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A Note on Chemical Trees with Maximal Inverse Sum Indeg Index

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Abstract

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The inverse sum indeg index of G is defined as $ISI(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$, where $d(u)$ is the degree of vertex $u \in V(G)$. This index has a nice predicting ability for the total surface area of octane isomers. In this note, we completely characterize the structure of chemical trees with the maximal inverse sum indeg index, which resolves a problem posed by Sedlar, Stevanović, and Vasilyev (2015).

1 Introduction

Let $G = (V, E)$ be a simple graph, where $V(G) = \{v_0, v_1, \ldots, v_{n-1}\}$ and $E(G)$ are the vertex set and edge set of G, respectively. For $v_i \in V(G)$, let $d_i = d(v_i)$ denote the degree of v_i in G, and let $\Delta(G)$ denote the maximum degree of G. The degree sequence of G is $\pi(G) = (d_0, d_1, \ldots, d_{n-1})$, where $d_0 \geq d_1 \geq \cdots \geq d_{n-1}$. A tree is a connected acyclic graph, and a chemical tree is a tree T with $\Delta(T) \leq 4$.

The inverse sum indeg (ISI for short) index of a graph G is defined as [15]

$$ISI(G) = \sum_{v_iv_j\in E(G)} f(d_i, d_j) = \sum_{v_iv_j\in E(G)} \frac{d_id_j}{d_i + d_j},$$

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where $f(x,y) = \frac{xy}{x+y}$ for $x, y \geq 1$. This recently developed topological index was shown to has a nice predicting ability for the total surface area of octane isomers [15]. Some extremal values of ISI index have been determined by Sedlar et al. [14] for connected graphs, trees, chemical graphs, chemical trees, graphs with given maximum degree, minimum degree, or number of pendent vertices, and trees with k leaves. An and Xiong [2] later obtained the extremal ISI index among graphs with given matching number, vertex connectivity, or independence number. Similar results were also derived by Chen and Deng [3] for graphs with given connectivity, chromatic number, clique number, independence number, covering number, or vertex bipartiteness. In addition, Falahati-Nezhad et al. [6] established sharp bounds on ISI index in terms of various graph invariants, including the order, radius, size, and number of pendent vertices. Gutman et al. [8] presented several inequalities on ISI index and characterized the graphs attaining the equalities. Several lower bounds were also given by Gutman et al. [9]. For more results concerning ISI index, we refer to [1, 5, 7, 10–13].

For trees, Sedlar et al. [14] showed that the star uniquely has the minimal ISI index, and they also left the problem of determining the maximal ISI index in the classes of trees and chemical trees at the end of their paper. Recently, some structural properties of trees with the maximal ISI index were observed and proven by Chen et al. [4], but the problem is still open. In this note, we would completely resolve the problem for the case of chemical trees.

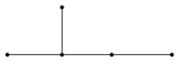
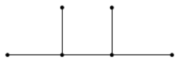
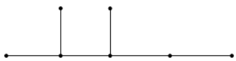
Let $\mathcal{T}_n$ be the set of all chemical trees on n vertices. For $n \leq 7$, the chemical trees with the maximal ISI index (optimal chemical trees, for short) can be easily determined by a direct calculation (see Table 1). So, in the following we always assume that $n = 7k + r \geq 8,\ k, r \in \mathbb{Z}$, and $0 \leq r \leq 6$. For $T \in \mathcal{T}_n$, an edge $uv \in E(T)$ with $d(u) = i$ and $d(v) = j$ is called an (i,j)-edge, and the number of (i,j)-edges in T is denoted by $m_{i,j}$. For $x \in \mathbb{R}$, let $\lfloor x \rfloor = \max\{a \in \mathbb{Z} \,|\, a \leq x\}$ and $\lceil x \rceil = \min\{a \in \mathbb{Z} \,|\, a \geq x\}$. We now denote by $\mathcal{T}_n^*(\subset \mathcal{T}_n)$ the set of all chemical trees on n vertices satisfying the following condition:

$m_{4,4} = k - 1$, $m_{4,3} = 2k - 1 + \lfloor \frac{r}{2} \rfloor$, $m_{4,1} = 3 - \lceil \frac{r}{2} \rceil$,

$m_{3,3} = n_{(3,2)} = 0$, $m_{3,1} = 4k - 2 + 2\lfloor \frac{r}{2} \rfloor$,

$m_{4,2} = m_{2,1} = 0$ if $r \in \{0, 2, 4, 6\}$, and $m_{4,2} = m_{2,1} = 1$ if $r \in \{1, 3, 5\}$.

Table 1. The optimal chemical trees of order 2–7.

n	optimal chemcial tree *T*	*ISI(T)*
2		$\frac{1}{2}$
3		$\frac{4}{3}$
4		$\frac{7}{3}$
5		$\frac{101}{30}$
6		$\frac{9}{2}$
7		$\frac{337}{60}$

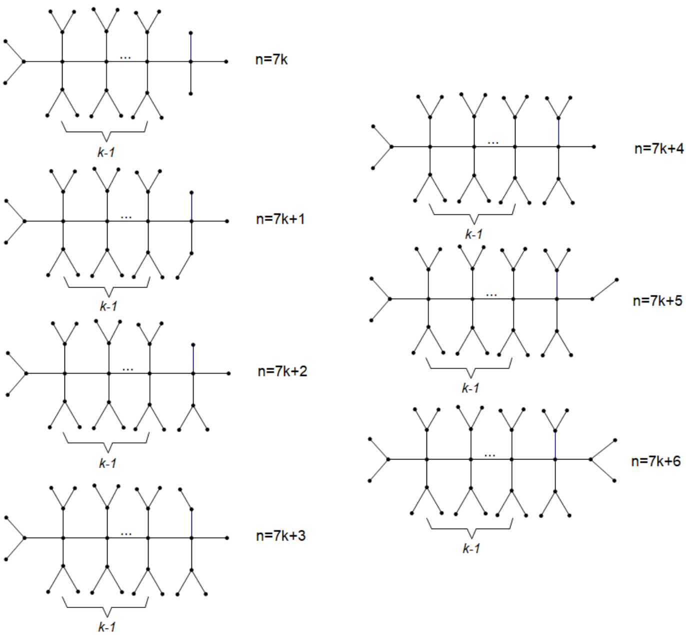


Figure 1. Some chemical trees in $\mathcal{T}_n^*(n \geq 8)$.

Note that for any $n \geq 8$, $\mathcal{T}_n^* \neq \varnothing$ (see Figure 1 for some chemical trees in $\mathcal{T}_n^*$), and for any $T^* \in \mathcal{T}_n^*$, it is easy to see that $n_4 = k$, $n_3 = 2k - 1 + \lfloor \frac{r}{2} \rfloor$, $n_1 = 4k + 1 + \lfloor \frac{r}{2} \rfloor$, $n_2 = 0$ if $r \in \{0, 2, 4, 6\}$, and $n_2 = 1$ if $r \in \{1, 3, 5\}$, where $n_i = |\{v \in V(T^*) \,|\, d(v) = i\}|$, $i \in \{1, 2, 3, 4\}$. Moreover, by a direct calculation, we have

$$ISI(T^*) = \frac{1}{70}\left(590k - 197 + 84r + \left\lfloor \frac{r}{2} \right\rfloor\right).$$

The main result of this note is as follows.

Theorem 1 *Let $n = 7k + r \geq 8$, $k, r \in \mathbb{Z}$, and $0 \leq r \leq 6$. For any $T \in \mathcal{T}_n$, we have*

$$ISI(T) \leq \frac{1}{70}\left(590k - 197 + 84r + \left\lfloor \frac{r}{2} \right\rfloor\right).$$

Moreover, the equality holds if and only if $T \in \mathcal{T}_n^*$.

The proof of Theorem 1 will be presented in the following section.

2 Proof of Theorem 1

We first recall the concept of BFS-graphs. For a rooted graph G with root v_0, the length of a shortest $v - v_0$ path (a path connecting v and v_0) in G, is called the height of a vertex v and denoted by $h(v)$.

Definition ([4]) *Let G be a connected rooted graph with root v_0. A well-ordering $\prec$ of the vertices is called a breadth-first searching ordering (with non-increasing degrees) if the following conditions hold for all vertices $u, v \in V(G)$:*

(B1) $u \prec v$ implies $h(u) \leq h(v)$;

(B2) $u \prec v$ implies $d(u) \geq d(v)$;

(B3) Let $uv, xy \in E(G)$ and $uy, xv \notin E(G)$ with $h(u) = h(x) = h(v) - 1 = h(y) - 1$. If $u \prec x$, then $v \prec y$.

A graph having a BFS-ordering of its vertices is called a BFS-graph. If a BFS-graph is a tree, then it is also called a BFS-tree.

To prove Theorem 1, we need some auxiliary results.

Lemma 2 ([4]) *Given a degree sequence π, there exists a BFS-graph with the maximal ISI index in $\mathcal{C}(\pi)$, where $\mathcal{C}(\pi)$ denotes the set of graphs with the degree sequence π.*

Lemma 2 suggests that, to find the optimal chemical trees, one can first determine their degree sequences $(4^{(n_4)}, 3^{(n_3)}, 2^{(n_2)}, 1^{(n_1)})$, where $a^{(k)}$ stands for k successive a's. Let $P = u_0u_1 \cdots u_l\ (l \geq 1)$ be a path of a graph G with $d(u_0) \geq 3$, $d(u_l) = 1$, and $d(u_i) = 2$ for $1 \leq i \leq l-1$. Then P is said to be a pendent path of G.

Lemma 3 ([4]) *An optimal chemical tree has no pendent paths of length* ≥ 3.

Lemma 4 ([4]) *An optimal chemical tree has at most one pendent path of length* 2.

Lemma 5 ([4]) *An optimal chemcial tree does not contain a path* $v_0v_1 \cdots v_l$ *of length* $l \geq 2$ *such that* $d(v_0) > d(v_i)$ *and* $d(v_l) > d(v_i)$ *for some* $i \in \{1, 2, \ldots, l-1\}$.

Although Lemmas 3, 4, and 5 were proved for trees in [4], we can use the same way to prove them for chemical trees. Now, by Lemmas 3, 4, and 5, we have the following.

Lemma 6 *If* $n \geq 8$, *then the degree sequence* $(4^{(n_4)}, 3^{(n_3)}, 2^{(n_2)}, 1^{(n_1)})$ *of an optimal chemical tree satisfies* $n_2 \in \{0, 1\}$.

Lemma 7 *If* $n \geq 8$, *then the degree sequence* $(4^{(n_4)}, 3^{(n_3)}, 2^{(n_2)}, 1^{(n_1)})$ *of an optimal chemical tree satisfies* $n_4 \geq 1$.

Proof. Let $T \in \mathcal{T}_n$ be an optimal chemical tree with degree sequence $(4^{(n_4)}, 3^{(n_3)}, 2^{(n_2)}, 1^{(n_1)})$. By contradiction, we can suppose that $n_4 = 0$. Now, by Lemma 6, we have $n_2 \in \{0, 1\}$. Since $3n_3 + 2n_2 + (n - n_3 - n_2) = 2(n-1)$, we get $n_3 = \frac{1}{2}(n - 2 - n_2)$.

If $n_2 = 0$, then we have $n_3 = \frac{n}{2} - 1$ and $n_1 = \frac{n}{2} + 1$, and hence,

$$ISI(T) = (n_3 - 1)f(3,3) + n_1 f(3,1) = \tfrac{9}{8}n - \tfrac{9}{4}.$$

If $n_2 = 1$, then we have $n_3 = \frac{1}{2}(n-3)$ and $n_1 = \frac{1}{2}(n+1)$, and hence

$$\begin{aligned} ISI(T) &= (n_3 - 1)f(3,3) + f(3,2) + (n_1 - 1)f(3,1) + f(2,1) \\ &= \tfrac{9}{8}n - \tfrac{271}{120} < \tfrac{9}{8}n - \tfrac{9}{4}. \end{aligned}$$

Since $n \geq 8$, we obtain $\frac{6}{5}n - \frac{9}{8}n = \frac{3}{40}n \geq 0.6 > \frac{197}{70} - \frac{9}{4}$. Consequently,

$$\begin{aligned} ISI(T) &\leq \tfrac{9}{8}n - \tfrac{9}{4} < \tfrac{6}{5}n - \tfrac{197}{70} = \tfrac{1}{70}(588k - 197 + 84r) \\ &< \tfrac{1}{70}\left(590k - 197 + 84r + \left\lfloor \tfrac{r}{2} \right\rfloor\right) = ISI(T^*), \end{aligned}$$

where $T^* \in \mathcal{T}_n^* \subset \mathcal{T}_n$, which contradicts the assumption that T is optimal. This proves that $n_4 \geq 1$, completing the proof of Lemma 7. ■

Lemma 8 *Let $n = 7k + r \geq 8$, $k, r \in \mathbb{Z}$, and $0 \leq r \leq 6$. For any $T \in \mathcal{T}_n$, if $n_2 = 0$, then*

$$ISI(T) \leq \begin{cases} \frac{59}{7}k + \frac{169}{140}r - \frac{197}{70}, & \textit{if } r \in \{0,2,4,6\}, \\ \frac{59}{7}k + \frac{169}{140}r - \frac{397}{140}, & \textit{if } r \in \{1,3,5\}, \end{cases} \tag{1}$$

and if $n_2 = 1$, then

$$ISI(T) \leq \begin{cases} \frac{59}{7}k + \frac{169}{140}r - \frac{199}{70}, & \textit{if } r \in \{0,2,4,6\}, \\ \frac{59}{7}k + \frac{169}{140}r - \frac{395}{140}, & \textit{if } r \in \{1,3,5\}. \end{cases} \tag{2}$$

Proof. Without loss of generality, we can suppose that $T \in \mathcal{T}_n$ is a chemical tree with degree sequence $\pi = (4^{(n_4)}, 3^{(n_3)}, 2^{(n_2)}, 1^{(n_1)})$. Since $4n_4 + 3n_3 + 2n_2 + n_1 = 2(n-1)$ and $n_4 + n_3 + n_2 + n_1 = n$, we have $n_3 = \frac{1}{2}(n - 2 - 3n_4 - n_2)$ and $n_1 = \frac{1}{2}(n + 2 + n_4 - n_2)$. Moreover, by Lemmas 6 and 7, we know that $n_2 \in \{0,1\}$ and $n_4 \geq 1$. On the other hand, from Lemma 2 it follows that there exists a BFS-tree $T' \in \mathcal{C}(\pi) \subset \mathcal{T}_n$ such that $ISI(T') \geq ISI(T)$. So, we can further assume that T is a BFS-tree. Consequently, we have $m_{4,3} + m_{4,2} + m_{4,1} = 4n_4 - 2m_{4,4} = 4n_4 - 2(n_4 - 1) = 2n_4 + 2$.

Case 1. $n_2 = 0$.

In this case, we have $n_3 = \frac{1}{2}(n - 2 - 3n_4)$ and $n_1 = \frac{1}{2}(n + 2 + n_4)$. If $n_3 \leq 2n_4 + 2$, then $\frac{1}{2}(n - 2 - 3n_4) \leq 2n_4 + 2$, which means that $n_4 \geq \lceil \frac{n-6}{7} \rceil = k$. Thus, we obtain

$$\begin{aligned} ISI(T) &= (n_4 - 1)f(4,4) + n_3 f(4,3) + (2n_4 + 2 - n_3)f(4,1) + 2n_3 f(3,1) \\ &= 2(n_4 - 1) + \frac{12}{7}n_3 + \frac{4}{5}(2n_4 - n_3 + 2) + \frac{3}{2}n_3 = \frac{1}{70}(-28 + 252n_4 + 169n_3) \\ &= \frac{1}{70}(-28 + 252n_4 + \frac{169}{2}(n - 2 - 3n_4)) = \frac{1}{140}(-394 + 169n - 3n_4) \\ &\triangleq g_1(n, n_4) \ . \end{aligned}$$

Moreover, since $g_1(n, n_4)$ is strictly decreased with n_4, and $n_3, n_1 \in \mathbb{Z}$, we have

$$ISI(T) = g_1(n, n_4) \leq \begin{cases} g_1(n,k) = \frac{59}{7}k + \frac{169}{140}r - \frac{197}{70}, & \text{if } r \in \{0,2,4,6\}, \\ g_1(n,k+1) = \frac{59}{7}k + \frac{169}{140}r - \frac{397}{140}, & \text{if } r \in \{1,3,5\}. \end{cases}$$

If $n_3 \geq 2n_4 + 3$, then $\frac{1}{2}(n - 2 - 3n_4) \geq 2n_4 + 3$, which means that $n_4 \leq \lfloor \frac{n-8}{7} \rfloor \leq k - 1$. Thus, we get

$$\begin{aligned} ISI(T) &= (n_4 - 1)f(4,4) + (2n_4 + 2)f(4,3) + (n_3 - 2n_4 - 2)f(3,3) \\ &+ (n - n_4 - n_3)f(3,1) \\ &= 2(n_4 - 1) + \tfrac{12}{7}(2n_4 + 2) + \tfrac{3}{2}(n_3 - 2n_4 - 2) + \tfrac{3}{4}(n - n_4 - n_3) \\ &= \tfrac{1}{28}(-44 + 21n + 47n_4 + 21n_3) = \tfrac{1}{28}(-44 + 21n + 47n_4 + \tfrac{21}{2}(n - 2 - 3n_4)) \\ &= \tfrac{1}{56}(-130 + 63n + 31n_4) \triangleq g_2(n, n_4) \ . \end{aligned}$$

Moreover, since $g_2(n, n_4)$ is strictly increased with n_4, we obtain

$$\begin{aligned} ISI(T) = g_2(n,n_4) \leq g_2(n,k-1) &= \frac{59}{7}k + \frac{9}{8}r - \frac{23}{8} \\ &< \frac{59}{7}k + \frac{169}{140}r - \frac{397}{140} = g_1(n,k+1) < g_1(n,k). \end{aligned}$$

Now, by combining the above arguments, we may obtain the desired bound (1).

Case 2. $n_2 = 1$.

In this case, we have $n_3 = \frac{1}{2}(n-3-3n_4)$ and $n_1 = \frac{1}{2}(n+1+n_4)$. If $n_3 \leq 2n_4+1$, then $\frac{1}{2}(n-3-3n_4) \leq 2n_4+1$, which means that $n_4 \geq \lceil \frac{n-5}{7} \rceil$. Thus, we obtain

$$\begin{aligned} ISI(T) &= (n_4-1)f(4,4) + n_3 f(4,3) + f(4,2) + (2n_4+2-n_3)f(4,1) \\ &+ 2n_3 f(3,1) + f(2,1) = \tfrac{1}{70}(56 + 252n_4 + 169n_3) \\ &= \tfrac{1}{140}(-395 + 169n - 3n_4) \triangleq g_3(n,n_4) \end{aligned}$$

Moreover, since $g_3(n, n_4)$ is strictly decreased with n_4, and $n_3, n_1 \in \mathbb{Z}$, we have

$$g_3(n,n_4) \leq \begin{cases} g_3(n,k+1) = \frac{59}{7}k + \frac{169}{140}r - \frac{199}{70}, & \text{if } r \in \{0,2,4,6\}, \\ g_3(n,k) = \frac{59}{7}k + \frac{169}{140}r - \frac{395}{140}, & \text{if } r \in \{1,3,5\}. \end{cases}$$

If $n_3 \leq 2n_4+2$, then $\frac{1}{2}(n-3-3n_4) \geq 2n_4+2$, which means that $n_4 \leq \lfloor \frac{n-7}{7} \rfloor = k-1$. Thus, we get

$$\begin{aligned} ISI(T) &= (n_4-1)f(4,4) + (2n_4+2)f(4,3) + (n_3-2n_4-2)f(3,3) + f(3,2) \\ &+ (n-n_4-n_3-2)f(3,1) + f(2,1) = \tfrac{1}{420}(-506 + 315n + 705n_4 + 315n_3) \\ &= \tfrac{1}{840}(-1957 + 945n + 465n_4) \triangleq g_4(n,n_4) \end{aligned}$$

Moreover, since $g_4(n, n_4)$ is strictly increased with n_4, we have

$$\begin{aligned} ISI(T) = g_4(n,n_4) \leq g_4(n,k-1) &= \frac{59}{7}k + \frac{9}{8}r - \frac{173}{60} \\ &< \frac{59}{7}k + \frac{169}{140}r - \frac{199}{70} = g_3(n,k+1) < g_3(n,k). \end{aligned}$$

Now, by combining the above arguments, we may obtain the desired bound (2). The proof of Lemma 8 is thus completed. ■

We are now ready to present the proof of Theorem 1.

Proof of Theorem 1. Let $n = 7k + r \geq 8$, $k, r \in \mathbb{Z}$, and $0 \leq r \leq 6$, and let $T \in \mathcal{T}_n$. Now, by combining Lemmas 7 and 8, we have

$$ISI(T) \leq \begin{cases} \frac{59}{7}k + \frac{169}{140}r - \frac{197}{70}, & \text{if } r \in \{0,2,4,6\}, \\ \frac{59}{7}k + \frac{169}{140}r - \frac{395}{140}, & \text{if } r \in \{1,3,5\}, \end{cases}$$

$$= \frac{1}{70}\left(590k - 197 + 84r + \left\lfloor \frac{r}{2} \right\rfloor\right). \tag{3}$$

Moreover, from the proof of Lemma 8, we know that the equality holds in (3) if and only if T satisfies the following conditions:

(a) $(4^{(n_4)}, 3^{(n_3)}, 2^{(n_2)}, 1^{(n_1)}) = (4^{(k)}, 3^{(2k-1+\lfloor \frac{r}{2} \rfloor)}, 2^{(\xi(r))}, 1^{(4k+1+\lfloor \frac{r}{2} \rfloor)})$;

(b) $m_{4,4} = k-1, m_{4,3} = 2k-1+\lfloor \frac{r}{2} \rfloor, m_{4,1} = 3 - \lceil \frac{r}{2} \rceil, m_{3,3} = m_{3,2} = 0, m_{3,1} = 4k-2+2\lfloor \frac{r}{2} \rfloor, m_{4,2} = m_{2,1} = \xi(r)$, where $\xi(r) = 0$ if $r \in \{0,2,4,6\}$ and $\xi(r) = 1$ if $r \in \{1,3,5\}$.

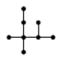
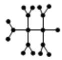
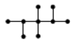
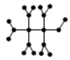
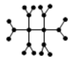
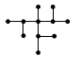
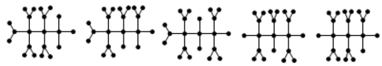
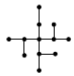
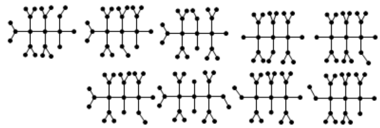
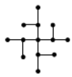
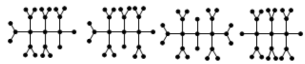
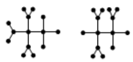
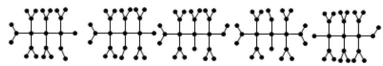
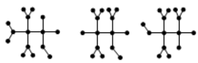
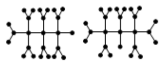
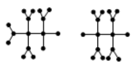
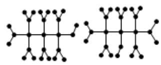
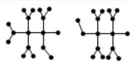
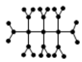
Since the condition (b) implies the condition (a), we can conclude that the equality holds in (3) if and only if $T \in \mathcal{T}_n^*$.

This completes the proof of Theorem 1. ■

3 Concluding remarks

For any $n \geq 2$, it is easy to see that the degree sequence of an optimal chemical tree is unique, but the optimal chemical trees need not be unique. Indeed, for $n \geq 28$, since $n_4 \geq 4$ and hence, the chemical trees in Figure 1 are not BFS-trees, which means that the optimal chemical trees are always not unique (Lemma 2 indicates that there always exists an optimal chemical tree which is a BFS-tree). For $2 \leq n \leq 27$, Tables 1 and 2 list all possible optimal chemical trees, which would yield that the optimal chemical trees are unique if and only if $n \in \{2, 3, \ldots, 13\} \cup \{18, 19, 20, 27\}$.

Table 2. The optimal chemical trees in $\mathcal{T}_n^*$ for $8 \le n \le 27$.

n	T_n^*	n	T_n^*
8		18	
9		19	
10		20	
11		21	
12		22	
13		23	
14		24	
15		25	
16		26	
17		27	

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