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BOUNDS OF F-INDEX FOR UNICYCLIC GRAPHS WITH FIXED PENDENT VERTICES

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ABSTRACT. Furtula and Gutman [J. Math. Chem., 53 (4) (2015), 1184-1190] reinvestigated the F-index as a sum of cubes of the degrees of all the vertices in a chemical graph and proved its various properties. A connected graph with equal order and size is called unicyclic graph, where order is number of vertices and size is number of edges. In this paper, we characterize the extremal graphs in a family of graphs called by unicyclic graphs with fixed number of pendent vertices. We also investigate the bound on F-index in the same family of graphs i.e

$$4(2n + 3\alpha) \leq F(G) \leq 8n + \alpha(\alpha + 2)(\alpha + 3)$$

for each $G \in \mathcal{U}_{\mathbf{n}}^{\alpha}$, where $\mathcal{U}_{\mathbf{n}}^{\alpha}$ is a class of all the unicyclic graphs such that the order of each graph is n with α pendent vertices.

Key words : Forgotten index; Unicyclic graphs; Extremal graphs.
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1. Introduction

A non-empirical numeric quantity associated with a molecular graph that remained invariant under graph isomorphism and encode at least one physical or chemical property of underlying organic molecules, is called topological index (TI). It turned out that TI's exhibit pivotal role in predicting the physical as well as chemical properties (boiling point, volatility, stability, solubility, connectivity, chirality and melting point) of chemical compounds. Furthermore, cheminformatics is a latest field that unifies chemistry, mathematics

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and information science that enable quantitative structure activity relationship (QSAR) and quantitative structure property relationship (QSPR) which primarily depend on suitable TI's and resulted in examining the bioactivities and chemical re-activities of the chemical compounds, see [5].

Although, graph theory has immense applications in diversified areas like computer science, optimization, biology, engineering, social sciences and particularly in chemistry. Consequently, several books [27, 28, 29, 30, 31, 32, 33, 34] and research articles [35, 36, 37, 38, 39] have been authored on the applications in the area of mathematical chemistry and chemical graph theory. In literature, for a simple-connected graph, TI's are distributed into four major classes, namely, degree-based, distance-based, counting polynomial related and spectral-based TI's. Among these types, the degree-based TI's are vastly studied and explored, see the recent survey [13].

Harry Wiener (1947) was the first who established the correlation between a distance based topological index and the boiling point of paraffin, see [20]. Initially this index was called Wiener number but later on this extensively investigated index was popularized by the name Wiener index. Numerous topological indices of valuable and practical nature were introduced after the Wiener index such as first, second, multiplicative, augmented and generalized Zagreb indices as well as co-indices, Randić indices, atom bond connectivity (ABC) index, fourth version of ABC, geometric-arithmetic (GA) index and fifth version of GA, see [1, 2, 4, 6, 7, 9, 12, 14, 15, 26, 10, 11].

In 1972, Furtula and Gutman [14] defined a degree based index as sum of cubes of degrees of end vertices of each edge of molecular graph. Approximately 43 years after the inception of this index, Furtula and Gutman (2015) [8], reconsidered and reinvestigated by offering lower and upper bounds as well as establishing its vitality in determining physico-chemical properties of chemical compounds. The years long state of obliviousness of this index gives rise to its name, forgotten topological index (F-index).

Che and Chen [41] offered improved lower and upper bounds for F-index, as compared to [8], with regard to size, minimum and maximum degrees, irregularity and Zagreb indices. In addition they provide characterization for all graphs analogous to benzenoid systems. Recently, Gao *et al.* [40] exhibited the F-index of some substantial drug molecular structures. Milovanovic et al. [16] and De et al. [3] workout and described the F-index and F-coindex for certain families of graphs. Basavanagoud and Timmanaikar [17] computed F-index of Kragujevac trees. Khaksari and Ghorbani [18] investigated F-index for the certain product of graphs. Akhter et al. [19] established the ordering among the few graphs with respect to F-index belonging to the class of unicyclic and bicyclic graphs.

In present article, we provide the existence of the extremal graphs with respect to F-index in the class of unicyclic graphs with certain pendent vertices. We also investigate the lower and upper bounds of the F-index in the same class of graphs. The rest of the paper is organized as; Section 2 includes the basic definitions and results, Section 3 consists of the main results on the graphs with minimum and maximum F-index and also covers the result related to the lower and upper bounds of F-index in the family of unicyclic graphs with certain pendent vertices.

2. Preliminaries

Let $G(V(G), E(G))$ be a graph with vertex-set V(G) and edge-set E(G) such that $v = |V(G)|$ and $e = |E(G)|$ are order and size of the graph G, respectively. Also the edge $e = uv$ shows connection between two vertices u and v i.e. u and v are adjacent. Two or more edges with same end points are called parallel edges or multi-edges and an edge which connects a vertex to itself is called a loop. A graph is connected if there is some path between each pair of vertices. A connected graph G without any cycle is called a tree having that $|V(G)| = |E(G)| - 1$ and a graph that contains at least one cycle is called cyclic. A vertex of a graph is called a cycle-vertex if it is on its some cycle, otherwise it is a tree-vertex. Moreover, $d(u)$ represents the degree of vertex $u \in G$. In the present study, all the graphs are simple (without parallel edges and loops) and undirected. For the further study about the graph theoretic terminologies, we refer [21]. Now, we define some topological indices which will be useful in the main results.

Definition 2.1 For a molecular graph G, the first Zagreb index and the second Zagreb index are defined as

$$M_1(G) = \sum_{rs \in E(G)} [d(r) + d(s)] \text{ and } M_2(G) = \sum_{rs \in E(G)} [d(r) \times d(s)].$$

Definition 2.2. Let G be a molecular graph. Then, general Randić index $(R_\alpha(G))$ is defined as follows:

$$R_\alpha(G) = \sum_{rs \in E(G)} [d(r) \times d(s)]^\alpha.$$

For $\alpha = -\frac{1}{2}$, $\alpha = \frac{1}{2}$ and $\alpha = 1$, we obtain Randić index, reciprocal Randić index and the second Zagreb index respectively.

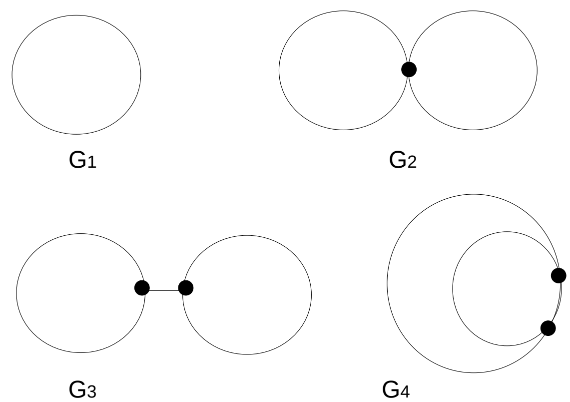

FIGURE 1. G_1 (cycle), G_2 (two cycles with common vertex), G_3 (two cycles with no common vertex or edge) and G_4 (two cycles with common edge).

Definition 2.3. Let G be a molecular graph. Then, the forgotten index (F-index) is defined as follow:

$$F(G) = \sum_{s \in V(G)} [d(s)]^3.$$

The general form of first Zagreb index is $M_1^{\beta}(G) = \sum_{rs \in E(G)} [d(r)^{\beta-1} + d(s)^{\beta-1}]$, where $\beta \in R, \beta \neq 0, 1$. The first general Zagreb index becomes Forgotten index if $\beta = 3$. For the detailed studies of the foresaid indices, we refer (Gutman and Trinajsti; 1972) [14], (Milan Randić; 1975) [22], Bollobás and Erdös; 1998) [23], (Amic et al.; 1998) [24], (Furtula and Gutman; 2015) [25].

A connected graph is ω-cyclic if $m = n - 1 + \omega$, where n is order and m is size of the graph. For $\omega = 0$, $\omega = 1$ or $\omega = 2$, it is called tree, unicyclic or bicyclic respectively. Moreover, in a unicyclic (1-cyclic) graph there is a unique cycle and a bicyclic (2-cyclic) graph contains two or three cycles. To understand ω-cyclic structure of graphs, the base-graph(s) (minimum subgraph(s)) G_1 and G_2, G_3 & G_4 of the unicyclic and bicyclic graphs with no pendant vertices are shown in FIGURE 1 respectively.

Now, we define some more unicyclic graphs from its base-graph. Let $\mathcal{U}(n, r, l)$ be a unicyclic graph with n vertices obtained by attaching r pendent vertices to any $l \geq 2$ vertices of the cycle C_p, where $p = n - rl$. Similarly the unicyclic graph $\mathcal{U}'(n, r', k)$ is obtained by identifying one end point of a path of order k (graph with $k-2$ vertices of degree two and 2 pendent vertices) with a vertex of the cycle C_q and the other end with the central vertex of the star $S_{1,r'}$ (graph with r' pendent vertices and one vertex of degree r'), where $q = n - r' - k + 1$ and $2 \leq k \leq n - r' - 2$. Assume that $\mathcal{U}(n, r, l)$= $\mathbf{U}$ and $\mathcal{U}'(n, r', k)$= $\mathbf{U}'$, then the partitions of their vertex set with respect to degrees of vertices are as follows;

$d(v)$, for $v \in \mathbf{U}$	1	2	$r+2$
$\lvert d(v) \rvert$	rl	$p-l$	l

Table 2.1.

$d(v)$, for $v \in \mathbf{U}'$	1	2	$r'+1$	3
$\lvert d(v) \rvert$	r'	$q+k-3$	1	1

Table 2.2.

Now, we obtain $\mathbf{U_1}$ from $\mathbf{U}$ by deleting r pendent vertices from a vertex of degree $r+2$ and joining these vertices to another vertex of degree $r+2$. Moreover, we derive $\mathbf{U_2}$ from $\mathbf{U_1}$ by deleting $2r$ pendent vertices from the vertex of degree $2r+2$ and joining these vertices to the vertex of degree $r+2$. If we continue this pattern, after $l-1$ iterations we obtain $\mathbf{U_{l-1}}$ from $\mathbf{U_{l-2}}$ by deleting $(l-1)r$ pendent vertices from a vertex of degree $(l-1)r+2$ and joining these vertices to the last vertex of degree $r+2$, where $2 \leq l \leq p$.

Let $\mathcal{U}_{\mathbf{n}}^{\alpha}$ be a class of all the unicyclic graphs such that the order of each graph is n with α pendent vertices. Moreover, assume that $\mathcal{U}_{\mathbf{1}}$, $\mathcal{U}_{\mathbf{2}}$ and $\mathcal{U}_{\mathbf{3}}$ be three subclasses of $\mathcal{U}_{\mathbf{n}}^{\alpha}$ such that the pendent vertices are attached with the cycle-vertices, tree-vertices and both of them respectively.

3. Main Results

In this section, we present the main results of the paper. Before to the final results, we establish some basic lemmas which will be frequently used in the main results.

Lemma 3.1 Let G_1 and G_2 be any two connected graphs of same order and size with degree sequences $< d_1^1, d_2^1, d_3^1, ..., d_n^1 >$ and $< d_1^2, d_2^2, d_3^2, ..., d_n^2 >$ respectively such that $d_i^1 = d_i^2$ for $1 \leq i \leq n$, where d_i^j is degree of vertices v_i^j in G_i^j for $1 \leq j \leq 2$ and $n = |V(G_1)| = |V(G_2)|$. Then, $F(G_1) = F(G_2)$.

Proof. If G_1 and G_2 are isomorphic then there is nothing to prove. Assume that G_1 and G_2 are non-isomorphic. Since $d_i^1 = d_i^2$ for $1 \leq i \leq n$, therefore

$$< d_1^1, d_2^1, d_3^1, ..., d_n^1 > = < d_1^2, d_2^2, d_3^2, ..., d_n^2 > .$$

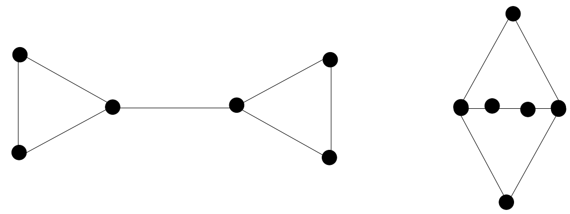

FIGURE 2. Non-isomorphic graphs of equal order and size have same F-index.

Consequently $\sum_{i=1}^{n}(d_i^1)^3 = \sum_{i=1}^{n}(d_i^2)^3$ which implies that

$$F(G_1) = F(G_2).$$

Lemma 3.2 Let u and v be any two vertices of the graph G such that $uv \in E(G)$. Assume that $G^{'}$ is obtained from G by the deletion of uv and joining u to an other vertex of G say w i.e $G^{'} = G - uv + uw$. Then

(i) $F(G^{'}) = F(G)$ if $d(w) = d(v) - 1$,
(ii) $F(G^{'}) > F(G)$ if $d(w) > d(v) - 1$ and
(ii) $F(G^{'}) < F(G)$ if $d(w) < d(v) - 1$,

where $d(v)$ and $d(w)$ are degrees of v and w in G respectively.

Proof. Since $d(v)$ and $d(w)$ denote the degrees of v and w in G respectively. Therefore, by definition of F-index, we have

$$F(G) - F(G^{'}) = d(v)^3 + d(w)^3 - (d(v) - 1)^3 - (d(w) + 1)^3$$

$$= -3(d(w) + d(v))[d(w) - (d(v) - 1)].$$

Using $d(w) = d(v) - 1$, $d(w) > d(v) - 1$ and $d(w) < d(v) - 1$ in the above equality, we obtain $F(G^{'}) = F(G)$, $F(G^{'}) > F(G)$ and $F(G^{'}) < F(G)$ respectively. This complete the proof.

Lemma 3.3 For $r \geq 2$, $p, q \geq 3$, $2 \leq l \leq p$, $2 \leq k \leq q - 3$ and $0 \leq i \leq l - 1$, F-index of the unicyclic graphs $\mathbf{U_i}$ and $\mathbf{U}^{'}$ are

$(i) F(\mathbf{U_i}) = rl+(l-i-1)(r+2)^3+8(p-l+i)+[(i+1)r+2]^3$

$(ii) F(\mathbf{U}^{'}) = 8(q+k-3)+(r+1)^3+r+27.$

Proof. Proof is obvious by Definition 2.3, Table 2.1 and Table 2.2.

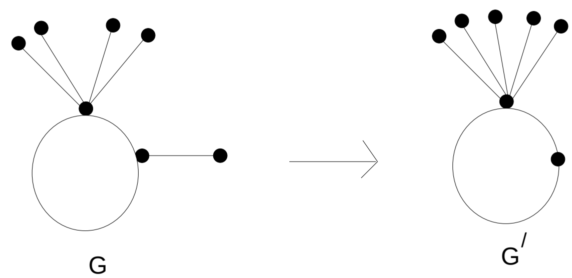

FIGURE 3. G' is obtained by applying a transformation on G.

Taking $i = 0$ in the above lemma, we obtain the following corollary;
Corollary 3.4. For $r \geq 2$, $p \geq 3$ and $2 \leq l \leq p$, F-index of the unicyclic graph $\mathbf{U}$ is

$$F(\mathbf{U}) = rl + l(r+2)^3 + 8(p-l).$$

Theorem 3.5. Let $r \geq 2$, $p, q \geq 3$, $2 \leq l \leq p$, $2 \leq k \leq q-3$ and $0 \leq i \leq l-1$. Then

(**i**) $F(\mathcal{U}'(n,r,2)) < F(\mathcal{U}(n,r,1))$,

(**ii**) $F(\mathcal{U}'(n,r,k)) = F(\mathcal{U}'(n,r,k+1))$,

(**iii**) $F(\mathcal{U}(n,r,l)) < F(\mathcal{U}'(n,r,2))$,

(**iv**) $F(\mathbf{U_0}) < F(\mathbf{U_1}) < ... < F(\mathbf{U_{l-1}})$,

(**v**) $F(\mathcal{U}'(n,r,k)) < F(\mathcal{U}(n,r,1))$.

Proof.(i) Putting $l = 1$ in Corollary 3.4, we obtain,

$$F(\mathcal{U}(n,r,l)) = r + 8(p-1) + (r+2)^3.$$

For $k = 2$, Lemma 3.3(ii) yields

$$F(\mathcal{U}'(n,r',2)) = r + 8(q-1) + (r'+1)^3 + 27.$$

Since $p = n - rl$, $q = n - r' - k + 1$, $r' = rl$ and $p - q = r' - r + 1$, for $l = 1$ and $k = 2$ we have

$$F(\mathcal{U}(n,r,1)) - F(\mathcal{U}'(n,r',2)) = 3r^2 + 9r - 20 > 0$$

Consequently, $F(\mathcal{U}'(n,r',2)) < F(\mathcal{U}(n,r,1))$ for $r \geq 2$.

(ii) By Lemma 3.3 (ii),

$$F(\mathcal{U}'(n,r',k)) = 8(q+k-3) + (r'+1)^3 + r' + 27.$$

Since for $k = k+1$, we have $q = q-1$. Therefore

$$F(\mathcal{U}^{'}(n, r^{'}, k+1)) = 8(q+k-3) + (r^{'}+1)^3 + r^{'} + 27.$$

Thus, $F(\mathcal{U}^{'}(n, r^{'}, k)) = F(\mathcal{U}^{'}(n, r, k+1))$.

(iii) Using Lemma 3.3 (ii) and Corollary 3.4, we have

$$F(\mathcal{U}^{'}(n, r^{'}, 2)) = 8(q-1) + (r^{'}+1)^3 + r^{'} + 27\text{and}$$

$$F(\mathcal{U}(n, r, l)) = rl + l(r+2)^3 + 8(p-l).$$

Since $p - q = r^{'} - rl + 1$, $r^{'} = rl$ and $k = 2$ therefore

$$F(\mathcal{U}(n, r, l)) - F(\mathcal{U}^{'}(n, r^{'}, 2)) = r^3 l(1-l^2) + 3lr^2(2-l) + 9lr - 12 < 0.$$

Consequently, $F(\mathcal{U}(n, r, l)) < F(\mathcal{U}^{'}(n, r^{'}, 2))$.

(iv) Using Lemma 3.3 (i), we have

$$F(\mathbf{U_i}) - F(\mathbf{U_{i+1}}) = 8 - 12r^2(i+1) - 3r^3 i(i+3).$$

By Lemma 3.1(iii), $F(\mathbf{U_i}) < F(\mathbf{U_{i+1}})$. Using $i = 0, 1, 2, 3, ..., l-2$, we have $F(\mathbf{U_0}) < F(\mathbf{U_1}) < ... < F(\mathbf{U_{l-1}})$.

(v) Since by (i) and (ii), we have

$$F(\mathcal{U}^{'}(n, r, 2)) < F(\mathcal{U}(n, r, 1)) \text{ and } F(\mathcal{U}^{'}(n, r, k)) = F(\mathcal{U}^{'}(n, r, k+1)).$$

Consequently,

$$F(\mathcal{U}^{'}(n, r, 2)) = F(\mathcal{U}^{'}(n, r, 3)) = ... = F(\mathcal{U}^{'}(n, r, q-3))$$

Thus, $F(\mathcal{U}^{'}(n, r, k)) < F(\mathcal{U}(n, r, 1))$ for $2 \le k \le q-3$.

Theorem 3.6. If $r \ge 2$, $p \ge 3$, $2 \le l \le p$, $\alpha = rl$ and $n \ge 5$. Then, for each $G \in \mathcal{U}_{\mathbf{n}}^{\alpha}$

(**a**) $F(\mathcal{U}(n, r, l)) \le F(G)$,

(**b**) $F(G) \le F(\mathcal{U}(n, r, 1))$,

where $\mathcal{U}_{\mathbf{n}}^{\alpha}$ is a class of all the unicyclic graphs such that each graph has n order and α pendent vertices. Moreover, equality holds if $G \cong \mathcal{U}(n, r, l)$ and $G \cong \mathcal{U}(n, r, l)$ respectively.

Proof.(a) We consider the following cases;
Case 1: Assume that $G \in \mathcal{U}_{\mathbf{1}}$ such that $G \cong \mathbf{U_i}$ for some $1 \le i \le l-1$. Since, $\mathcal{U}(n, r, l) = \mathbf{U_0}$ therefor by Theorem 3.5 (iv) $\mathcal{U}(n, r, l)) \le G \cong \mathbf{U_i}$ for $1 \le i \le l-1$.

Case 2: If $G \in \mathcal{U}_{\mathbf{2}}$ such that $G \cong \mathcal{U}^{'}(n, r^{'}, k)$. By Theorem 3.5 (iii) and (ii), we have

$F(\mathcal{U}(n, r, l)) < F(\mathcal{U}^{'}(n, r^{'}, 2))$ and

$F(\mathcal{U}^{'}(n, r^{'}, 2)) = F(\mathcal{U}^{'}(n, r^{'}, 3)) = ... = F(\mathcal{U}^{'}(n, r^{'}, k))$.

Therefore $F(\mathcal{U}(n, r, l)) < F(\mathcal{U}^{'}(n, r^{'}, k))$ for each $k \geq 2$. If $G \in \mathcal{U}_{\mathbf{2}}$ is other than $\mathcal{U}^{'}(n, r^{'}, k)$, then using the transformation of deletion and addition of an edge, we obtain $G \cong \mathcal{U}^{'}(n, r^{'}, k)$. Then by Lemma 3.2 and Theorem 3.5 (ii), we get $F(\mathcal{U}(n, r, l)) < F(\mathcal{U}^{'}(n, r^{'}, k))$. Consequently, $F(\mathcal{U}(n, r, l)) < G$ for each $G \in \mathcal{U}_{\mathbf{2}}$.

Case 3: If $G \in \mathcal{U}_{\mathbf{3}}$, then we have two possibilities. (i) There exists $G^{*} \in G_1 \cup G_2$ such that the degree sequences of G and G^{*} are same. Then, by Lemma 3.1 $F(G) = F(G^{*})$. (ii) After using some transformations of the deletion and addition of the edges, we obtain $G^{*} \in \mathcal{U}_{\mathbf{1}}$ or $G^{*} \in \mathcal{U}_{\mathbf{2}}$ such that $F(G^{*}) \leq F(G)$ (by Lemma 3.2). Finally, we follow case (i) or case (ii) (proved above) and get the result.

From all the cases, $F(\mathcal{U}(n, r, l)) \leq F(G)$ for each $G \in \mathcal{U}_{\mathbf{n}}^{\alpha}$.

(b) The proof is same as of part **(a)** using Lemmas 3.1-3.4 and Theorem 3.5.

Theorem 3.7. Let $\mathcal{U}_{\mathbf{n}}^{\alpha}$ be a class of all the unicyclic graphs such that the order of each graph is n with α pendent vertices. Then,

$$4(2n + 3\alpha) \leq F(G) \leq 8n + \alpha(\alpha + 2)(\alpha + 3)$$

for each $G \in \mathcal{U}_{\mathbf{n}}^{\alpha}$, where the lower bound is achieved if and only if $G \cong \mathcal{U}(n, 1, l)$ and the upper bound is achieved if and only if $G \cong \mathcal{U}(n, r, 1)$.

Proof. Using corollary 3.4, we obtain $F(\mathcal{U}(n, 1, l)) = 4(2n+3\alpha)$ and $F(\mathcal{U}(n, r, 1)) = 8n+\alpha(\alpha+2)(\alpha+3)$ for $\alpha = rl$ pendent vertices. Moreover, by Theorem 3.6 (a) $F(\mathcal{U}(n, r, l)) \leq F(G)$ implies that $F(\mathcal{U}(n, 1, l)) \leq F(\mathcal{U}(n, r, l)) \leq F(G)$ and $F(G) \leq F(\mathcal{U}(n, r, 1))$ for each $G \in \mathcal{U}_{\mathbf{n}}^{\alpha}$. Consequently, we obtain $4(2n + 3\alpha) \leq F(G) \leq 8n + \alpha(\alpha + 2)(\alpha + 3)$ for each $G \in \mathcal{U}_{\mathbf{n}}^{\alpha}$. Moreover, the lower bound is achieved if and only if $G \cong \mathcal{U}(n, 1, l)$ and the upper bound is achieved if and only if $G \cong \mathcal{U}(n, r, 1)$.

4. Conclusion

In this paper, we have characterized the extremal graphs with minimum and maximum F-index in the class of unicyclic graphs with certain pendent vertices. A mathematical inequality consisting on the lower and upper bounds of the F-index is also established in the terms of order of the graphs and the attached pendent vertices.

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