Harmonic index of graphs with more than one cut-vertex

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Abstract

The harmonic index $H(G)$ of a graph G is defined as the sum of the weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u in G. In this work we compute the harmonic index of a graph with a cut-vertex and with more than one cut-vertex. As an application, this topological index is computed for Bethe trees and dendrimer trees. Also, the harmonic indices of Fasciagraph and a special type of trees, namely, polytree are computed.

Keywords : Graph; Degree; Cut-vertex; Cut-edge; Block; Harmonic Index

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The Randić Index of G is one of the most successful molecular descriptors in structure-property and structure-activity relationship studies. It is defined as $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$ where $d(u)$ is the degree of the vertex u in G [12]. The mathematical properties of this invariant have been studied extensively in [8] [11]. Motivated by the success of Randić index, various generalizations and modifications were introduced, such as the sum connectivity and the general sum connectivity index.

In this paper, we consider another variant of the Randić index, known as the harmonic index $H(G)$. For a graph G, the harmonic index $H(G)$ is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$ where $d(u)$ is the degree of the vertex u in G. As far as we know, this index first appeared in [7]. Zhong found the minimum and maximum values of the harmonic index for simple connected graphs, trees and unicyclic graphs and characterized the corresponding extremal graphs [17] [18]. Zhong *et al.* studied the harmonic index of bicyclic graphs and characterized the corresponding extremal graphs [19]. Deng *et al.* determined the trees with the second to the sixth maximum harmonic indices, and bicyclic graphs with the first four maximum harmonic indices [6]. The same authors considered the relation between the harmonic index $H(G)$ and the chromatic number and proved that $\chi(G) \leq 2H(G)$ by using the effect of removal of a minimum degree vertex on the harmonic index [5]. Wu *et al.* gave a best possible lower bound for the harmonic index of a triangle-free graph with minimum degree at least two and characterized the extremal graphs [14]. Zhong *et al.* gave some sharp lower bounds for harmonic index in terms of the other vertex-degree-based topological indices such as Zagreb index, Randić index, sum-connectivity index and ABC index [16]. Gutman gave a survey of selected degree-based topological indices and summarized their properties [9]. Xu *et al.* found the first and the second Zagreb indices of the set of connected graphs of order n and size m and characterized the extremal graphs [15].

Assuming that the graph G has more than one cut-vertex, Balakrishnan *et al.* obtained an expression for Wiener Index of the graph G in terms of the blocks of G and other quantities [3]. Similar to this, we obtain an expression for the harmonic index of a graph with a cut-vertex and with more than one cut-vertex. As an application, this topological index is computed for Bethe trees and dendrimer trees. Also, the harmonic index of Fasciagraph and a special type of trees, namely, polytree are computed.

We conclude this section with some notation and terminology. Let G be a graph. The degree of a vertex v of G is denoted by $d(v)$. If $d(v) = 1$ then v is said to be a pendant vertex in G and the edge incident with v is referred to as pendant edge. The set of neighbours of v is denoted by $N_G(v)$. For an edge $e = uv$, the weight of e in G is $w_G(e) = \dfrac{2}{d(u) + d(v)}$. A connected non trivial graph having on cut-vertices is called a block. A block of a graph is a subgraph that is a block and is maximal with respect to this property. As usual, P_n and S_n denote the path and the star on n vertices respectively. For other notations in graph theory, please refer to [2] [4].

2 Harmonic index of graphs with more than one cut-vertex

In this section, we compute the harmonic index of a graph with a cut-vertex and with more than one cut-vertex in terms of the harmonic index of the blocks of the graph.

Theorem 1. *Let G be a simple connected graph with a cut-vertex u. Let H_i, $1 \leq i \leq r$, be the components of $G - u$. Let $G_i = G\left[V\left(H_i\right) \bigcup \{u\}\right]$.*

Then

$$H(G)=\sum_{i=1}^{r}H\left(G_i\right)-2\sum_{i=1}^{r}\sum_{w\in N_{G_i}(u)}\left\{\frac{k-k_i}{\left[k_i+d\left(w\right)\right]\left[k+d\left(w\right)\right]}\right\} \tag{1}$$

where $d_G\left(u\right)=k$ *and* $d_{G_i}\left(u\right)=k_i$.

Proof.

$$\begin{aligned} H(G) &= \sum_{i=1}^{r}H(G_i)-\sum_{i=1}^{r}\sum_{w\in N_{G_i}(u)}\frac{2}{k_i+d(w)}+\sum_{i=1}^{r}\sum_{w\in N_{G_i}(u)}\frac{2}{k+d(w)} \\ &= \sum_{i=1}^{r}H\left(G_i\right)-2\sum_{i=1}^{r}\sum_{w\in N_{G_i}(u)}\left\{\frac{k-k_i}{\left[k_i+d\left(w\right)\right]\left[k+d\left(w\right)\right]}\right\} \end{aligned}$$

■

Our result in this work can be regarded as a generalization of (1). So we have the following theorem.

Theorem 2. *Let* $\mathscr{C}=\{v_1,v_2,\ldots,v_l\}$ *be the set of all cut-vertices and* $\mathscr{B}=\{B_1,B_2,\ldots,B_k\}$ *be the set of all blocks of a simple connected graph* G*. Then*

$$\begin{aligned} H(G) = \sum_{i=1}^{k}H(B_i) &- 2\sum_{i=1}^{l}\sum_{B\in B_i'}\sum_{\substack{x\in N_B(v_i)\\ x\notin\mathscr{C}}}\left\{\frac{1}{d_B(v_i)+d_B(x)}-\frac{1}{d_G(v_i)+d_G(x)}\right\} \\ &-\sum_{i=1}^{l}\sum_{B\in B_i'}\sum_{\substack{x\in N_B(v_i)\\ x\in\mathscr{C}}}\left\{\frac{1}{d_B(v_i)+d_B(x)}-\frac{1}{d_G(v_i)+d_G(x)}\right\} \end{aligned} \tag{2}$$

where $B_i'=\{B\in\mathscr{B}|v_i\in B\},\quad 1\le i\le l$.

Proof. Clearly $d_G(v_i)=\sum_{B\in B_i'}d_B(v_i)$, for $1\le i\le l$ and $E(G)=\bigcup_{i=1}^{k}E(B_i)$. Let $e=uv\in E(G)$. Obviously $e\in B_i$ for some i. If $u,v\notin\mathscr{C}$, then the weight of e in G is the same as the weight of e in B_i. Let us consider the case that either u or $v \in \mathscr{C}$. Without loss of generality, assume that $u \in \mathscr{C}$. The weight of e in B_i is less by $2\left\{\frac{1}{d_{B_i}(u)+d_{B_i}(v)} - \frac{1}{d_G(u)+d_G(v)}\right\}$ from the weight of e in G. Similarly if $u, v \in \mathscr{C}$ then the weight of e in B_i is less by $\left\{\frac{1}{d_{B_i}(u)+d_{B_i}(v)} - \frac{1}{d_G(u)+d_G(v)}\right\}$ from the weight of e in G. Hence

$$H(G) = \sum_{i=1}^{k} H(B_i) - 2\sum_{i=1}^{l}\sum_{B\in B_i'}\sum_{\substack{x\in N_B(v_i)\\ x\notin\mathscr{C}}}\left\{\frac{1}{d_B(v_i)+d_B(x)} - \frac{1}{d_G(v_i)+d_G(x)}\right\}$$
$$-\sum_{i=1}^{l}\sum_{B\in B_i'}\sum_{\substack{x\in N_B(v_i)\\ x\in\mathscr{C}}}\left\{\frac{1}{d_B(v_i)+d_B(x)} - \frac{1}{d_G(v_i)+d_G(x)}\right\}$$

∎

Using the above theorem we can calculate the harmonic index of a graph with a cut-edge as follows.

Corollary 1. *Let $uv \in E(G)$ be a cut-edge of G and let G_1 and G_2 be the two components of $G - uv$. Then*

$$H(G) = H(G_1) + H(G_2) - 2\left\{\sum_{w\in N(u)-\{v\}}\frac{1}{[d(u)+d(w)-1][d(u)+d(w)]}\right.$$
$$\left. + \sum_{w\in N(v)-\{u\}}\frac{1}{[d(v)+d(w)-1][d(v)+d(w)]} - \frac{1}{d(u)+d(v)}\right\}$$

Using the equation (2), we also find the upper and lower bounds for harmonic index of trees as follows.

3 Harmonic Index of Generalized Bethe Trees

In a tree, any vertex can be chosen as the root vertex. Suppose T is an unweighted rooted tree such that its vertices at the same level have equal degrees. The root vertex is at level 1 and T has k levels. In [1], Rojo and Robbiano, called such a tree as generalized Bethe tree. They donoted the class of generalized Bethe tree of k levels by B_k.

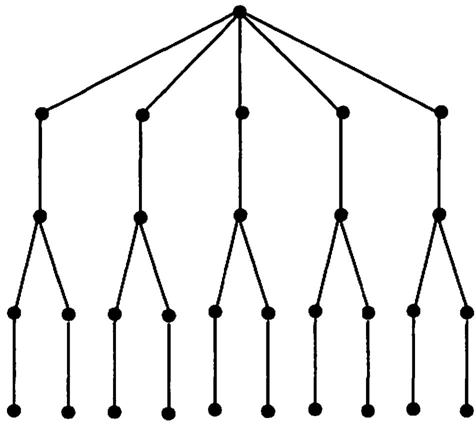

Figure 1: Generalized Bethe Tree of 5 levels

In this section we compute the harmonic index of Bethe tree using (2).

Theorem 3. *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. If d_1 denotes the degree of rooted vertex, d_i+1 denotes degree of the vertices on the i^{th} level of B_{k+1} for $1 < i < k+1$ and n_i denotes the number of vertices on the i^{th} level of B_{k+1} for $1 \leq i \leq k+1$, then the harmonic index of B_{k+1} is computed as follows.*

$$H(B_{k+1}) = 2\left\{\frac{n_2}{d_1+d_2+1} + \sum_{i=2}^{k-1} \frac{n_{i+1}}{d_i + d_{i+1} + 2} + \frac{n_{k+1}}{d_k+2}\right\} \tag{3}$$

Proof. Clearly $n_1 = 1$ and $n_i = d_1 d_2 d_3 \cdots d_{i-1}$ for $1 < i \leq k+1$. Also $|V(B_{k+1})| = 1 + \sum_{i=1}^{k} \prod_{j=1}^{i} d_j$ and each block of B_{k+1} is K_2, nothing but the edges of B_{k+1}. In B_{k+1} the rooted vertex belongs to d_1 blocks and the vertices in i^{th} level of B_{k+1} belongs to d_i+1 blocks, $2 \leq i \leq k$. Using equation (2)

$$H(B_{k+1}) = \sum_{i=1}^{k}\prod_{j=1}^{i} d_j - 2d_1d_2d_3\cdots d_k\left(\frac{1}{2}-\frac{1}{d_k+2}\right)$$
$$-2\left\{d_1\left(\frac{1}{2}-\frac{1}{d_1+d_2+1}\right)+d_1d_2\left(\frac{1}{2}-\frac{1}{d_2+d_3+2}\right)+\cdots\right.$$
$$\left.+d_1d_2d_3\cdots d_{k-1}\left(\frac{1}{2}-\frac{1}{d_{k-1}+d_k+2}\right)\right\}$$
$$=2\left\{d_1\frac{1}{d_1+d_2+1}+d_1d_2\frac{1}{d_2+d_2+2}+\cdots\right.$$
$$\left.+d_1d_2\cdots d_{k-1}\frac{1}{d_{k-1}+d_k+2}+d_1d_2\cdots d_k\frac{1}{d_k+2}\right\}$$
$$=2\left\{\frac{n_2}{d_1+d_2+1}+\sum_{i=2}^{k-1}\frac{n_{i+1}}{d_i+d_{i+1}+2}+\frac{n_{k+1}}{d_k+2}\right\}$$

∎

A dendrimer tree $T_{k,d}$ is a rooted tree such that degree of whose non-pendant vertices is equal to d and distance between the rooted vertex and pendant vertices is equal to k. So $T_{k,d}$ can be considered as a generalized Bethe tree with $k+1$ levels such that non-pendant vertices have equal degree. We can compute the harmonic index of dendrimer tree as follows using equation (3).

Corollary 2. *Let $T_{k,d}$ be a dendrimer tree of $k+1$ levels whose degree of the non-pendant vertices is equal to d. Then*

$$H(T_{k,d}) = \frac{(2d-1)(d-1)^k-(d+1)}{(d+1)(d-2)} \tag{4}$$

Proof. Comparing this $T_{k,d}$ with B_{k+1}, we have $d_1 = d, d_i+1 = d; 2 \le i \le k$

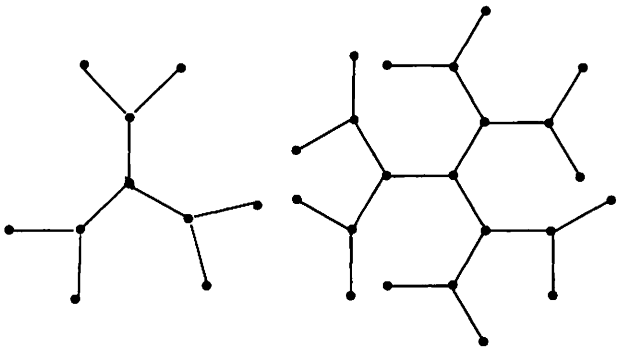

Figure 2: $T_{2,3}$ $T_{3,3}$

and $n_i = d(d-1)^{i-2}$; $2 \leq i \leq k+1$.

$$\begin{aligned}
H(T_{k,d}) &= 2\left\{\frac{d}{d+d-1+1} + \sum_{i=2}^{k-1}\frac{d(d-1)^{i-1}}{d-1+d-1+2} + \frac{d(d-1)^{k-1}}{d-1+2}\right\} \\
&= 1 + \sum_{i=2}^{k-1}(d-1)^{i-1} + 2\frac{d(d-1)^{k-1}}{d+1} \\
&= \frac{(d-1)^{k-1}-1}{d-2} + \frac{2d(d-1)^{k-1}}{d+1} \\
&= \frac{(2d-1)(d-1)^k-(d+1)}{(d+1)(d-2)}
\end{aligned}$$

■

Remark 1. *Chemically more interesting, special cases of the equation* (4) *correspond to* $d = 3, 4$

$$H(T_{k,3}) = 5(2^{k-2}) - 1$$

and

$$H(T_{k,4}) = \left(\frac{7}{10}\right)3^k - \frac{1}{2}$$

4 Harmonic index of fasciagraph and polytree

In this section we give the exact formula of harmonic index for growing graphs namely fasciagraph and growing tree namely polytree.

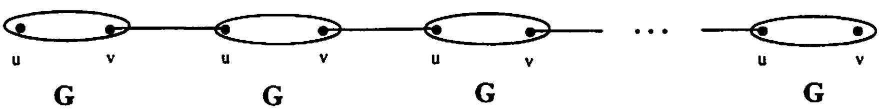

Figure 3: G_k

Theorem 4. *Let G be a simple connected graph and $u, v \in V(G)$ such that u and v are non adjacent. Let G_k be a graph obtained from k copies of G such that the vertex u of one copy of G is adjacent to the vertex v of the next copy of G except the terminals(see figure 3). Then*

$$H(G_k) = kH(G) - 2(k-1)\left\{ \sum_{w \in N_G(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]} + \sum_{w \in N_G(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2} \right\} \tag{5}$$

Proof. We can prove this by the method of induction on k. Let $k = 2$.

Then

$$H(G_2) = 2H(G) - \sum_{w\in N(u)} \frac{2}{d(u)+d(w)} - \sum_{w\in N(v)} \frac{2}{d(v)+d(w)}$$

$$+ \sum_{w\in N(u)} \frac{2}{d(u)+d(w)+1} + \sum_{w\in N(v)} \frac{2}{d(v)+d(w)+1} + \frac{2}{d(u)+d(v)+2}$$

$$= 2H(G) - 2\Bigg\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}$$

$$+ \sum_{w\in N(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2}\Bigg\}$$

Assume the result for G_{k-1} . Let u and v be the vertices corresponding to $(k-1)^{th}$ and k^{th} copies of G in G_k respectively. Then

$$H(G_k) = H(G_{k-1}) + H(G) - \sum_{w\in N(u)} \frac{2}{d(u)+d(w)} - \sum_{w\in N(v)} \frac{2}{d(v)+d(w)}$$

$$+ \sum_{w\in N(u)} \frac{2}{d(u)+d(w)+1} + \sum_{w\in N(v)} \frac{2}{d(v)+d(w)+1} + \frac{2}{d(u)+d(v)+2}$$

$$= H(G_{k-1}) + H(G) - 2\Bigg\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}$$

$$+ \sum_{w\in N(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2}\Bigg\}$$

$$= (k-1)H(G) - 2(k-2)\Bigg\{ \sum_{w\in N_G(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}$$

$$+ \sum_{w\in N_G(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2}\Bigg\}$$

$$+ H(G) - 2\Bigg\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}$$

$$+ \sum_{w\in N(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2}\Bigg\}$$

$$= kH(G) - 2(k-1)\Bigg\{ \sum_{w\in N_G(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}$$

$$+ \sum_{w\in N_G(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2}\Bigg\}$$

■

Fasciagraph is a class of polygraph. The structure of the simplest fasciagraph F is uniquely specified by the structure of the monomer unit G and the number of monomer units. Every unit of F is adjacent with two units except the terminal units.

A fasciagraph is a polygraph with k copies of a fixed graph G such that the vertex u in the i^{th} copy is adjacent to the vertex v in the $(i+1)^{th}$ copy of G, $i = 1, 2, \ldots, k-1$

Corollary 3. *Let F be a fasciagraph composed of k copies of a graph G. Then*

$$H(F) = kH(G) - 2(k-1)\Bigg\{ \sum_{w \in N_G(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]} + \sum_{w \in N_G(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2} \Bigg\}$$

Theorem 5. *Let G be a simple connected graph and $u \in V(G)$. Let G_k be a graph obtained from $k \geq 3$ copies of G such that the vertex u of one copy of G is adjacent to the same vertex u of the next copy of G except the terminals. Then*

$$H(G_k) = kH(G) - 4\Bigg\{ \sum_{w \in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]} + (k-2) \sum_{w \in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+2]} - \frac{1}{2d(u)+3} - (k-3)\frac{1}{4[d(u)+2]} \Bigg\}$$

Proof. We can prove this by the method of induction on k. Let $k = 3$.

Then

$$H(G_3) = 3H(G) - 3 \sum_{w\in N(u)} \frac{2}{d(u)+d(w)} + 2 \sum_{w\in N(u)} \frac{2}{d(u)+d(w)+1}$$
$$+ \sum_{w\in N(u)} \frac{2}{d(u)+d(w)+2} + 2\frac{2}{d(u)+1+d(u)+2}$$
$$= 3H(G) - 4\left\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}\right.$$
$$\left. + \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+2]} - \frac{1}{2d(u)+3}\right\}$$

Let us consider G_{k-1}. Let u be the vertex corresponding to $(k-1)^{th}$ and k^{th} copies of G in G_k.

$$H(G_k) = H(G_{k-1}) + H(G) - \sum_{w\in N(u)} \frac{2}{d(u)+1+d(w)} - \sum_{w\in N(u)} \frac{2}{d(u)+d(w)}$$
$$+ \sum_{w\in N(u)} \frac{2}{d(u)+d(w)+2} + \sum_{w\in N(u)} \frac{2}{d(u)+d(w)+1} + \frac{2}{d(u)+2+d(u)+2}$$
$$= H(G_{k-1}) + H(G) - 4\left\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+2]} + \frac{1}{4(d(u)+2)}\right\}$$
$$= (k-1)H(G) - 4\left\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}\right.$$
$$+ (k-3) \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+2]} - \frac{1}{2d(u)+3}$$
$$\left. - (k-4)\frac{1}{4[d(u+2)]}\right\} + H(G) - 4\left\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+2]}\right.$$
$$\left. + \frac{1}{4(d(u)+2)}\right\}$$
$$= kH(G) - 4\left\{ \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+1]}\right.$$
$$+ (k-2) \sum_{w\in N(u)} \frac{1}{[d(u)+d(w)][d(u)+d(w)+2]} - \frac{1}{2d(u)+3}$$
$$\left. - (k-3)\frac{1}{4[d(u)+2]}\right\}$$

■

Consider a chemical polytree F_{nk} consisting of k copies of the star S_n such that u is the centre vertex of S_n (see figure 4). Using the above theorem we have harmonic index of polytree in terms of order of the star.

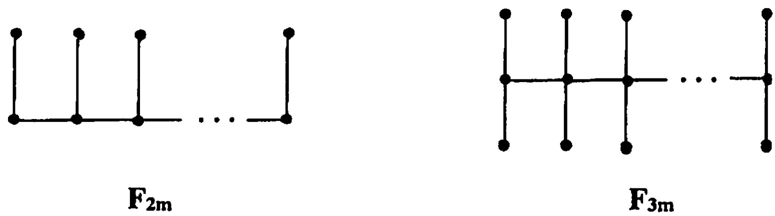

Figure 4: Chemical Polytrees

Corollary 4. *Let F_{nk} be a chemical polytree consisting of k copies of the star S_n such that u is the centre vertex of S_n. Then*

$$H(F_{nk}) = \frac{2k(n-1)}{n} - 4\left\{\frac{n-1}{n(n+1)} + \frac{(k-2)(n-1)}{n(n+2)} - \frac{1}{2n+1} - \frac{k-3}{2(n+1)}\right\}$$

Proof. Since u is the centre vertex of S_n, $d(u) = n-1$ and $d(w) = 1$, we get the result. ■

Remark 2. *Chemically relevant fasciagraphs F_{nk} correspond to the cases $n = 2$ and $n = 3$.*

$$H(F_{2k}) = \frac{15k-22}{6}$$

and

$$H(F_{3k}) = \frac{189k-213}{105}$$

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