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Some sufficient conditions for Hamiltonian property in terms of Wiener-type invariants

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Abstract. The Wiener-type invariants of a simple connected graph $G = (V, E)$ can be expressed in terms of the quantities $W_f = \sum_{\{u,v\}\subseteq V} f(d_G(u, v))$ for various choices of the function $f(x)$, where $d_G(u, v)$ is the distance between vertices u and v in G. In this paper, we give some sufficient conditions for a connected graph to be Hamiltonian, a connected graph to be traceable, and a connected bipartite graph to be Hamiltonian in terms of the Wiener-type invariants.

Keywords. Wiener-type invariant; degree sequence; traceable; Hamilton.

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1. Introduction

In theoretical chemistry, molecular structure descriptors, also called topological indices, are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. One of the oldest, best studied and most often applied molecular structure descriptor is the Wiener index [16]

$$W(G) = \sum_{\{u,v\}\subseteq V} d_G(u, v)$$

where $G = (V, E)$ is the graph representing the molecule under consideration, and $d_G(u, v)$ is the distance between vertices u and v in graph G. More details on vertex distances and Wiener index can be found in the reviews [6, 7].

Several generalizations and modification of the Wiener index were put forward. Many of these Wiener-type invariants can be expressed in terms of the quantities

$$W_f = W_f(G) = \sum_{\{u,v\}\subseteq V} f(d_G(u, v))$$

for various choices of the function $f(x)$. In particular, W_x coincides with the ordinary Wiener index, $W_{\frac{1}{x^2}}$ was named the Harary index [13], but later the same name was used for $W_{\frac{1}{x}}$ [14]; other authors call $W_{\frac{1}{x}}$ the reciprocal Wiener index [5]. $W_{\frac{x+x^2}{2}}$ is called the hyper-Wiener index [15] denoted by WW. The quantity W_{x^λ} was studied for the first time by Gutman [8], and is called the modified Wiener index and denoted by W_λ, where $\lambda \neq 0$ is a real number. There are many papers devoted to the Wiener-type invariants W_f, see [4, 9, 11, 12] and the references cited therein.

Recall that a path or cycle which contains every vertex of a graph is called a Hamilton path or Hamilton cycle of the graph. A graph is traceable if it contains a Hamilton path, and Hamiltonian if it contains a Hamilton cycle. Concerning the existence of Hamiltonian path or Hamiltonian cycle, there are many famous sufficient conditions in terms of its vertex degrees, such as Dirac's condition [3], Chvátal's condition [2] and so on. Recently, Yang [17] and Hua and Wang [10] gave a sufficient condition for a connected graph to be traceable by using its Wiener index and Harary index, respectively. Zeng [18] also gave a sufficient condition, in terms of Harary index, for a connected bipartite graph to be Hamiltonian. In this paper, we will provide some new sufficient conditions in terms of the Wiener-type index W_f for a connected graph to be traceable or Hamiltonian.

Before proceeding, we introduce some further notation. For a simple connected graph $G = (V, E)$, $d_G(v)$ denotes the degree of a vertex v in G, and $d_G(u, v)$ denotes the distance between two vertices u and v in G. The maximum vertex distance in G is the diameter D of G. Let G and H be two vertex-disjoint graphs. The join of G and H, denoted by $G \vee H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{uv | u \in V(G) \text{ and } v \in V(H)\}$. Let K_n be the complete graph on n vertices. K_n^* denotes the graph obtained from K_n by deleting $n - 2$ edges incident with the same vertex. Let $K_{n,m}$ be the complete bipartite graph with bipartition (X, Y) and $|X| = n$, $|Y| = m$. $K_{n,n}^*$ denotes the bipartite graph obtained from $K_{n,n}$ by deleting $n - 1$ edges incident with the same vertex. For other notations and terminologies not defined here, the readers are referred to [1].

This paper is organized as follows: in §2, we give a sufficient condition for a connected graph to be Hamiltonian by means of the Wiener-type index. In §3, we give a sufficient condition for a connected graph to be traceable. In §4, we give a sufficient condition for a connected bipartite graph to be Hamiltonian.

2. Wiener-type index condition for a connected graph to be Hamiltonian

In this section, we will give a sufficient condition of a connected graph to be Hamiltonian by means of the Wiener-type index. First we introduce the following Chvátal condition for a connected graph to be Hamiltonian.

Lemma 1 [2]. *Let G be a nontrivial graph of order n, $n \geq 3$, with degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$. Suppose that there is no integer $k < \frac{n}{2}$, such that $d_k \leq k$ and $d_{n-k} \leq n - k - 1$, then G is Hamiltonian.*

Theorem 2. *Let G be a connected simple graph of order $n \geq 3$. If $W_f(G) \leq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - 2[f(2) - f(1)]$ for a monotonically increasing function $f(x)$ on $x \in [1, D]$, or $W_f(G) \geq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - 2[f(2) - f(1)]$ for a monotonically decreasing function $f(x)$ on $x \in [1, D]$, then G is Hamiltonian, unless $G \cong K_n^*$ or $K_2 \vee 3K_1$.*

Proof. Assume that G is not a Hamiltonian graph with degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$ and $n \geq 3$. By Lemma 1, there is a integer $k < \frac{n}{2}$, such that $d_k \leq k$ and $d_{n-k} \leq n-k-1$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, D]$, then

$$\begin{aligned}
W_f(G) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} f(d_G(v_i, v_j)) \\
&\geq \frac{1}{2}\sum_{i=1}^{n}[f(1)d_i + f(2)(n-1-d_i)] \\
&= \frac{1}{2}\sum_{i=1}^{n}[(n-1)f(2) + (f(1) - f(2))d_i] \\
&= \frac{f(2)}{2}n(n-1) - \frac{f(2)-f(1)}{2}\sum_{i=1}^{n} d_i \\
&\geq \frac{f(2)}{2}n(n-1) - \frac{f(2)-f(1)}{2}[k^2 + (n-2k)(n-k-1) \\
&\quad +k(n-1)] \\
&= \frac{f(2)}{2}n(n-1) - \frac{f(2)-f(1)}{2} \\
&\quad \times[(n^2-3n+4) - (k-1)(2n-3k-4)] \\
&= \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - 2[f(2) - f(1)] \\
&\quad +\frac{f(2)-f(1)}{2}(k-1)(2n-3k-4) \\
&\geq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - 2[f(2) - f(1)].
\end{aligned}$$

If $f(x)$ is a monotonically decreasing function for $x \in [1, D]$, then

$$\begin{aligned}
W_f(G) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} f(d_G(v_i, v_j)) \\
&\leq \frac{1}{2}\sum_{i=1}^{n}[f(1)d_i + f(2)(n-1-d_i)] \\
&= \frac{1}{2}\sum_{i=1}^{n}[(n-1)f(2) + (f(1) - f(2))d_i] \\
&= \frac{f(2)}{2}n(n-1) + \frac{f(1)-f(2)}{2}\sum_{i=1}^{n} d_i \\
&\leq \frac{f(2)}{2}n(n-1) + \frac{f(1)-f(2)}{2} \\
&\quad \times[k^2 + (n-2k)(n-k-1) + k(n-1)] \\
&= \frac{f(2)}{2}n(n-1) - \frac{f(2)-f(1)}{2} \\
&\quad \times[(n^2-3n+4) - (k-1)(2n-3k-4)] \\
&= \frac{f(1)}{2}n^2 + \left[f(2) - \frac{3}{2}f(1)\right]n - 2[f(2) - f(1)]
\end{aligned}$$

$$
\begin{aligned}
&+\frac{f(2)-f(1)}{2}(k-1)(2n-3k-4)\\
&\le \frac{f(1)}{2}n^2+\left[f(2)-\frac{3}{2}f(1)\right]n-2[f(2)-f(1)].
\end{aligned}
$$

Combining this fact and our assumption, we get $W_f(G)=\frac{f(1)}{2}n^2+[f(2)-\frac{3}{2}f(1)]n-2[f(2)-f(1)]$. So, all equalities above should be attained. Thus, we have (a) the diameter of G is no more than two; (b) $d_1=\cdots=d_k=k$, $d_{k+1}=\cdots=d_{n-k}=n-k-1$ and $d_{n-k+1}=\cdots=d_n=n-1$; and (c) $k=1$ or $2n=3k+4$.

If $k=1$, then $d_1=1$, $d_2=\cdots=d_{n-1}=n-2$, $d_n=n-1$, which implies that $G\cong K_n^*$. If $2n=3k+4$, then $n=5$ and $k=2$ due to the fact $k<\frac{n}{2}$. G is a connected graph of order 5 with $d_1=d_2=d_3=2$, $d_4=d_5=4$, which implies that $G\cong K_2\vee 3K_1$. It is easy to check that none of the graphs K_n^* or $K_2\vee 3K_1$ is Hamiltonian. This completes the proof. □

Let $f(x)=x$, $\frac{1}{x}$, $\frac{x^2+x}{2}$, x^λ in Theorem 2, respectively. We can get the following sufficient conditions in terms of the Wiener index, Harary index, hyper-Wiener index, modified Wiener index, respectively, for a connected graph to be Hamiltonian.

COROLLARY 3

Let G be a connected simple graph of order $n\ge 3$. If its Wiener index $W(G)\le \frac{1}{2}n^2+\frac{1}{2}n-2$, then G is Hamiltonian, unless $G\cong K_n^*$ or $K_2\vee 3K_1$.

COROLLARY 4

Let G be a connected simple graph of order $n\ge 3$. If its Harary index $H(G)\ge \frac{1}{2}n^2-n+1$, then G is Hamiltonian, unless $G\cong K_n^*$ or $K_2\vee 3K_1$.

COROLLARY 5

Let G be a connected simple graph of order $n\ge 3$. If its hyper-Wiener index $WW(G)\le \frac{1}{2}n^2+\frac{3}{2}n-4$, then G is Hamiltonian, unless $G\cong K_n^*$ or $K_2\vee 3K_1$.

COROLLARY 6

Let G be a connected simple graph of order $n\ge 3$. If its modified Wiener index $W_\lambda(G)\le \frac{1}{2}n^2+(2^\lambda-\frac{3}{2})n-2(2^\lambda-1)$ for $\lambda>0$, or $W_\lambda(G)\ge \frac{1}{2}n^2+(2^\lambda-\frac{3}{2})n-2(2^\lambda-1)$ for $\lambda<0$, then G is Hamiltonian, unless $G\cong K_n^*$ or $K_2\vee 3K_1$.

3. Wiener-type index condition for a graph to be traceable

In this section, we will give a sufficient condition of a connected graph to be traceable by means of the Wiener-type index. First we introduce the following condition for a connected graph to be traceable.

Lemma 7 [2]. *Let G be a graph of order n, $n\ge 4$, with degree sequence $(d_1,d_2,\ldots,d_n)$, where $d_1\le d_2\le\cdots\le d_n$. Suppose that there is no integer $k<\frac{n+1}{2}$, such that $d_k\le k-1$ and $d_{n-k+1}\le n-k-1$, then G is traceable.*

Now, we use Lemma 7 to give a new sufficient condition, in terms of the Wiener-type index, for a connected graph to be traceable.

Theorem 8. *Let G be a connected simple graph of order $n \geq 9$. If $W_f(G) \leq \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n + 5[f(1) - f(2)]$ for a monotonically increasing function $f(x)$ on $x \in [1, D]$, or $W_f(G) \geq \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n + 5[f(1) - f(2)]$ for a monotonically decreasing function $f(x)$ on $x \in [1, D]$, then G is traceable, unless $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$ or $K_4 \vee 6K_1$.*

Proof. Suppose that G is a non-traceable connected graph with degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$ and $n \geq 9$. By Lemma 7, there is a integer $k < \frac{n+1}{2}$, i.e., $k \leq \lfloor \frac{n}{2} \rfloor$, such that $d_k \leq k - 1$ and $d_{n-k+1} \leq n - k - 1$. Since G is connected and $1 \leq d_k \leq k - 1$, we have $k \geq 2$. Then

$$\begin{aligned}\sum_{i=1}^{n} d_i &\leq k(k-1) + (n-2k+1)(n-k-1) + (k-1)(n-1) \\ &= 3k^2 - (2n+1)k + n^2 - n = g(k).\end{aligned}$$

For $n \geq 9$ and $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$, we have $g(k) \leq g(2) = n^2 - 5n + 10$, i.e., $\sum_{i=1}^{n} d_i \leq n^2 - 5n + 10$ with equality if and only if (i) $k = 2, 5$ for $n = 10$ or (ii) $k = 2$ for $n \neq 10$.

If $f(x)$ is a monotonically increasing function for $x \in [1, D]$, then

$$\begin{aligned}W_f(G) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} f(d_G(v_i, v_j)) \\ &\geq \frac{1}{2}\sum_{i=1}^{n}[f(1)d_i + f(2)(n-1-d_i)] \\ &= \frac{1}{2}\sum_{i=1}^{n}[f(2)(n-1) + (f(1) - f(2))d_i] \\ &= \frac{f(2)}{2}n(n-1) - \frac{1}{2}[f(2) - f(1)]\sum_{i=1}^{n} d_i \\ &\geq \frac{f(2)}{2}n(n-1) - \frac{1}{2}[f(2) - f(1)][n^2 - 5n + 10] \\ &= \frac{f(1)}{2}n^2 + \left[2f(2) - \frac{5}{2}f(1)\right]n + 5[f(1) - f(2)].\end{aligned}$$

If $f(x)$ is a monotonically decreasing function for $x \in [1, D]$, then

$$\begin{aligned}W_f(G) &\leq \frac{1}{2}\sum_{i=1}^{n}[f(1)d_i + f(2)(n-1-d_i)] \\ &= \frac{1}{2}\sum_{i=1}^{n}[f(2)(n-1) + (f(1) - f(2))d_i] \\ &= \frac{f(2)}{2}n(n-1) + \frac{1}{2}[f(1) - f(2)]\sum_{i=1}^{n} d_i\end{aligned}$$

$$\leq \frac{f(2)}{2}n(n-1) + \frac{1}{2}[f(1) - f(2)][n^2 - 5n + 10]$$
$$= \frac{f(1)}{2}n^2 + \left[2f(2) - \frac{5}{2}f(1)\right]n + 5[f(1) - f(2)].$$

By our assumption, we have $W_f(G) = \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n + 5[f(1) - f(2)]$. So, all the above equalities should be attained. And we have (a) the diameter of G is no more than two; (b) $d_1 = \cdots = d_k = k-1$, $d_{k+1} = \cdots = d_{n-k+1} = n-k-1$ and $d_{n-k+2} = \cdots = d_n = n-1$; and (c) $k = 2$, or $k = 5$ and $n = 10$.

If $k = 2$, then G is a connected simple graph with $d_1 = d_2 = 1$, $d_3 = \cdots = d_{n-1} = n-3$ and $d_n = n-1$, which implies that $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$.

If $k = 5$, then $n = 10$. And G is a connected simple graph of order 10 with $d_1 = \cdots = d_6 = 4$, $d_7 = \cdots = d_{10} = 9$, which implies that $K_4 \vee 6K_1$.

It is easy to check that none of the graphs $K_1 \vee (K_{n-3} \cup 2K_2)$ and $K_4 \vee 6K_1$ is traceable. This complete the proof. □

Let $f(x) = x, \frac{1}{x}, \frac{x^2+x}{2}, x^\lambda$ in Theorem 2, respectively. We can get the following sufficient conditions in terms of the Wiener index, Harary index, hyper-Wiener index, modified Wiener index, respectively, for a connected graph to be traceable. Note that the following Corollaries 9 and 10 are also given in [17] and [10], respectively, but there is a flaw in the proof of their theorems for $4 \leq n \leq 8$.

COROLLARY 9 [17]

Let G be a connected simple graph of order $n \geq 9$. If its Wiener index $W(G) \leq \frac{1}{2}n^2 + \frac{3}{2}n - 5$, then G is traceable, unless $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$ or $K_4 \vee 6K_1$.

COROLLARY 10 [10]

Let G be a connected simple graph of order $n \geq 9$. If its Harary index $W(G) \leq \frac{1}{2}n^2 - \frac{3}{2}n + \frac{5}{2}$, then G is traceable, unless $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$ or $K_4 \vee 6K_1$.

COROLLARY 11

Let G be a connected simple graph of order $n \geq 9$. If its hyper-Wiener index $WW(G) \leq \frac{1}{2}n^2 + \frac{7}{2}n - 10$, then G is traceable, unless $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$ or $K_4 \vee 6K_1$.

COROLLARY 12

Let G be a connected simple graph of order $n \geq 9$. If its modified Wiener index $W_\lambda(G) \leq \frac{1}{2}n^2 + (2^{\lambda+1} - \frac{5}{2})n + 5(1 - 2^\lambda)$ for $\lambda > 0$, or $W_\lambda(G) \geq \frac{1}{2}n^2 + (2^{\lambda+1} - \frac{5}{2})n + 5(1 - 2^\lambda)$ for $\lambda < 0$, then G is traceable, unless $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$ or $K_4 \vee 6K_1$.

4. Wiener-type index condition for a connected bipartite graph to be Hamiltonian

In this section, we will give a sufficient condition of a connected bipartite graph to be Hamiltonian by using of the Wiener-type index.

Lemma 13 [2]. *Let $G = G[X, Y]$ be a connected simple and bipartite graph with $|X| = |Y| = n \geq 2$ and degree sequence $(d_1, d_2, \ldots, d_{2n})$, where $d_1 \leq d_2 \leq \cdots \leq d_{2n}$. Suppose that there is no integer $k \leq \frac{n}{2}$, such that $d_k \leq k$ and $d_n \leq n - k$. Then G is Hamiltonian.*

Theorem 14. *Let $G = G[X, Y]$ be a connected simple and bipartite graph with $|X| = |Y| = n \geq 2$. If $W_f(G) \leq [f(1)+f(2)]n^2 - [f(1)+f(2)-f(3)]n + [f(1)-f(3)]$ for a monotonically increasing function $f(x)$ on $x \in [1, D]$, or $W_f(G) \geq [f(1)+f(2)]n^2 - [f(1)+f(2)-f(3)]n + [f(1)-f(3)]$ for a monotonically decreasing function $f(x)$ on $x \in [1, D]$, then G is Hamiltonian, unless $G \cong K^*_{n,n}$.*

Proof. By contradiction, suppose that G is not a Hamiltonian connected bipartite graph. By Lemma 13, there exists an integer $k \leq \frac{n}{2}$ such that $d_k \leq k$ and $d_n \leq n - k$. Then

$$\sum_{i=1}^{2n} d_i \leq k^2 + (n-k)^2 + n^2 = 2(k^2 - kn + n^2) \leq 2n^2 - 2n + 2$$

with equalities if and only if $k = 1$, $d_1 = 1$, $d_2 = \cdots = d_n = n - 1$ and $d_{n+1} = \cdots = d_{2n} = n$, i.e., $G \cong K^*_{n,n}$.

If $f(x)$ is a monotonically increasing function for $x \in [1, D]$, then

$$\begin{aligned} W_f(G) &= \frac{1}{2}\sum_{i=1}^{2n}\sum_{j=1}^{2n} f(d_G(v_i, v_j)) \\ &\geq \frac{1}{2}\sum_{i=1}^{2n}[f(1)d_i + f(2)(n-1) + f(3)(n-d_i)] \\ &= f(2)n(n-1) + f(3)n^2 - \frac{f(3)-f(1)}{2}\sum_{i=1}^{2n} d_i \\ &\geq f(2)n(n-1) + f(3)n^2 - \frac{f(3)-f(1)}{2}[2n^2 - 2n + 2] \\ &= [f(1)+f(2)]n^2 - [f(1)+f(2)-f(3)]n + [f(1)-f(3)]. \end{aligned}$$

If $f(x)$ is a monotonically decreasing function for $x \in [1, D]$, then

$$\begin{aligned} W_f(G) &= \frac{1}{2}\sum_{i=1}^{2n}\sum_{j=1}^{2n} f(d_G(v_i, v_j)) \\ &\leq \frac{1}{2}\sum_{i=1}^{2n}[f(1)d_i + f(2)(n-1) + f(3)(n-d_i)] \\ &= f(2)n(n-1) + f(3)n^2 + \frac{f(1)-f(3)}{2}\sum_{i=1}^{2n} d_i \\ &\leq f(2)n(n-1) + f(3)n^2 + \frac{f(1)-f(3)}{2}[2n^2 - 2n + 2] \\ &= [f(1)+f(2)]n^2 - [f(1)+f(2)-f(3)]n + [f(1)-f(3)]. \end{aligned}$$

Combining this fact and our assumption, we get $W_f(G) = [f(1) + f(2)]n^2 - [f(1) + f(2) - f(3)]n + [f(1) - f(3)]$, and all equalities above should be attained. So, we have $G \cong K^*_{n,n}$. This completes the proof. □

Let $f(x) = x, \frac{1}{x}, \frac{x^2+x}{2}, x^\lambda$ in Theorem 14, respectively. We can get the following sufficient conditions in terms of the Wiener index, Harary index, hyper-Wiener index, modified Wiener index, respectively, for a connected bipartite graph to be Hamiltonian.

COROLLARY 15

Let $G = G[X, Y]$ be a connected simple and bipartite graph with $|X| = |Y| = n \geq 2$. If its Wiener index $W(G) \leq 3n^2 - 2$, then G is Hamiltonian, unless $G \cong K^*_{n,n}$.

COROLLARY 16

Let $G = G[X, Y]$ be a connected simple and bipartite graph with $|X| = |Y| = n \geq 2$. If its Harary index $H(G) \geq \frac{3}{2}n^2 - \frac{7}{6}n + \frac{2}{3}$, then G is Hamiltonian, unless $G \cong K^*_{n,n}$.

COROLLARY 17

Let $G = G[X, Y]$ be a connected simple and bipartite graph with $|X| = |Y| = n \geq 2$. If its hyper-Wiener index $WW(G) \leq 4n^2+2n-5$, then G is Hamiltonian, unless $G \cong K^*_{n,n}$.

COROLLARY 18

Let $G = G[X, Y]$ be a connected simple and bipartite graph with $|X| = |Y| = n \geq 2$. If its modified Wiener index $W_\lambda(G) \leq (1 + 2^\lambda)n^2 - (1 + 2^\lambda - 3^\lambda)n + (1 - 3^\lambda)$ for $\lambda > 0$, or $W_\lambda(G) \geq (1 + 2^\lambda)n^2 - (1 + 2^\lambda - 3^\lambda)n + (1 - 3^\lambda)$ for $\lambda < 0$, then G is Hamiltonian, unless $G \cong K^*_{n,n}$.

Corollaries 16 and 17 improve the results in [18].

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