, where M_n has the same meaning as in Lemma 4. Furthermore, by Lemma 1, if U is a direct or indirect ascendant of a graph in $\tilde{\mathcal{U}}_{n,3} \setminus A$, then $EU(U) < M_n$. Two cases remain: $U \in A$ or U is a direct or indirect ascendant of a graph in A. For the first case, by Lemmas 3 and 4, if $U \in A$ then $EU(U) > M_n$. For the second case, note first that by Lemma 4 if $U = U^{\mathrm{I}}_{0,0,n-3}(0)$, then $EU(U) > M_n$. Second, by Lemmas 5 and 1 if U is a direct or indirect ascendant of a graph in A other than $U^{\mathrm{I}}_{0,0,n-3}(0)$ then $EU(U) < M_n$. Thus, the only unicyclic graphs U of order n with $EU(U) > M_n$ are $U_{0,0,n-3}$, $U_{0,1,n-4}$ and $U^{\mathrm{I}}_{0,0,n-3}(0)$, and their order with respect to the Euler Sombor index is established by Lemmas 3 and 4. ■

3 Minimal unicyclic graphs with respect to the Euler Sombor index

We shall denote by $C_p + P_{x_1 x_k}$, with $k \geq 2$ the graph obtained by attaching the pendent path $P_{x_1 x_k}$ to a vertex of the cycle C_p. Let $m \geq n > 0$. An edge xy will be called a (m,n)-edge whenever $d(x) = m$ and $d(y) = n$.

Similar to the definition given in the previous section, the next notion is useful in what follows.

Definition 2. Let G and G' be two graphs of order n. If G can be obtained by applying the inverse of the transform given in Lemma 1 once to G', we say that G is a direct descendant of G'. If the minimum number of times needed to apply the inverse transform to G' in order to obtain G is greater than 1, we say that G is an indirect descendant of G'.

Before we give the next results, we need the following examples.

Example 3. If $n \geq 4$, C_n has one family of direct descendants, namely the family of graphs $C_{n-k+1} + P_{x_1 x_k}$, where $2 \leq k \leq n-2$. For brevity, denote it by ${}^{\mathrm{I}}C_n(k)$.

Example 4. If $n \geq 9$, for each $3 \leq k \leq n-2$ the graph ${}^{\mathrm{I}}C_n(k)$ has 12 (families of) direct descendants denoted by ${}^{\mathrm{II},i}C_n(k)$ for $1 \leq i \leq 12$ and detailed in figure 4.

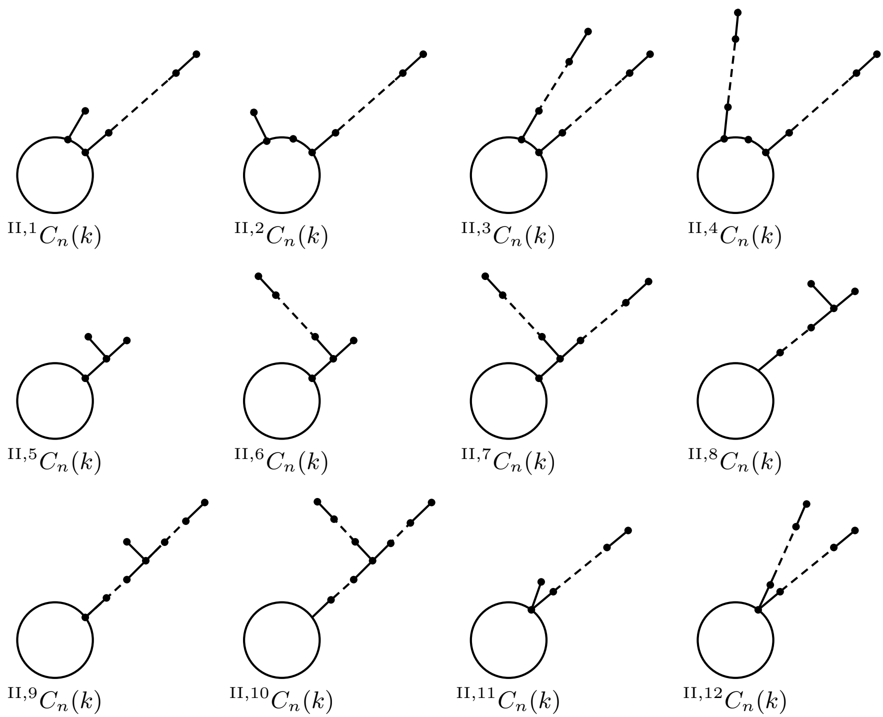


Figure 4. The direct descendants of ${}^{\mathrm{I}}C_n(k)$ for $n \geq 9$ and $3 \leq k \leq n-2$

Lemma 6. *If $n \geq 7$, then*

$$EU(C_n) < EU({}^{\mathrm{I}}C_n(k)) < EU({}^{\mathrm{I}}C_n(2)) < EU({}^{\mathrm{II},i}C_n(l))$$

for all $3 \leq k \leq n-2$, $3 \leq l \leq n-2$ and $1 \leq i \leq 12$.

Proof. Direct computations give $EU(C_n) = n\sqrt{12} \approx (n-3)\sqrt{12} + 10.39$, $EU({}^{\mathrm{I}}C_n(k)) = (n-4)\sqrt{12} + 3\sqrt{19} + \sqrt{7} \approx (n-3)\sqrt{12} + 12.25$ for all $3 \leq k \leq n-2$ and $EU({}^{\mathrm{I}}C_n(2)) = (n-3)\sqrt{12} + 2\sqrt{19} + \sqrt{13} \approx (n-3)\sqrt{12} + 12.32$, thus establishing the first two inequalities.

For the last one, not first that for $i \in \{4, 7, 9\}$ the class of graphs ${}^{\mathrm{II},i}C_n(l)$ exist only if $n \geq 8$ and for $i = 10$ the class of graphs ${}^{\mathrm{II},i}C_n(l)$ exist only if $n \geq 9$.

Observe now that each graph in the classes ${}^{\mathrm{II},i}C_n(l)$ for $i \in \{1, 6\}$ contains one $(1,2)$-edge, one $(1,3)$-edge, three $(2,3)$-edges, one $(3,3)$-edge, and $n-6$ $(2,2)$-edges, which implies that for $i \in \{1, 6\}$

$$EU({}^{\mathrm{II},i}C_n(l)) = (n-6)\sqrt{12} + 3\sqrt{19} + \sqrt{7} + \sqrt{13} + \sqrt{27} \approx (n-3)\sqrt{12} + 14.13 \quad (9)$$

Similarly, each graph in the classes ${}^{\mathrm{II},i}C_n(l)$ for $i \in \{2, 9\}$ contains one $(1,2)$-edge, one $(1,3)$-edge, five $(2,3)$-edges, and $n-7$ $(2,2)$-edges, which implies that for $i \in \{2, 9\}$

$$EU({}^{\mathrm{II},i}C_n(l)) = (n-7)\sqrt{12} + 5\sqrt{19} + \sqrt{7} + \sqrt{13} \approx (n-3)\sqrt{12} + 14.18 \quad (10)$$

Likewise, each graph in the classes ${}^{\mathrm{II},i}C_n(l)$ for $i \in \{3, 7\}$ contains two $(1,2)$-edges, four $(2,3)$-edges, one $(3,3)$-edge, and $n-7$ $(2,2)$-edges, which implies that for $i \in \{3, 7\}$

$$EU({}^{\mathrm{II},i}C_n(l)) = (n-7)\sqrt{12} + 4\sqrt{19} + 2\sqrt{7} + \sqrt{27} \approx (n-3)\sqrt{12} + 14.06 \quad (11)$$

By the same token, each graph in the classes ${}^{\mathrm{II},i}C_n(l)$ for $i \in \{4, 10\}$ contains two $(1,2)$-edges, six $(2,3)$-edges, and $n-8$ $(2,2)$-edges, which implies that for $i \in \{4, 10\}$

$$EU({}^{\mathrm{II},i}C_n(l)) = (n-8)\sqrt{12} + 6\sqrt{19} + 2\sqrt{7} \approx (n-3)\sqrt{12} + 14.12 \quad (12)$$

Moreover,

$$EU(^{\mathrm{II},5}C_n(l)) = (n-5)\sqrt{12}+2\sqrt{13}+2\sqrt{19}+\sqrt{27} \approx (n-3)\sqrt{12}+14.19, \quad (13)$$

$$EU(^{\mathrm{II},8}C_n(l)) = (n-6)\sqrt{12}+4\sqrt{19}+2\sqrt{13} \approx (n-3)\sqrt{12}+14.25, \quad (14)$$

$$EU(^{\mathrm{II},11}C_n(l)) = (n-5)\sqrt{12}+3\sqrt{28}+\sqrt{21}+\sqrt{7} \approx (n-3)\sqrt{12}+16.7, \quad (15)$$

$$EU(^{\mathrm{II},12}C_n(l)) = (n-6)\sqrt{12}+4\sqrt{28}+2\sqrt{7} \approx (n-3)\sqrt{12}+16.06. \quad (16)$$

By comparing (9)-(16) with the value of $EU(^{\mathrm{I}}C_n(2))$ the last inequality follows. ■

Theorem 2. *If $n \geq 7$, then the first, second and third smallest (families of) graphs with respect to the Euler Sombor index in the class of unicyclic graphs of order n are C_n, $^{\mathrm{I}}C_n(k)$ with $3 \leq k \leq n-2$ and $^{\mathrm{I}}C_n(2)$, respectively.*

Proof. Let U be an arbitrarily fixed unicyclic graph of order n. Applying to U as many times as possible the inverse of the transform given in Lemma 1, we always obtain the same graph, namely C_n. Thus, C_n is the minimal unicyclic graph of order n with respect to the Euler Sombor index, and any unicyclic graph of order n other than C_n is a direct or indirect descendant of it. The first two inequalities of Lemma 6 establish the ordering between C_n and its direct descendants. Lastly, by the last inequality of Lemma 6, by Lemma 1, and taking into account examples 3 and 4, for any unicyclic indirect descendant U of C_n we have $EU(C_n) < EU(^{\mathrm{I}}C_n(k)) < EU(^{\mathrm{I}}C_n(2)) < EU(U)$. ■

Note. After the present paper was completed and submitted for publication, the authors learned that results analogous to Theorem 2 are contained in the, then unpublished, paper [7].

Remark. The results obtained so far establish the top three minimal and maximal unicyclic graphs of order $n \geq 7$ with respect to the Euler Sombor index. We analyze the remaining cases here.

For $n = 3$ there exists only one unicyclic graph, $C_3 = U_{0,0,0}$. It is at the same time the minimal and maximal unicyclic graph of order 3 with respect to the Euler Sombor index.

For $n = 4$ there exist two unicyclic graphs, C_4 and $U_{0,0,1}$. They are the minimal and, respectively, maximal unicyclic graphs of order 4 with respect to the Euler Sombor index since $EU(C_4) = 4\sqrt{12}$ and $EU(U_{0,0,1}) = 2\sqrt{19} + \sqrt{13} + \sqrt{12}$.

For $n = 5$ there exist five unicyclic graphs, C_5, ${}^{\mathrm{I}}C_5(3)$, ${}^{\mathrm{I}}C_5(2) = U^{\mathrm{I}}_{0,0,1}(0)$, $U_{0,1,1}$ and $U_{0,0,2}$, listed here in ascending order with respect to the Euler Sombor index, by a direct computation.

For $n = 6$ there exist 13 unicyclic graphs, which we omit for brevity. A direct computation gives $U_{0,0,3}$, $U_{0,1,2}$ and $U^{\mathrm{I}}_{0,0,3}(0)$, in this order, as the top three maximal unicyclic graphs and C_6, ${}^{\mathrm{I}}C_6(k)$ with $3 \leq k \leq 4$ and ${}^{\mathrm{I}}C_6(2)$, in this order, as the top three minimal unicyclic graphs of order 6 with respect to the Euler Sombor index.

In conclusion, Theorems 1 and 2 establishing the top three minimal and maximal unicyclic graphs of order n hold whenever $\left|\mathcal{U}_n\right| \geq 3$ (i.e. for all $n \geq 5$) and furthermore, the graphs C_n and $U_{0,0,n-3}$ were shown to be the minimal and respectively maximal unicyclic graphs of order n whenever $\mathcal{U}_n \neq \emptyset$ (i.e. for all $n \geq 3$).

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