*Appl. Math. J. Chinese Univ.*
2022, 37(3): 350-365

# Unicyclic graphs with extremal Lanzhou index

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**Abstract.** Very recently D. Vukičević et al. [8] introduced a new topological index for a molecular graph $G$ named Lanzhou index as $Lz(G) = \sum_{u\in V(G)} \overline{d_u} d_u^2$, where $d_u$ and $\overline{d_u}$ denote the degree of vertex $u$ in $G$ and in its complement respectively. Lanzhou index $Lz(G)$ can be expressed as $(n-1)M_1(G) - F(G)$, where $M_1(G)$ and $F(G)$ denote the first Zagreb index and the forgotten index of $G$ respectively, and $n$ is the number of vertices in $G$. It turns out that Lanzhou index outperforms $M_1(G)$ and $F(G)$ in predicting the logarithm of the octanol-water partition coefficient for octane and nonane isomers. It was shown that stars and balanced double stars are the minimal and maximal trees for Lanzhou index respectively. In this paper, we determine the unicyclic graphs and the unicyclic chemical graphs with the minimum and maximum Lanzhou indices separately.

## §1 Introduction

Let $G$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For any $u \in V(G)$, the neighborhood of $u$, written $N(u)$, is the set of vertices adjacent to $u$. The degree of vertex $u$ in a graph $G$, denoted by $d_u$, is the number of edges incident to $u$. An isolated vertex is a vertex of degree zero. A leaf or pendant vertex is a vertex of degree one. The degree sequence of a graph is the list of vertex degrees, usually written in nonincreasing order.

The first Zagreb index and forgotten index [7] of a graph $G$ are defined as

$$M_1(G) = \sum_{u\in V(G)} d_u^2, \quad F(G) = \sum_{u\in V(G)} d_u^3.$$

After the two indices were introduced in the same paper, many mathematical and chemical properties had been considered in [6, 14-16] for the first Zagreb index, while the forgotten index was unpopular for many years until it was reintroduced in [3]. It turns out that the Furtula-Gutman linear combination $M_1(G)+\lambda F(G)$, $\lambda \in [-20, 20]$ is an excellent correlation to predict the octanol-water partition coefficient. And a sharp peak is obtained at $\lambda = -0.140$ for octane

Received: 2019-02-27. Revised: 2020-02-25.
MR Subject Classification: 05C05, 05C07, 05C35, 05C09, 05C92.
Keywords: Lanzhou index, unicyclic graph, extremal graph, Zagreb index, forgotten index.
Digital Object Identifier(DOI): https://doi.org/10.1007/s11766-022-3768-3.
Supported by the National Natural Science Foundation of China(11871256), and the Chinese-Croatian bilateral project(7-22).
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isomers, but it is not good for nonane isomers. Very recently Vukičević et al. found that 0.140 is very close to $\frac{1}{7}$, and the value of the denominator is the largest possible degree of a vertex in octanes with 8 vertices, but nonanes are molecular graphs with 9 vertices. Therefore, Vukičević et al. defined a new index for a molecular graph $G$ named the Lanzhou index [8], which is denoted by $Lz(G)$. They first interpret the free parameter $\lambda$ as $-\frac{1}{n-1}$ in the Furtula-Gutman linear combination, then multiply $n-1$ to get rid of fractions. That is,

$$Lz(G) = (n-1)M_1(G) - F(G) = \sum_{u\epsilon V(G)} d_u^2[(n-1) - d_u] = \sum_{u\epsilon V(G)} \overline{d_u} d_u^2,$$

where $\overline{d_u}$ denotes the degree of the vertex $u$ in $\overline{G}$, the complement of $G$. Lanzhou index $Lz(G)$ behaves better in predicting the octanol-water partition coefficient of octane and nonane isomers than $M_1(G)$, $F(G)$ and $Lz(\overline{G})$. Thus, it is a good topological index [5].

As is well known, finding extremal graphs and values of the topological indices over some classes of graphs attracts the attention of many researchers. In [8], extremal graphs with $n$ vertices are illustrated. More precisely, complete and empty graphs are of minimum Lanzhou index 0, and $\frac{2}{3}(n-1)$-regular graphs with $n \equiv 1 \pmod 3$ are of maximum Lanzhou index $\frac{4}{27}n(n-1)^3$. For trees with $n$ vertices, star and balanced double star are the minimal and maximal graphs respectively. For chemical trees on $n$ vertices, extremal graphs have been determined (see Proposition 4.2). Actually, extremal values on a number of other indices, such as the Wiener index [2], the first and second Zagreb indices [1, 10, 12, 17], and the Kirchhoff index [4, 11, 13], have been already investigated for unicyclic graphs. In this paper, we consider the extremal Lanzhou indices of unicyclic graphs and corresponding extremal graphs.

In order to exhibit our results, we present some notations. Let $C_k$ $(k \geq 3)$ be a cycle on $k$ vertices, and $S_k$ $(k \geq 1)$ be a star with $k$ vertices, which is a tree consisting of one vertex and the other $k-1$ vertices adjacent to it. A double star $S_{k,l}$ is a tree obtained from $K_2$ by attaching $k-1$ leaves to one of its vertices and $l-1$ leaves to the other one. Hence, $S_{k,l}$ has one vertex of degree $k$, one of degree $l$, and $k+l-2$ vertices of degree one. A double star on $n$ vertices is balanced if the difference between $k$ and $l$ is as small as possible. We denote the balanced double star on $n$ vertices by $BDS(n) = S_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. A graph is called unicyclic if it is connected and contains exactly one cycle. We represent a unicyclic graph $G$ with the unique cycle $C_k = v_1 v_2 \cdots v_k v_1$ as $U(C_k; T_1, T_2, \ldots, T_k)$, where $T_i$ (a tree) is the component of $G - E(C_k)$ containing $v_i$ for each $1 \leq i \leq k$. We may regard $v_i$ as the root of $T_i$. The order of $T_i$, written $t_i + 1$ $(t_i \geq 0)$, is the number of vertices in $T_i$. We say $T_i$ is trivial if it contains only one vertex; Otherwise, it is non-trivial. In particular, when $T_i = S_{t_i+1}$, it is a star with $t_i$ leaves. Let $\mathcal{U}(n,k)$ be the set of unicyclic graphs with $n$ vertices and a unique cycle $C_k$ such that the vertices not on the cycle are pendent. That is, any graph $G \in \mathcal{U}(n,k)$ can be written as $U(C_k; S_{t_1+1}, S_{t_2+1}, \ldots, S_{t_k+1})$, where some stars $S_{t_i+1}$ may be trivial, i.e. $t_i = 0$. Let $i_0$ be the number of non-trivial components in $G - E(C_k)$. We make a convention that $S_{t_1+1}$, $S_{t_2+1}, \ldots,$ $S_{t_{i_0}+1}$ are the $i_0$ non-trivial components, where $1 \leq t_1 \leq t_2 \leq \cdots \leq t_{i_0}$. Also $d_{v_i} = t_i + 2$ for each $i$, and $3 \leq d_{v_1} \leq d_{v_2} \leq \cdots \leq d_{v_{i_0}}$. The non-trivial components $S_{t_1+1}$, $S_{t_2+1}, \ldots,$ $S_{t_{i_0}+1}$ are uniform if $\max\limits_{1 \leq i < j \leq i_0} |t_j - t_i| \leq 1$. A unicyclic graph containing $n$ vertices is called minimal or maximal according as it has minimum or maximum Lanzhou index among all unicyclic graphs with $n$ vertices. Minimal and maximal graphs are called extremal graphs.

In this paper, we use $d_u$, $k$, $i_0$ to represent related parameters of graph $G$. Similarly, using same superscripts as $G'$ and $G^\star$ to them, we get corresponding parameters of $G'$ and $G^\star$. Precisely, $d'_u$, $k'$, $i'_0$ and $d^\star_u$, $k^\star$, $i^\star_0$ represent degree of vertex $u$, length of the unique cycle, the number of non-trivial components (after removing all edges of the cycle) of $G'$ and $G^\star$ respectively. For other terminologies used but not defined, we may refer to Ref. [8]. Next we give a transformation, which reduces all unicyclic graphs to graphs in $\mathcal{U}(n) = \cup_{k=3}^{n}\mathcal{U}(n,k)$ without changing their Lanzhou indices.

**Transformation** $A$**:** *Let $G = U(C_k; T_1, T_2, \ldots, T_k)$ be a unicyclic graph. For a vertex $y \in T_j$ not on $C_k$ with $d_y \geq 2$, let $u$ be a vertex on the path between $v_j$ and $y$ such that $u$ is adjacent to $y$, and $y_1, \ldots, y_r$ be the neighbors of $y$ other than $u$. Let $G' = G - \{v_iv_{i+1}, uy, y_ry\} + \{uy_r, v_iy, v_{i+1}y\}$. We say $G'$ is obtained from $G$ by Transformation A. For example, see Fig. 1.*

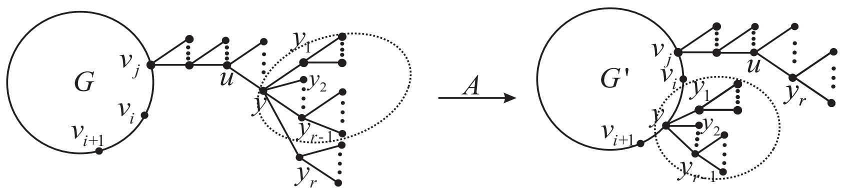


Fig. 1. Transformation $A$ from graph $G$ to $G'$.

**Proposition 1.1.** *Let $G'$ be obtained from a unicyclic graph $G$ by Transformation A. Then $G'$ is also a unicyclic graph, and $Lz(G') = Lz(G)$.*

*Proof.* Clearly, the vertices $y, u, y_r, v_i, v_{i+1}$ have the same degrees in $G$ and $G'$. So $G$ and $G'$ have the same degree sequence, which implies that $Lz(G') = Lz(G)$. □

**Corollary 1.2.** *The minimum and maximum Lanzhou indices of all unicyclic graphs with $n$ vertices are equal to those of graphs in $\mathcal{U}(n)$.*

*Proof.* For a unicyclic graph $G$ with $n$ vertices, if it has a vertex $u$ not on its cycle with degree at least two, then we obtain a new unicyclic graph $G'$ by applying Transformation $A$ so that the number of such vertices decreases by one. By Proposition 1.1 we obtain that $G$ and $G'$ have the same Lanzhou index. By repeating Transformation $A$ to $G$ finite times, finally we get a unicyclic graph in $\mathcal{U}(n)$ whose Lanzhou index is equal to that of $G$. That is, for any unicyclic graph $G$ with $n$ vertices, we can find a unicyclic graph in $\mathcal{U}(n)$ with the same Lanzhou index as $G$. □

By Corollary 1.2, we know that extremal values of Lanzhou indices of all unicyclic graphs achieve on some unicyclic graphs in $\mathcal{U}(n)$. Therefore, we only need to consider unicyclic graphs in $\mathcal{U}(n)$. Clearly, for each $3 \leq k \leq n-1$, the vertices not on its cycle of a graph in $\mathcal{U}(n,k)$ are leaves. For a graph $G \in \mathcal{U}(n,k)$ with two non-trivial components, the next transformation and proposition tell us that if the total number of leaves of the two non-trivial components is less than $\frac{2(n-7)}{3}$, then $G$ is not a maximal graph. And if the above total number is more than $\frac{2(n-7)}{3}$, then $G$ is not a minimal graph.

**Transformation** $B$**:** *Suppose that* $G \in \mathcal{U}(n,k)$ *and for* $v_i,\ v_j \in V(C_k),\ i \neq j,\ N(v_i)\backslash V(C_k) = \{x_1, x_2, \ldots, x_{t_1}\},\ N(v_j)\backslash V(C_k) = \{y_1, y_2, \ldots, y_{t_2}\}$ *with* $t_1, t_2 \geq 1$. *Let* $G' = G - \{v_jy_1, v_jy_2, \ldots, v_jy_{t_2}\} + \{v_iy_1, v_iy_2, \ldots, v_iy_{t_2}\}$. *We say* $G'$ *is obtained from* $G$ *by Transformation* $B$. *For example, see Fig. 2.*

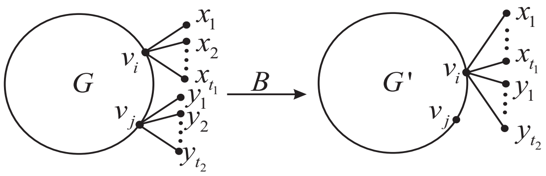



Fig. 2. Transformation $B$ from graph $G$ to $G'$.

**Proposition 1.3.** *Let* $G'$ *be obtained from a unicyclic graph* $G \in \mathcal{U}(n,k)$ *by Transformation* $B$. *Then* $G' \in \mathcal{U}(n,k)$ *with* $i_0' = i_0 - 1$. *Moreover, if* $t_1 + t_2 < \frac{2(n-7)}{3}$, *then* $Lz(G') > Lz(G)$. *Otherwise,* $Lz(G') \leq Lz(G)$.

*Proof.* By Transformation $B$, we know $G' \in \mathcal{U}(n,k)$, $d'_{v_i} = t_1+t_2+2$, $d'_{v_j} = 2$, and other vertices remain unchanged in their degrees. So, $T_{v_j}$ becomes trivial from a non-trivial component. Let $D = \{v_i,\ v_j\}$, and the difference of their Lanzhou indices is

$$\begin{aligned} Lz(G') - Lz(G) &= \sum_{u\in D}[(n-1-d'_u)d'^2_u - (n-1-d_u)d^2_u] \\ &= (n-t_1-t_2-3)(t_1+t_2+2)^2 - (n-t_1-3)(t_1+2)^2 \\ &+ 4(n-3) - (n-t_2-3)(t_2+2)^2 \\ &= t_1t_2[2(n-7) - 3t_1 - 3t_2]. \end{aligned}$$

Thus, if $t_1 + t_2 < \frac{2(n-7)}{3}$, then $Lz(G') > Lz(G)$. Otherwise, $Lz(G') \leq Lz(G)$. □

The outline of this paper is given as follows. In Section 2, we obtain the minimal unicyclic graphs by some transformations to unicyclic graphs in $\mathcal{U}(n)$. In Section 3, we obtain the maximal unicyclic graphs in two steps. First, we reduce maximal graphs to two possible specific classes of $\mathcal{U}(n)$. Then, we get the maximum values of all unicyclic graphs by comparing their maximum Lanzhou indices. In Section 4, we focus on the extremal chemical graphs and give some relations between extremal chemical trees and unicyclic graphs.

## §2 Minimal unicyclic graphs

In this section, we partition the set of graphs $\mathcal{U}(n,k)$ into two parts according to $i_0 \geq 2$ and $i_0 \leq 1$. For the former, we will prove that their Lanzhou indices are larger than those of some graphs in $\mathcal{U}(n,k)$ with $i_0 = 1$. Therefore, minimum values must be obtained from some graphs in $\mathcal{U}(n,k)$ with $i_0 \le 1$. For convenience, let $\mathcal{U}_0(n,k) = \{G \in \mathcal{U}(n,k) | i_0 \ge 2\}$. Then $\mathcal{U}_0(n) = \cup_{k=3}^{n} \mathcal{U}_0(n,k)$. To prove the main conclusion, we introduce a transformation as follows.

**Transformation C:** *Suppose that $G \in \mathcal{U}(n,k)$ and $N(v_i)\backslash V(C_k) = \{x_1, x_2, \ldots, x_{t_1}\}$ with $t_1 \ge 1$. Let $G' = G - \{v_{i-1}v_i\} + \{v_{i-1}x_1\}$, where subscripts are integers modulo $k$. We say $G'$ is obtained from $G$ by Transformation $C$ at specified vertex $v_i$; Conversely, we say $G$ is obtained from $G'$ by $C^{-1}$ (the reversal of Transformation $C$) at specified vertex $v_i$. For example, see Fig. 3.*

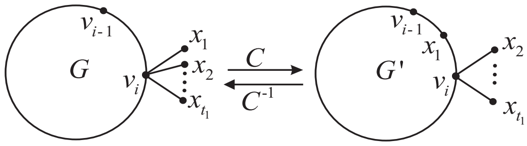



Fig. 3. Graphs $G$ and $G'$ in Transformations $C$ and $C^{-1}$.

**Proposition 2.1.** *Let $G$ be obtained from a unicyclic graph $G' \in \mathcal{U}(n,k+1)$ by Transformation $C^{-1}$, as shown in Fig. 3. Then $G \in \mathcal{U}(n,k)$, and*

$$Lz(G) - Lz(G') = (d'_{v_i} - 1)(-3d'_{v_i} + 2n - 8).$$

*Proof.* By Transformation $C^{-1}$, $d_{v_i} = d'_{v_i} + 1$, $d_{x_1} = d'_{x_1} - 1 = 1$, and other vertices remain unchanged in their degrees. So, let $D = \{v_i, x_1\}$, and the difference of their Lanzhou indices is

$$\begin{aligned} Lz(G) - Lz(G') &= \textstyle\sum_{u \in D} [(n-1-d_u)d_u^2 - (n-1-d'_u)d'^2_u] \\ &= (n-2-d'_{v_i})(d'_{v_i}+1)^2 - (n-1-d'_{v_i})d'^2_{v_i} + (n-2) - 4(n-3) \\ &= (d'_{v_i} - 1)(-3d'_{v_i} + 2n - 8). \end{aligned}$$ □

**Lemma 2.2.** *For any $G \in \mathcal{U}_0(n,k)$ with $n \ge 14$, let $v_i$ be a vertex of minimum degree among roots of non-trivial trees in $G - E(C_k)$ and $G'$ be obtained from $G$ by Transformation $C$ at specified vertex $v_i$. Then $Lz(G') < Lz(G)$.*

*Proof.* By Transformation $C$, $G' \in \mathcal{U}(n,k+1)$, $d'_{v_i} = d_{v_i} - 1$, $d'_{x_1} = 2$, and the other vertices remain unchanged in their degrees. Substituting $d_{v_i} - 1$ for $d'_{v_i}$ in Proposition 2.1, we obtain that $Lz(G) - Lz(G') = (d_{v_i} - 2)(-3d_{v_i} + 2n - 5)$.

Since a unicyclic graph has the same number of vertices and edges, by Degree-Sum Formula, $2n = \Sigma_{u \in V(G)} d_u \ge (n-k) + 2(k-i_0) + d_{v_i} i_0$. Since $i_0 \ge 2$, $d_{v_i} \le \frac{n-k}{i_0} + 2 \le \frac{n-3}{2} + 2 = \frac{n+1}{2}$. For $n \ge 14$, we have $\frac{n+1}{2} < \frac{2n-5}{3}$. So $Lz(G) - Lz(G') > 0$. □

**Corollary 2.3.** *If a graph $G \in \mathcal{U}_0(n,k)$ with $n \ge 14$, then there exists $G^\star \in \mathcal{U}(n,k^\star)$ with $i_0^\star = 1$ such that $Lz(G^\star) < Lz(G)$.*

*Proof.* By the convention before Transformation $A$, the $v_i$'$s, i \in [1, i_0]$, are roots of non-trivial trees in $G - E(C_k)$ and $d_{v_1} \le d_{v_2} \le \cdots \le d_{v_{i_0}}$. First, taking $v_1$ as specified vertex, we apply Transformation $C$ on graph $G$ $d_{v_1} - 2$ times, and denote the resulting graph by $G'$. So $G' \in \mathcal{U}_0(n, k+t_1)$ with $d'_{v_1} = 2$, $i'_0 = i_0 - 1$. Next, taking $v_i$, $i = 2, \ldots, i_0 - 1$, as specified vertices in turn, we apply Transformation $C$ from $G'$ $d_{v_i} - 2$ times successively and denote the last graph by $G^\star$. That is, $G^\star = U(C_{n-t_{i_0}}; S_{t_{i_0}+1}, v_2, v_3, \ldots, v_{n-t_{i_0}})$ with $k^\star = n - t_{i_0}$ and $i_0^\star = 1$. It follows that $Lz(G^\star) < Lz(G)$ by Lemma 2.2. Consequently, $G^\star \in \mathcal{U}(n, k^\star)$ is a required graph. □

**Lemma 2.4.** *$U(C_3; S_{n-2}, v_2, v_3)$ is the minimal graph in $\mathcal{U}(n)\backslash\mathcal{U}_0(n)$ for $n \geq 3$.*

*Proof.* Let $G$ be a graph in $\mathcal{U}(n)\backslash\mathcal{U}_0(n)$, and $k$ be the length of a unique cycle of $G$. Then $3 \leq k \leq n$, and $i_0 = 0$ or 1. Hence

$$\begin{aligned} Lz(G) &= (n-k)(n-2) + 4(k-1)(n-3) + (k-3)(n+2-k)^2 \\ &= k^3 - (2n+7)k^2 + (n^2+13n+6)k - (2n^2+18n). \end{aligned}$$

So $g(k) := Lz(G)$ is a cubic function of $k$. We claim that $g(k)$ takes the minimum value only at $k = 3$ in the integer-interval $[3, n]$ by an analytical approach. First, $g'(k) = 3k^2 - 2(2n+7)k + n^2 + 13n + 6$. Then, the equation $g'(k) = 0$ has roots $k_1 = \frac{2n+7-\sqrt{n^2-11n+31}}{3}$ and $k_2 = \frac{2n+7+\sqrt{n^2-11n+31}}{3}$. For $n \geq 3$, we can confirm that $k_1 > 3$ and $k_2 > n$. Thus, $g(k)$ is strictly monotone increasing in $[3, k_1]$. So, if $n \leq k_1$, then $3 \leq n \leq 6$, and the claim is true. Otherwise, $n \geq 7$, and $g(k)$ is strictly monotone decreasing in $[k_1, n]$. Therefore, the minimum value of $g(k)$ is $g(3) = n^2 + 3n - 18$ or $g(n) = 4n^2 - 12n$. In fact, we have $g(3) \leq g(n)$ for $n \geq 3$, and equality holds if and only if $n = 3$, which also yields the claim.

Consequently, $Lz(G)$ takes the minimum value when $k = 3$, and $G = U(C_3; S_{n-2}, v_2, v_3)$ is the required minimal graph for Lanzhou index. □

**Theorem 2.5.** *If $G$ is a minimal unicyclic graph with $n \geq 3$ vertices for Lanzhou index, then $G = U(C_3; S_{n-2}, v_2, v_3)$ and $Lz(G) = n^2 + 3n - 18$.*

*Proof.* For $n \geq 14$, by Corollary 2.3, we know any graph in $\mathcal{U}_0(n)$ has larger Lanzhou index than some graph in $\mathcal{U}(n)$ with $i_0 = 1$. Hence, the minimal graph in $\mathcal{U}(n)$ for Lanzhou index must be one with $i_0 \leq 1$. By Lemma 2.4, $U(C_3; S_{n-2}, v_2, v_3)$ is of the minimum Lanzhou index for any graphs in $\mathcal{U}(n)$ with $i_0 \leq 1$. Therefore, $U(C_3; S_{n-2}, v_2, v_3)$ is the minimal graph in $\mathcal{U}(n)$.

For $9 \leq n \leq 13$, if $G \in \mathcal{U}(n)$ and $i_0 \geq 3$, then there exists $G^\star \in \mathcal{U}(n, k^\star)$ with $i_0^\star = 2$ such that $Lz(G^\star) < Lz(G)$ by similar arguments as Lemma 2.2 and Corollary 2.3. Therefore, minimal graphs must be in $\mathcal{U}(n)$ with $i_0 \leq 2$. We only need to consider graphs with $i_0 = 2$. Denote the two non-trivial components by $S_{t_1+1}$ and $S_{t_2+1}$ with $1 \leq t_1 \leq t_2$. By Transformation $B$ and Proposition 1.3, if $t_1 + t_2 > \frac{2(n-7)}{3}$, then $G$ is not minimal and there exists a graph with $i_0 = 1$ having smaller Lanzhou index. For $n = 9$, $t_1 + t_2 > \frac{2(n-7)}{3} = \frac{4}{3}$. Thus, for any $G$ with $i_0 = 2$, $G$ is not minimal. Combining Lemma 2.4, we know $U(C_3; S_7, v_2, v_3)$ is the minimal graph. We can verify the cases that $n = 10,\ 11,\ 12,\ 13$ similarly. Take $n = 13$ for example. Since $\frac{2(13-7)}{3} = 4$, we need to consider graphs with $t_1 + t_2 \leq 4$. That is, $G$ is a graph with $t_1 = t_2 = 1,\ k = 11$ or $t_1 = 1,\ t_2 = 2,\ k = 10$ or $t_1 = 1,\ t_2 = 3,\ k = 9$ or $t_1 = t_2 = 2,\ k = 9$. Their Lanzhou indices are 544 or 562 or 580 or 580, but all of them are larger than $Lz(U(C_3; S_{11}, v_2, v_3)) = 190$.

For $3 \leq n \leq 8$, we first find the minimal graphs in $\mathcal{U}_0(n)$ by enumeration according to $i_0$ $(2 \leq i_0 \leq \lfloor \frac{n}{2} \rfloor)$, then compare Lanzhou indices of the minimal unicyclic graphs in $\mathcal{U}_0(n)$ with $U(C_3; S_{n-2}, v_2, v_3)$. By a simple calculation, results are consistent with the above conclusion.

Now we turn to consider the unicycle graphs $G \notin \mathcal{U}(n)$. If $G$ is of minimum Lanzhou index, then $G$ can be transformed into a unicycle graph $G'$ in $\mathcal{U}(n)$ by a series of Transformation $A$ such that $G$ and $G'$ have the same Lanzhou index and the length of the cycle of $G'$ is larger than that of $G$. This implies that $G'$ is also a minimal graph in $\mathcal{U}(n)$ whose cycle is of length at least 4, which is impossible since $G = U(C_3; S_{n-2}, v_2, v_3)$ is the unique minimal graph in $\mathcal{U}(n)$. Thus, the minimal unicycle graphs must belong to $\mathcal{U}(n)$. By the above arguments we have that for each $n \geq 3$, $U(C_3; S_{n-2}, v_2, v_3)$ is the minimal graph in all unicyclic graphs with $n$ vertices. □

So far, we have obtained the minimal unicyclic graphs $U(C_3; S_{n-2}, v_2, v_3)$ for $n \geq 3$. We also note that the removal of edge $v_2v_3$ from $U(C_3; S_{n-2}, v_2, v_3)$ results in the minimal tree $S_n$. Conversely, adding an edge between two leaves of $S_n$ yields the minimal unicyclic graph.

## §3 Maximal unicyclic graphs

In this section, we will determine the maximal unicyclic graphs for Lanzhou index by reducing maximal graphs to two possible specific classes of graphs and then comparing Lanzhou indices of the two specific classes of graphs.

For each integer $n \geq 3$, let $\overline{\mathcal{U}(n)}$ be the set of graphs in $\mathcal{U}(n)$ with the maximum Lanzhou index. For $G \in \overline{\mathcal{U}(n)}$, let $C_k$ denote the cycle of $G$, and recall that $i_0$ is the number of non-trivial components in $G - E(C_k)$. Next lemma tells us that $i_0$ is at most three in the majority of maximal unicyclic graphs.

**Lemma 3.1.** *Let $G \in \overline{\mathcal{U}(n)}$. If $n \geq 17$, then $1 \leq i_0 \leq 3$; If $8 \leq n \leq 16$, then $1 \leq i_0 \leq 4$.*

*Proof.* Since $G \in \overline{\mathcal{U}(n)}$, $G \in \mathcal{U}(n,k)$ for some $k \geq 3$. By Transformation $B$ and Proposition 1.3, for any $i, j \in [1, i_0]$ and $i \neq j$, we have $t_i + t_j \geq \frac{2(n-7)}{3}$. Otherwise, we will obtain a new graph whose Lanzhou index is larger than $G$ by Transformation $B$. It contradicts $G \in \overline{\mathcal{U}(n)}$.

First we claim that $i_0 \geq 1$. If not, then $G \in \overline{\mathcal{U}(n)}$ is isomorphic to $C_n$, and $Lz(C_n) = 4n(n-3)$. For every integer $n \geq 8$, the unicyclic graph $U(C_{n-1}; S_2, v_2, v_3, \ldots, v_{n-1})$ has Lanzhou index $4n^2 - 10n - 14$ which is larger than $Lz(C_n)$, a contradiction.

For $n \geq 17$, suppose that $i_0 \geq 4$. Then $n - k = \sum_{j=1}^{i_0} t_j \geq \sum_{j=1}^{4} t_j \geq 2 \times \frac{2(n-7)}{3}$, which implies that $k \leq \frac{28-n}{3}$. Since $k \geq i_0 \geq 4$, we have $n \leq 16$, a contradiction. So $1 \leq i_0 \leq 3$.

For $n \geq 8$, suppose that $i_0 \geq 5$. Then $n-k \geq \sum_{j=1}^{5} t_j \geq 2\times\frac{2(n-7)}{3}+1$, which implies that $k \leq \frac{25-n}{3}$. Since $k \geq i_0 \geq 5$, we have $n \leq 10$. The possible graph must be $U(C_5; S_2, S_2, S_2, S_2, S_2) \in \mathcal{U}(10, 5)$. However, $Lz(U(C_5; S_2, S_2, S_2, S_2, S_2)) = 310 < Lz(U(C_4; S_2, S_2, S_3, S_3)) = 316$, a contradiction. So $1 \leq i_0 \leq 4$. □

**Theorem 3.2.** *Let $G \in \overline{\mathcal{U}(n)}$ with $n \geq 11$. Then $G \in \mathcal{U}(n, 3)$ and $i_0 = 2$ or $3$.*

*Proof.* Let $k$ be the length of the cycle of $G$. We have $1 \leq i_0 \leq 4$ by Lemma 3.1.

We first claim that $i_0 \geq k - 1$. To the contrary suppose that $i_0 \leq k - 2$. Then there must be at least two vertices of degree two on its cycle $C_k$, which may be assumed to be adjacent for Lanzhou index of a graph is determined by its degree sequence. Let $v_{k-1}$ and $v_k$ be such two vertices with $v_{k-1}v_k \in E(C_k)$. There exists a vertex $v_1 \neq v_{k-1}$ but adjacent to $v_k$. If $k \geq 4$, let $G'$ be obtained from $G$ by Transformation $C^{-1}$ at specified vertex $v_{k-1}$, where $x_1 = v_k$. Then by Proposition 2.1, the difference of their Lanzhou indices is $Lz(G') - Lz(G) = (d_{v_{k-1}} - 1)(-3d_{v_{k-1}} + 2n - 8) = 2n - 14 > 0$, a contradiction. For $k = 3$, $i_0 = 1$ and $G = U(C_3; S_{n-2}, v_2, v_3)$. By Lemma 2.4, we know that $Lz(G) < Lz(C_n)$, which contradicts.

If $i_0 \leq 2$, then $k = 3$ and $i_0 = 2$, so the theorem holds.

From now on we may suppose $3 \leq i_0 \leq 4$. We claim that $i_0 = k$. Suppose that $i_0 \leq k - 1$. Then $k \geq i_0 + 1 \geq 4$. By the convention immediately before Transformation $A$, $v_1, v_k \in V(C_k)$ with $d_{v_1} \geq 3$ and $d_{v_k} = 2$. Let $G'$ be obtained from $G$ by Transformation $C^{-1}$ at specified vertex $v_1$, where $x_1 = v_k$. Then by Proposition 2.1, the difference of their Lanzhou indices is $Lz(G') - Lz(G) = (d_{v_1} - 1)(-3d_{v_1} + 2n - 8)$. If $d_{v_1} \geq \frac{2n-8}{3}$, then $d_{v_3} \geq d_{v_2} \geq d_{v_1} \geq \frac{2n-8}{3}$, and

$$n - k = \sum_{i=1}^{i_0} t_i \geq t_1 + t_2 + t_3 \geq 3d_{v_1} - 6 \geq 2n - 14 \geq n - 3 \text{ for } n \geq 11,$$

which implies that $k \leq 3$, a contradiction. So $d_{v_1} < \frac{2n-8}{3}$, and $Lz(G') > Lz(G)$, contradicting that $G \in \overline{\mathcal{U}(n)}$. Therefore, the claim $i_0 = k$ holds.

Further we claim that $i_0 \neq 4$. Suppose that $i_0 = k = 4$. For $n \geq 11$, by Lemma 3.1, we have $11 \leq n \leq 16$, and $G$ must be $U(C_4; S_2, S_3, S_3, S_3)$, $U(C_4; S_3, S_3, S_3, S_3)$, $U(C_4; S_3, S_3, S_3, S_4)$, and $U(C_4; S_4, S_4, S_4, S_4)$ by Proposition 1.3, which have the Lanzhou indices smaller than $U(C_3; S_3, S_4, S_4)$, $U(C_3; S_4, S_4, S_4)$, $U(C_3; S_4, S_4, S_5)$ and $U(C_3; S_5, S_5, S_6)$ respectively. This contradiction implies that $k = i_0 = 3$. □

For $n \geq 11$, by Theorem 3.2, maximal graphs in $\mathcal{U}(n)$ belong to $\mathcal{U}(n, 3)$ with $i_0 = 2$ or 3. Next, we will investigate the two specific cases.

**Lemma 3.3.** *For $n \geq 5$, let $G \in \mathcal{U}(n, 3)$ with $i_0 = 2$ be the maximal graph. Then $G = U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3)$. Moreover,*

$$Lz(G) = \begin{cases} \frac{1}{4}n^3 + \frac{3}{4}n^2 - \frac{5}{2}n - 8, & \text{if } n \text{ is even;} \\ \frac{1}{4}n^3 + \frac{3}{4}n^2 - \frac{9}{4}n - \frac{27}{4}, & \text{otherwise.} \end{cases}$$

*Proof.* $G$ can be written as $U(C_3; S_{t_1+1}, S_{t_2+1}, v_3)$, where $t_1 + t_2 + 3 = n$. Since $d_{v_i} = t_i + 2$ $(i = 1, 2)$, we have $d_{v_2} = n + 1 - d_{v_1}$.

$$\begin{aligned} Lz(G) &= (n-3)(n-1-1) + 4(n-1-2) + (n-1-d_{v_1})d_{v_1}^2 + (d_{v_1}-2)(n+1-d_{v_1})^2 \\ &= -(n+5)d_{v_1}^2 + (n+1)(n+5)d_{v_1} - n^2 - 5n - 8. \end{aligned}$$

Clearly, $Lz(G)$ is a quadratic function of $d_{v_1}$, and the image is symmetrical about $\frac{n+1}{2}$. Hence, $Lz(G)$ is maximized at $d_{v_1} = \lceil \frac{n}{2} \rceil$, and $d_{v_2} = n + 1 - \lceil \frac{n}{2} \rceil = \lfloor \frac{n+2}{2} \rfloor$. So the maximal graph is $G = U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3)$. Moreover, if $n$ is odd, then $d_{v_1} = \frac{n+1}{2}$, and $Lz(G) = \frac{1}{4}n^3 + \frac{3}{4}n^2 - \frac{9}{4}n - \frac{27}{4}$; Otherwise, $d_{v_1} = \frac{n}{2}$, and $Lz(G) = \frac{1}{4}n^3 + \frac{3}{4}n^2 - \frac{5}{2}n - 8$. □

**Lemma 3.4.** *For $n \geq 6$, let $G \in \mathcal{U}(n, 3)$ with $i_0 = 3$ be the maximal graph. Then $G = U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1})$ with $S_{t_1+1}, S_{t_2+1}$ and $S_{t_3+1}$ being uniform.*

*Proof.* $G$ can be written as $U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1})$. Since $G$ is the maximal graph, $d_{v_1}+d_{v_3} = t_1+t_3+4 \geq \frac{2(n-7)}{3}+4 = \frac{2n-2}{3}$ by Proposition 1.3. Similarly, $d_{v_1}+d_{v_2} \geq \frac{2n-2}{3}$. The convention before Transformation $A$ implies that $t_1 \leq t_2 \leq t_3$. Hence, $3 \leq d_{v_1} \leq d_{v_2} \leq d_{v_3}$.

Suppose to the contrary that $d_{v_3} - d_{v_1} \geq 2$. Then there are two cases.

**Case 1.** $d_{v_1} \leq d_{v_2} < d_{v_3}$.

Assume that $N(v_1)\backslash V(C_k) = \{x_1, x_2, \ldots, x_{t_1}\}$ and $N(v_3)\backslash V(C_k) = \{z_1, z_2, \ldots, z_{t_3}\}$. Let $G' = G - \{v_3z_{t_3}\} + \{v_1z_{t_3}\}$. Then $d'_{v_1} = d_{v_1}+1$, $d'_{v_3} = d_{v_3}-1$, and other vertices remain unchanged in their degrees. Let $D = \{v_1, v_3\}$, and the difference of their Lanzhou indices is

$$\begin{aligned} Lz(G') - Lz(G) &= \sum_{u\in D}[(n-1-d'_u)d'^2_u - (n-1-d_u)d_u^2] \\ &= -3d_{v_1}^2 + (2n-5)d_{v_1} + 3d_{v_3}^2 - (2n+1)d_{v_3} + 2n - 2 \\ &= (d_{v_3} - d_{v_1})[3(d_{v_1}+d_{v_3}) - 2n - 1] - 6d_{v_1} + 2n - 2. \end{aligned}$$

Since $d_{v_2} < d_{v_3}$, we have $d_{v_1}+d_{v_3} \geq d_{v_1}+d_{v_2}+1 \geq \frac{2n-2}{3}+1 = \frac{2n+1}{3}$. It suffices to prove that $d_{v_1} \leq \frac{n}{3} - \frac{1}{2}$. If so, then $-6d_{v_1} \geq -6(\frac{n}{3}-\frac{1}{2}) = -2n+3$. Consequently, $Lz(G') - Lz(G) \geq 2(3 \times \frac{2n+1}{3} - 2n - 1) - 2n + 3 + 2n - 2 = 1$, which contradicts that $G$ is maximal.

Suppose by the contrary that $d_{v_1} > \frac{n}{3} - \frac{1}{2}$. If $d_{v_1} \geq \frac{n}{3}+\frac{1}{2}$, then $n+3 = d_{v_1}+d_{v_2}+d_{v_3} \geq 3d_{v_1}+2 \geq 3(\frac{n}{3}+\frac{1}{2})+2 = n+3+\frac{1}{2}$, which is a contradiction. Otherwise, we have $\frac{n}{3}-\frac{1}{2} < d_{v_1} < \frac{n}{3}+\frac{1}{2}$. If $n \equiv 0 \pmod 3$, then $d_{v_1} = \frac{n}{3}$. Combining $d_{v_3}+d_{v_1} \geq 2d_{v_1}+2 = \frac{2n+6}{3}$, we have $Lz(G') - Lz(G) \geq 2[3(d_{v_1}+d_{v_3}) - 2n - 1] - 6d_{v_1} + 2n - 2 \geq 8$. Similarly, if $n \equiv 1 \pmod 3$, then $d_{v_1} = \frac{n-1}{3}$ and $Lz(G') - Lz(G) \geq 6$. Otherwise, $d_{v_1} = \frac{n+1}{3}$ and $Lz(G') - Lz(G) \geq 10$. All cases imply that $Lz(G') > Lz(G)$, which contradicts that $G$ is maximal.

**Case 2.** $d_{v_1} < d_{v_2} = d_{v_3}$.

Assume that $N(v_1)\backslash V(C_k) = \{x_1, x_2, \ldots, x_{t_1}\}$, $N(v_2)\backslash V(C_k) = \{y_1, y_2, \ldots, y_{t_2}\}$ and $N(v_3)\backslash V(C_k) = \{z_1, z_2, \ldots, z_{t_3}\}$. Let $G' = G - \{v_2y_{t_2}, v_3z_{t_3}\} + \{v_1y_{t_2}, v_1z_{t_3}\}$. Then $d'_{v_1} = d_{v_1}+2$, $d'_{v_2} = d_{v_2}-1$, $d'_{v_3} = d_{v_3}-1$, and other vertices remain unchanged in their degrees. Let $D = \{v_1,\ v_2,\ v_3\}$, and the difference of their Lanzhou indices is

$$\begin{aligned} Lz(G') - Lz(G) &= \sum_{u\in D}[(n-1-d'_u)d'^2_u - (n-1-d_u)d_u^2] \\ &= -6d_{v_1}^2 + 4(n-4)d_{v_1} + 4n - 12 + 6d_{v_2}^2 - 2(2n+1)d_{v_2} + 2n \\ &= (d_{v_2} - d_{v_1})[6(d_{v_1}+d_{v_2}) - 4n - 2] - 18d_{v_1} + 6n - 12. \end{aligned}$$

Since $n+3 = d_{v_1}+d_{v_2}+d_{v_3} \leq d_{v_2}-2+2d_{v_2} \leq 3d_{v_2}-2$, we obtain that $d_{v_2} \geq \frac{n+5}{3}$. On the other hand, $d_{v_2} = n+3-d_{v_1}-d_{v_3} \leq n+3-\frac{2n-2}{3} \leq \frac{n+11}{3}$. Hence, we obtain that $\frac{n+5}{3} \leq d_{v_2} \leq \frac{n+11}{3}$.

If $n \equiv 0 \pmod 3$, then $d_{v_2} = \frac{n+6}{3}$ or $\frac{n+9}{3}$. Hence, $d_{v_1}+d_{v_2} = n+3-d_{v_3} = \frac{2n+3}{3}$ or $\frac{2n}{3}$, $d_{v_1} = n+3-2d_{v_2} = \frac{n-3}{3}$ or $\frac{n-9}{3}$. Thus, $Lz(G') - Lz(G) = 18$ or $30$. Analogously, if $n \equiv 1 \pmod 3$, then $d_{v_2} = \frac{n+5}{3}$ or $\frac{n+8}{3}$ or $\frac{n+11}{3}$. We obtain that $Lz(G') - Lz(G) = 6$ or $30$ or $18$; If $n \equiv 2 \pmod 3$, then $d_{v_2} = \frac{n+7}{3}$ or $\frac{n+10}{3}$, and $Lz(G') - Lz(G) = 26$. Therefore, $Lz(G') - Lz(G) > 0$, which contradicts that $G$ is maximal. □

Next lemma determines Lanzhou indices of maximal graphs in $\mathcal{U}(n, 3)$ with $i_0 = 3$.

**Lemma 3.5.** *For $n \geq 6$, let $G \in \mathcal{U}(n,3)$ with $i_0 = 3$ be the maximal graph. Then*

$$Lz(G) = \begin{cases} \frac{2}{9}n^3 + \frac{5}{3}n^2 - 7n, & \text{if } n \equiv 0 \pmod 3; \\ \frac{2}{9}n^3 + \frac{5}{3}n^2 - 7n - \frac{26}{9}, & \text{if } n \equiv 1 \pmod 3; \\ \frac{2}{9}n^3 + \frac{5}{3}n^2 - 7n - \frac{22}{9}, & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

*Proof.* By Lemma 3.4, $G = U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1})$ with $\max\limits_{1\leq i<j\leq 3} |t_j - t_i| \leq 1$. By convention before Transformation $A$, we obtain that $0 \leq t_3 - t_1 \leq 1$.

If $t_3 - t_1 = 0$, then $t_1 = t_2 = t_3$; Otherwise, $t_1 = t_2,\ t_3 = t_1 + 1$ or $t_3 = t_2 = t_1 + 1$. Hence, the number of leaves in $G - E(C_3)$ is as follows. If $n \equiv 0 \pmod 3$, then $t_1 = t_2 = t_3 = \frac{n}{3} - 1$; If $n \equiv 1 \pmod 3$, then $t_1 = t_2 = \frac{n-4}{3},\ t_3 = \frac{n-1}{3}$. Otherwise, $t_1 = \frac{n-5}{3},\ t_2 = t_3 = \frac{n-2}{3}$. Since $d_{v_i} = t_i + 2$ for $i \in [1,3]$, Lanzhou index of graph $G$ with above three cases is as follows.

$$\begin{aligned} Lz(G) &= (n-3)(n-1-1) + 3(n-1-(\tfrac{n}{3}+1))(\tfrac{n}{3}+1)^2 \\ &= \tfrac{2}{9}n^3 + \tfrac{5}{3}n^2 - 7n, \\ Lz(G) &= (n-3)(n-1-1) + 2(n-1-\tfrac{n+2}{3})(\tfrac{n+2}{3})^2 + (n-1-\tfrac{n+5}{3})(\tfrac{n+5}{3})^2 \\ &= \tfrac{2}{9}n^3 + \tfrac{5}{3}n^2 - 7n - \tfrac{26}{9}, \\ Lz(G) &= (n-3)(n-1-1) + (n-1-\tfrac{n+1}{3})(\tfrac{n+1}{3})^2 + 2(n-1-\tfrac{n+4}{3})(\tfrac{n+4}{3})^2 \\ &= \tfrac{2}{9}n^3 + \tfrac{5}{3}n^2 - 7n - \tfrac{22}{9}. \end{aligned}$$

□

**Theorem 3.6.** *If $11 \leq n \leq 26$, then the maximal unicyclic graph is $U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1})$ with $S_{t_1+1}, S_{t_2+1}$ and $S_{t_3+1}$ being uniform; If $n = 27$, then the maximal unicyclic graphs are $U(C_3; S_{13}, S_{13}, v_3)$ and $U(C_3; S_9, S_9, S_9)$; If $n \geq 28$, then the maximal unicyclic graph is $U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3)$.*

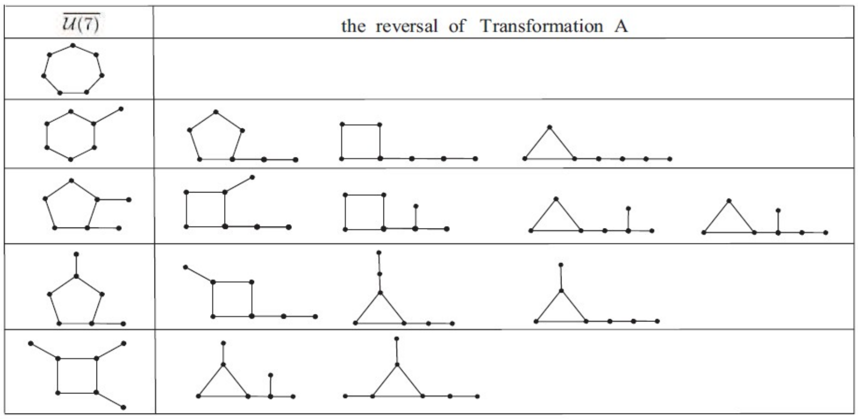
*Proof.* Let $G$ be a maximal graph in $\mathcal{U}(n)$. By Theorem 3.2, we know that $G \in \mathcal{U}(n,3)$ with $i_0 = 2$ or 3. If $i_0 = 2$, by Lemma 3.3, $G = U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3)$; If $i_0 = 3$, by Lemma 3.4, $G$ must be $U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1})$ with $S_{t_1+1}, S_{t_2+1}$ and $S_{t_3+1}$ being uniform. Comparing their Lanzhou indices, we obtain that for $7 \leq n \leq 26$, the former is less than the latter; For $n = 27$, theirs are equal; For $n \geq 28$, the former is more than the latter.

Now we consider unicycle graphs $G \notin \mathcal{U}(n)$. If $G$ is of maximum Lanzhou index, then, by Corollary 1.2 it can be transformed into a unicyclic graph $G'$ in $\mathcal{U}(n)$ by a series of Transformation $A$ such that $G$ and $G'$ have the same Lanzhou index and the length of the cycle of $G'$ is larger than that of $G$. That implies that $G'$ is also a maximal graph in $\mathcal{U}(n)$ whose cycle is of length at least 4, which contradicts Theorem 3.2. □

**Theorem 3.7.** *If $3 \leq n \leq 6$, then $C_n$ is the maximal unicyclic graph; If $n = 7$ and $8 \leq n \leq 10$, then the maximal unicyclic graphs are shown in Tables 1 and 2 respectively.*

*Proof.* For $3 \leq n \leq 7$, we first obtain that the maximal graphs in $\mathcal{U}(n)$ by an enumerative approach according to the value of $i_0$ $(0 \leq i_0 \leq \lfloor \frac{n}{2} \rfloor)$. Then by the reversal of Transformation $A$, we can get all maximal unicyclic graphs not in $\mathcal{U}(n)$. This way we can see that the maximal unicyclic graphs for $3 \leq n \leq 6$ are $C_n$, and for $n = 7$ the maximal unicyclic graphs are shown in Table 1.

Table 1. The maximal unicyclic graphs of $n = 7$.




From now on let $8 \le n \le 10$ and $G \in \overline{\mathcal{U}(n)}$ with the unique cycle $C_k$. Then we know that $1 \le i_0 \le 4$ by Lemma 3.1 and $i_0 \ge k-1$ is also true by the proof of Theorem 3.2. Hence, the maximal graphs belong to $\mathcal{U}(n,k)$ with $i_0 = 2$ and $k = 3$ or $3 \le i_0 \le 4$ and $k = i_0$ or $i_0+1$. For the former, by the proof of Theorem 3.6 we know that $Lz(U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3)) < Lz(U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1}))$ with $S_{t_1+1}, S_{t_2+1}$ and $S_{t_3+1}$ being uniform. Thus we need only to find maximal graphs in $\mathcal{U}(n,k)$ with $3 \le i_0 \le 4$ and $k = i_0$ or $i_0 + 1$.

We claim that except for $U(C_4, S_3, S_3, S_3, v_4)$, other graphs with $k = i_0+1$ are not maximal. For $n = 8$, $U(C_4; S_2, S_2, S_3, v_4)$ is the unique unicyclic graph with $k = i_0 + 1$, but $Lz(U(C_4; S_2, S_2, S_3, v_4)) = 164 < 168 = Lz(U(C_4; S_2, S_2, S_2, S_2))$. For $n = 9$ or 10, and $k = i_0 + 1$, we have $3 \le d_{v_1} \le 4$ and $d_{v_k} = 2$. Let $G' \in \mathcal{U}(n, i_0)$ be obtained from $G$ by Transformation $C^{-1}$ at specified vertex $v_1$. Then $Lz(G') - Lz(G) = (d_{v_1} - 1)(-3d_{v_1} + 2n - 8)$ by Proposition 2.1. So, for $n = 9$, we have $d_{v_1} = 3$, and $Lz(G') - Lz(G) = 2$, contradicting that $G \in \overline{\mathcal{U}(n)}$. For $n = 10$, $Lz(G') - Lz(G) \ge 0$, and equality holds if and only if $d_{v_1} = 4$. So $G = U(C_4, S_3, S_3, S_3, v_4)$. In a word we have $k = i_0$ or $G = U(C_4, S_3, S_3, S_3, v_4) \in \mathcal{U}(10, 4)$.

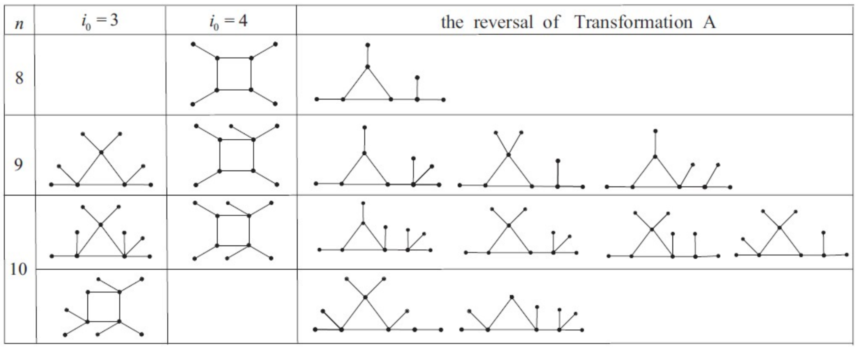
If $k = i_0 = 3$, then by Lemma 3.4, $G$ can be expressed as $U(C_3; S_{t_1+1}, S_{t_2+1}, S_{t_3+1})$ with $S_{t_1+1}, S_{t_2+1}$ and $S_{t_3+1}$ being uniform. If $k = i_0 = 4$, then $G = U(C_4; S_2, S_2, S_2, S_2)$ for $n = 8$, $G = U(C_4; S_2, S_2, S_2, S_3)$ for $n = 9$, $G = U(C_4; S_2, S_2, S_3, S_3)$ and $G = U(C_4; S_2, S_2, S_2, S_4)$ for $n = 10$. Combining it with some simple computations we have $G = U(C_4; S_2, S_2, S_2, S_2)$ for $n = 8$, $G = U(C_3; S_3, S_3, S_3)$ and $U(C_4; S_2, S_2, S_2, S_3)$ with the Lanzhou index 234 for $n = 9$, and $G = U(C_3; S_3, S_3, S_4), U(C_4; S_3, S_3, S_3, v_4)$ and $U(C_4; S_2, S_2, S_3, S_3)$ with the Lanzhou index 316 for $n = 10$.

Similar to the above case of $n = 7$ we can also generate all maximal unicyclic graphs not in $\mathcal{U}(n)$ for $8 \le n \le 10$ by the reversal of Transformation $A$, see Table 2. $\square$

In addition, there is a simple transformation between maximal unicyclic graphs and maximal trees for $n \ge 28$ as follows. The situation is complicated for the other cases.

**Corollary 3.8.** *Let $n \ge 28$. For the maximal unicyclic graph $U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3)$ with*

Table 2. The maximal unicyclic graphs for $n = 8, 9, 10$.




*cycle* $C_3 = v_1v_2v_3v_1$, $d_{v_1} = \lceil \frac{n}{2} \rceil$ *and* $d_{v_2} = \lfloor \frac{n+2}{2} \rfloor$, $U(C_3; S_{\lceil \frac{n-2}{2} \rceil}, S_{\lfloor \frac{n}{2} \rfloor}, v_3) - v_2v_3$ *is the maximal tree. Conversely, for the maximal tree* $BDS(n) = S_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ *with vertices* $v_1$ *and* $v_2$ *such that* $d_{v_1} = \lceil \frac{n}{2} \rceil$ *and* $d_{v_2} = \lfloor \frac{n}{2} \rfloor$, $BDS(n) + v_2v_3$ *is the maximal unicyclic graph for any leaf* $v_3$ *adjacent to* $v_1$.

## §4 Chemical graphs

In this section, we consider chemical unicyclic graphs (i.e. their maximum degree does not exceed four). Let $\mathcal{U}_n^{\Delta}$ denote the set of unicyclic graphs containing $n$ vertices with the maximum degree at most $\Delta$. For a graph $G$, let $n_i$ be the number of vertices with degree $i$ for a non-negative integer $i$. If each vertex of $G$ has degree between 1 and 4, we say $(n_1, n_2, n_3, n_4)$ is the degree-vector of $G$.

**Proposition 4.1.** *Let* $n \geq 11$ *and* $G \in \mathcal{U}_n^4$. *Then* $4n(n-3) \leq Lz(G) \leq 6n^2 + O(n)$. *The left equality holds if and only if* $G = C_n$. *The right equality is achieved just for unicyclic graphs with*

$$(n_1, n_2, n_3, n_4) = \begin{cases} (\frac{2n}{3}, 0, 0, \frac{n}{3}), & \textit{if } n \equiv 0 \pmod 3; \\ (\frac{2n-2}{3}, 1, 0, \frac{n-1}{3}), & \textit{if } n \equiv 1 \pmod 3; \\ (\frac{2n-1}{3}, 0, 1, \frac{n-2}{3}), & \textit{if } n \equiv 2 \pmod 3. \end{cases}$$

*Proof.* By Degree-Sum Formula, we have $n_1 + 2(n - n_1 - n_3 - n_4) + 3n_3 + 4n_4 = 2n$. So $n_1 = n_3 + 2n_4$, $n_2 = n - 2n_3 - 3n_4$, where $0 \leq 2n_3 + 3n_4 \leq n$. Then

$$\begin{aligned} Lz(G) &= (n_3 + 2n_4)(n-2) + 4(n - 2n_3 - 3n_4)(n-3) + 9n_3(n-4) + 16n_4(n-5) \\ &= 2(n-7)n_3 + 6(n-8)n_4 + 4n(n-3), \end{aligned}$$

which is an increasing function of $n_3$ and $n_4$ for $n \geq 8$. So it is minimized for $n_3 = n_4 = 0$. To find the maximum value, we need to maximize $2(n-7)n_3 + 6(n-8)n_4$ for integers $n_3$ and $n_4$ with $0 \leq 2n_3 + 3n_4 \leq n$. By an analogous argument as in [8], since a vertex of degree 4 has larger contribution to $Lz(G)$ than two vertices of degree 3 for $n \geq 11$, the right hand side is maximized for all chemical unicyclic graphs containing the largest possible number of vertices of degree 4. Thus, $n_4 = \frac{n}{3}, \frac{n-1}{3}$ or $\frac{n-2}{3}$ and $n_3 = 0, 0$ or 1 according to $n \equiv 0, 1$ or 2 (mod 3). Meanwhile, $Lz(G) \le 6n^2 - 28n,\ 6n^2 - 30n + 16$ or $6n^2 - 30n + 18$. Some corresponding maximal unicyclic graphs can be constructed: add two pendants to each of the $\lfloor \frac{n}{3} \rfloor$ vertices, and one pendant to the $n_1 - 2n_4$ vertex to a cycle of length $\lceil \frac{n}{3} \rceil$. □

**Remark 1.** The maximal graphs in $\mathcal{U}_n^4$ with $3 \le n \le 10$ have been determined; See the graphs in Tables 1 and 2 except for $U(C_3, S_3, S_3, S_4)$ in the case of $n = 10$, and all cycles $C_n$ with $3 \le n \le 6$. We can see that the upper bound on Lanzhou index in Proposition 4.1 is still effective for $n = 9$ and 10, but there are other maximal graphs with $(n_1, n_2, n_3, n_4) = (5, 0, 3, 1)$ and $(6, 0, 2, 2)$. For $3 \le n \le 8$, such upper bound no longer holds.

For $n \ge 9$ the minimal graphs in $\mathcal{U}_n^4$ are cycles $C_n$. For $3 \le n \le 8$ the minimal graphs in $\mathcal{U}_n^4$ are listed in Fig. 4, where $\mathcal{U}_8^4$ contains 10 minimal graphs. For $3 \le n \le 7$ the lower bound is no longer effective.

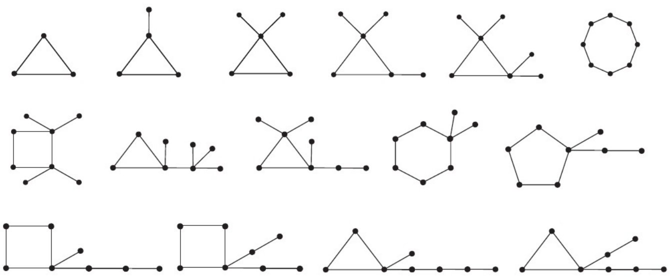


Fig. 4. The minimal graphs in $\mathcal{U}_n^4$ for $3 \le n \le 8$.

Let $\mathcal{T}_n^\Delta$ denote the set of all trees on $n$ vertices with the maximum degree at most $\Delta$. Proposition 6 in [8] gives the maximal and minimal Lanzhou indices of chemical trees in $\mathcal{T}_n^4$ for $n \ge 8$, and states that the maximal trees have largest possible number of vertices of degree 4. However, the maximal values for $n = 8$ and 9 are not correct. We can find that $G_2$ and $G_4$ with $n_4 \le 1$ have larger Lanzhou indices than $G_1$ and $G_3$ respectively (see Fig. 5). Even though, the proposition and its proof are correct for $n \ge 10$. So the proposition can be modified slightly as follows, and the corresponding maximal chemical trees always exist from the well-known Degree-Sum Formula (see Exercise 2.1.27 in [9]).

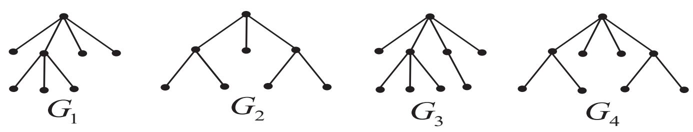



Fig. 5. Counterexamples for Proposition 6 in [8]: $Lz(G_1) = 132, Lz(G_2) = 138, Lz(G_3) = 194, Lz(G_4) = 196$.

**Proposition 4.2.** [8] *Let $n \ge 10$ and $T_n \in \mathcal{T}_n^4$. Then $4n^2 - 18n + 20 \le Lz(T_n) \le 6n^2 + O(n)$. The left equality holds if and only if $T_n = P_n$, and the maximum value of $Lz(T_n)$ is achieved* *just for any trees with*

$$(n_1, n_2, n_3, n_4) = \begin{cases} (\frac{2n}{3}, 1, 0, \frac{n-3}{3}), & \text{if } n \equiv 0 \pmod 3; \\ (\frac{2n+1}{3}, 0, 1, \frac{n-4}{3}), & \text{if } n \equiv 1 \pmod 3; \\ (\frac{2n+2}{3}, 0, 0, \frac{n-2}{3}), & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

For $n \geq 9$, the minimal unicyclic graph in $\mathcal{U}_n^4$ and minimal tree in $\mathcal{T}_n^4$ are $C_n$ and $P_n$ (a path with $n$ vertices) respectively. The following result gives some relations between their maximal graphs.

**Theorem 4.3.** *Let $n \geq 11$ with $n \equiv 1$ (mod 3). For any maximal tree $T_n \in \mathcal{T}_n^4$, by adding an edge between some pair of a vertex of degree 3 and a pendant, we can get a maximal graph in $\mathcal{U}_n^4$. Conversely, for a maximal graph $G \in \mathcal{U}_n^4$, the deletion of an edge in its cycle results in a maximal chemical tree if and only if one end of the edge has degree 2.*

*For $n \geq 11$ with $n \equiv 0$ or 2 (mod 3), any maximal graphs in $\mathcal{T}_n^4$ and in $\mathcal{U}_n^4$ cannot be transformed into each other by the addition and deletion of an edge.*

*Proof.* Let $n \geq 11$ with $n \equiv 1 \pmod 3$. For any maximal tree $T_n \in \mathcal{T}_n^4$, we have $(n_1, n_2, n_3, n_4) = (\frac{2n+1}{3}, 0, 1, \frac{n-4}{3})$ by Proposition 4.2. Hence, $T_n$ has at least 9 pendants and one vertex of degree 3. There must be a pendent that is not adjacent to the vertex of degree 3. By adding an edge between the two vertices to $T_n$, we can get a graph in $\mathcal{U}_n^4$ with degree-vector $(n_1, n_2, n_3, n_4) = (\frac{2n-2}{3}, 1, 0, \frac{n-1}{3})$, which is maximal by Proposition 4.1. Conversely, for a maximal graph $G \in \mathcal{U}_n^4$, we have $(n_1, n_2, n_3, n_4) = (\frac{2n-2}{3}, 1, 0, \frac{n-1}{3})$ by Proposition 4.1. Take an edge $e$ in the cycle of $G$. If one end of $e$ has degree 2, then the other end must have degree 4. So $G - e$ is a tree in $\mathcal{T}_n^4$ with $(n_1, n_2, n_3, n_4) = (\frac{2n+1}{3}, 0, 1, \frac{n-4}{3})$, which is maximal by Proposition 4.2. Otherwise, both ends of $e$ have degree 4. Hence, $G - e$ is a tree with $n_3 = 2$, which is not maximal in $\mathcal{T}_n^4$ by Proposition 4.2.

Let $n \geq 11$ with $n \equiv 0$ or 2 (mod 3) and $T_n$ be a maximal tree in $\mathcal{T}_n^4$. Then $n_2 \leq 1$ and $n_3 = 0$ by Proposition 4.2. In order to get a graph in $\mathcal{U}_n^4$ by adding an edge $e$ between two nonadjacent vertices of $T_n$, we know that one of such two vertices must be pendant. However, $T_n + e \in \mathcal{T}_n^4$ would be not maximal by Proposition 4.1, since it has a vertex of degree 2. Conversely, a maximal graph $G \in \mathcal{U}_n^4$ has $n_2 = 0$ and $n_3 \leq 1$ by Proposition 4.1. So any edge $e$ in the cycle of $G$ has an end of degree 4. Hence, $G - e \in \mathcal{T}_n^4$ and $n_3 \geq 1$, which is not maximal by Proposition 4.2. □

For the case $\Delta = 3$ we have similar results as Proposition 4.1 and Theorem 4.3.

**Proposition 4.4.** *Let $n \geq 8$ be an integer and $G \in \mathcal{U}_n^3$. Then $4n^2 - 12n \leq Lz(G) \leq 5n^2 - 19n - (n-7)\frac{1-(-1)^n}{2}$. The left equality holds if and only if $G = C_n$, and the right equality holds just for any unicyclic graphs with*

$$(n_1, n_2, n_3) = \begin{cases} (\frac{n}{2},\ 0,\ \frac{n}{2}), & \text{if } n \text{ is even}; \\ (\frac{n-1}{2}, 1, \frac{n-1}{2}), & \text{otherwise}. \end{cases}$$

*Proof.* By Degree-Sum Formula, we have $n_1 + 2(n - n_1 - n_3) + 3n_3 = 2n$. Then $n_1 = n_3$ and $n_2 = n - 2n_3$, where $0 \le 2n_3 \le n$. Therefore,

$$\begin{aligned} Lz(G) &= n_3(n-1-1) + 4(n-2n_3)(n-1-2) + 9n_3(n-1-3) \\ &= 2(n-7)n_3 + 4n(n-3), \end{aligned} \tag{1}$$

which is a strictly monotone increasing function of $n_3$ for $n \ge 8$. So it has the minimum value $4n(n-3)$ at $n_3 = 0$, and the maximum value $Lz(G) = 5n^2 - 19n - (n-7)\frac{1-(-1)^n}{2}$ obtained at $n_3 = \frac{n - \frac{1-(-1)^n}{2}}{2}$. Precisely, if $n$ is odd, then $n_3 = n_1 = \frac{n-1}{2}$, $n_2 = 1$; Otherwise, $n_3 = n_1 = \frac{n}{2}$, $n_2 = 0$. Some corresponding maximal unicyclic graphs can be constructed: add one pendant to each of the $\lfloor \frac{n}{2} \rfloor$ vertices to a cycle of length $\lceil \frac{n}{2} \rceil$. □

**Remark 2.** For $n = 7$, we can obtain that $Lz(G) = 4n(n-3) = 112$ for each $G \in \mathcal{U}_n^3$ from formula (1) (see Table 1), which is consistent to both upper and lower bounds in Proposition 4.4. For $3 \le n \le 6$, $Lz(G)$ is a strictly monotone decreasing function of $n_3$. Hence, $C_n$ is the only maximal graph, and the graphs shown in Fig. 6 are the minimal graphs. However, such bounds in Proposition 4.4 are no longer effective for $3 \le n \le 6$ by the monotonicity of $Lz(G)$.

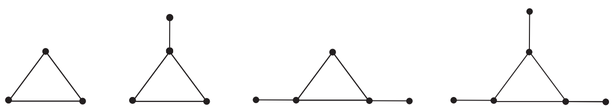


Fig. 6. The minimal graphs in $\mathcal{U}_n^3$ with $3 \le n \le 6$.

For maximal graphs in $\mathcal{T}_n^3$ and $\mathcal{U}_n^3$, we also have similar relations as in Theorem 4.3 as follows. The proof is also similar and omitted.

**Theorem 4.5.** *Let $n \ge 9$ be an odd number. For any maximal tree $T_n \in \mathcal{T}_n^3$, by adding an edge between some pair of a vertex of degree 2 and a pendant, we can get a maximal graph in $\mathcal{U}_n^3$. Conversely, for a maximal graph $G \in \mathcal{U}_n^3$, the deletion of an edge in its cycle results in a maximal tree in $\mathcal{T}_n^3$ if and only if one end of the edge has degree 2.*

*For an even number $n \ge 8$, any maximal graphs in $\mathcal{T}_n^3$ and in $\mathcal{U}_n^3$ cannot be transformed into each other by the addition and deletion of an edge.*

## §5 Conclusion

We have characterized all extremal unicyclic graphs with $n \ge 3$ vertices about Lanzhou index by three graph transformations. It turns out that the length of the cycle is 3 for all extremal unicyclic graphs except for some maximal graphs with $3 \le n \le 10$. Minimal unicyclic graphs and minimal trees can be transformed into each other by the addition and deletion of one edge. There are such simple transformations between maximal unicyclic graphs and maximal trees when $n \ge 28$. For chemical graphs with maximum degree at most 4 and 3 we have also determined respectively all extremal graphs. Our results show that in most cases there are no the above-mentioned transformations between extremal chemical unicyclic graphs and trees.

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