International Journal of Applied Engineering Research ISSN 0973-4562 Volume 15, Number 3 (2020) pp. 287-293

Zagreb Polynomials of Graph Operations

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Abstract:

In this paper, we present exact expressions for the *first and second Zagreb polynomials* of some graph operations namely union, join, cartesian product, composition and corona of graphs. These expressions in other way, establish some relations among Zagreb polynomials.

2010 Mathematics Subject Classification: 05C07, 05C31.

Keywords: Zagreb polynomial, degree, graph operation.

1. INTRODUCTION

Let G be a nontrivial, simple, finite, undirected graph with n vertices and m edges. The vertex set is $V(G)=\{v_1,v_2,...,v_n\}$ and an edge set is $E(G)=\{e_1,e_2,...,e_m\}$. The *degree* of a vertex v in G is the number of edges incident to v and is denoted by $d_G(v)=deg_G(v)$.

The *union* $G_1\cup G_2$ of graphs G_1 and G_2 is a graph whose vertex set is $V(G_1\cup G_2)=V(G_1)\cup V(G_2)$ and an edge set is $E(G_1\cup G_2)=E(G_1)\cup E(G_2)$. The graph pG where $p\geq 1$ is a graph which is union of p copies of G. The *join* G_1+G_2 of two graphs G_1 and G_2 is a graph obtained from G_1 and G_2 by joining every vertex of G_1 to all vertices of G_2. The *cartesian product* $G_1\times G_2$ of two graphs $G_1=(V_1(G_1),E_1(G_1))$

and $G_2=(V_2(G_2),E_2(G_2))$ is defined as follows: Consider any two vertices $u=(u_1,u_2)$ and $v=(v_1,v_2)$ in $V(G_1\times G_2)=V_1(G_1)\times V_2(G_2)$. The two vertices u and v are adjacent in $G_1\times G_2$ whenever ($u_1=v_1$ and $u_2v_2\in E(G_2)$) or ($u_2=v_2$ and $u_1v_1\in E(G_1)$). The *composition* $G_1[G_2]$ of two graphs G_1 and G_2 is defined as follows: Consider any two vertices $u=(u_1,u_2)$ and $v=(v_1,v_2)$ in $V(G_1[G_2])=V_1(G_1)\times V_2(G_2)$. The two vertices u and v are adjacent in $G_1[G_2]$ whenever $(u_1v_1\in E(G_1))$ or ($u_1=v_1$ and $u_2v_2\in E(G_2)$). The *corona* $G_1\circ G_2$ of graphs G_1 and G_2 is a graph obtained from G_1 and G_2 by taking one copy of G_1 and $|V(G_1)|$ copies of G_2 and then joining by an edge each vertex of the i^{th} copy of G_2 is named (G_2,i) with the i^{th} vertex of G_1. For details of graph operations, refer to [7].

For undefined graph theoretic terminologies and notations refer to [7] or [9].

2. TOPOLOGICAL INDICES AND GRAPH POLYNOMIALS

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in graph theoretical parameters. A molecular graph is a graph whose vertices correspond to the atoms of the chemical compound and edges to the chemical bonds. Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be used to characterize some property of the graph of a molecule is called a *topological index* of that graph. A topological index is a numerical parameter mathematically derived from the graph structure. It is a graph invariant, thus it does not depend on the labeling or pictorial representation of the graph. There are numerous molecular descriptors, which are also referred to as topological indices, see [6], that have found some applications in theoretical chemistry, especially in QSPR (Quantitative Structure-Property Relationship) and QSAR (Quantitative Structure-Activity Relationship) research. Zagreb indices are the best investigated topological indices, but their properties and chemical applications were always studied for the case of ordinary molecular graphs.

The first and second Zagreb indices [6] of a graph G are defined as

$$M_1(G)=\sum_{v\in V(G)} d_G(v)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v),$$

respectively.

The first Zagreb index [12] can also be expressed as

$$M_1(G) = \sum_{uv \in E(G)} \left(d_G(u) + d_G(v)\right).$$

The characterization of any graph by a *polynomial* is one of the open and important problems in graph theory. Some parameters of a graph allow to define polynomials related to a graph. Several polynomials are interesting since they compress information about the graph structure. Every polynomial defines a topological index and has proved to be useful in the study of several topological indices.

Following are some of the graph polynomials.

The *Wiener polynomial* [13] of a graph G is defined as

$$W(G;q) = \sum_{\{u,v\} \subset V(G)} q^{d_G(u,v)},$$

where $\frac{d}{dq}(W(G;q))|_{q=1} = W(G)$ and q is a parameter.

The *harmonic polynomial* [8] of a graph G is defined as

$$H(G,x) = 2 \sum_{uv \in E(G)} x^{d_G(u)+d_G(v)-1},$$

where $\int_0^1 H(G,x)dx = H(G)$ and x is a parameter.

The ***Zagreb polynomial*** is one of the degree based graph polynomials considered in chemical graph theory. Considering the Zagreb indices, Fath-Tabar in [5] defined first and second Zagreb polynomials as

$$M_1(G,x) = \sum_{v_i v_j \in E(G)} x^{d_G(v_i)+d_G(v_j)}$$

and

$$M_2(G,x) = \sum_{v_i v_j \in E(G)} x^{d_G(v_i) \cdot d_G(v_j)},$$

respectively, where x is a variable.

Just like Zagreb polynomials, in addition, Shuxian [11] defined two polynomials related to the first Zagreb index in the following form.

Proposition 2.1. *For a graph G,*

$$M_1^*(G,x) = \sum_{v_i \in V(G)} d_G(v_i) x^{d_G(v_i)},$$

$$M_0(G,x) = \sum_{v_i \in V(G)} x^{d_G(v_i)}.$$

In [4], Bindusree et al., gave the following polynomials.

Proposition 2.2. *For a graph G,*

$$M_4(G,x) = \sum_{v_i v_j \in E(G)} x^{d_G(v_i)(d_G(v_i)+d_G(v_j))},$$

$$M_5(G,x) = \sum_{v_i v_j \in E(G)} x^{d_G(v_j)(d_G(v_i)+d_G(v_j))},$$

$$M_{a,b}(G,x) = \sum_{v_i v_j \in E(G)} x^{a d_G(v_i)+b d_G(v_j)},$$

$$M'_{a,b}(G,x) = \sum_{v_i v_j \in E(G)} x^{(d_G(v_i)+a)(d_G(v_j)+b)}.$$

The Zagreb polynomials of generalized *xyz*-point-line transformation graphs are found in [1,2,3].

3. MAIN RESULTS

Proposition 3.1. *[7] If G_1 and G_2 are two graphs, then*

$$d_{G_1 \cup G_2}(v) = \begin{cases} d_{G_1}(v), & if\ v \in V(G_1), \\ d_{G_2}(v), & if\ v \in V(G_2). \end{cases}$$

Theorem 3.2. *If G_1 and G_2 are two graphs, then*

$$M_1(G_1 \cup G_2, x) = M_1(G_1, x) + M_1(G_2, x)$$

and

$$M_2(G_1 \cup G_2, x) = M_2(G_1, x) + M_2(G_2, x).$$

Proof. Using the definitions of first and second Zagreb polynomials with Propositions 2.1, 2.2 and 3.1, we get

$$M_1(G_1 \cup G_2, x) = \sum_{uv\in E(G_1\cup G_2)} x^{d_{G_1\cup G_2}(u)+d_{G_1\cup G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1\cup G_2}(u)+d_{G_1\cup G_2}(v)} + \sum_{uv\in E(G_2)} x^{d_{G_1\cup G_2}(u)+d_{G_1\cup G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1}(u)+d_{G_1}(v)} + \sum_{uv\in E(G_2)} x^{d_{G_2}(u)+d_{G_2}(v)}$$

$$= M_1(G_1, x) + M_1(G_2, x).$$

$$M_2(G_1 \cup G_2, x) = \sum_{uv\in E(G_1\cup G_2)} x^{d_{G_1\cup G_2}(u)\cdot d_{G_1\cup G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1\cup G_2}(u)\cdot d_{G_1\cup G_2}(v)} + \sum_{uv\in E(G_2)} x^{d_{G_1\cup G_2}(u)\cdot d_{G_1\cup G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1}(u)\cdot d_{G_1}(v)} + \sum_{uv\in E(G_2)} x^{d_{G_2}(u)\cdot d_{G_2}(v)}$$

$$= M_2(G_1, x) + M_2(G_2, x).$$

Proposition 3.3. *[7] If* G_1 *is an* (n_1, m_1) *-graph and* G_2 *is an* (n_2, m_2) *-graph, then*

$$d_{G_1+G_2}(v) = \begin{cases} d_{G_1}(v) + n_2, & \text{if } v \in V(G_1), \\ d_{G_2}(v) + n_1, & \text{if } v \in V(G_2). \end{cases}$$

Theorem 3.4. *If* G_1 *is an* (n_1, m_1) *-graph and* G_2 *is an* (n_2, m_2) *-graph, then*

$$M_1(G_1 + G_2, x) = x^{2n_2} M_1(G_1, x) + x^{2n_1} M_1(G_2, x) + x^{n_1+n_2} M_0(G_1, x) M_0(G_2, x),$$

and $M_2(G_1 + G_2, x) = M'_{n_2,n_2}(G_1, x) + M'_{n_1,n_1}(G_2, x) + x^{(n_1+n_2)} M_0(G_1, x) M_0(G_2, x).$

Proof. Using the definitions of first and second Zagreb polynomials with Propositions 2.1, 2.2 and 3.3, we get

$$M_1(G_1 + G_2, x) = \sum_{uv\in E(G_1+G_2)} x^{d_{G_1+G_2}(u)+d_{G_1+G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1+G_2}(u)+d_{G_1+G_2}(v)} + \sum_{uv\in E(G_2)} x^{d_{G_1+G_2}(u)+d_{G_1+G_2}(v)} + \sum_{u\in V(G_1), v\in V(G_2)} x^{d_{G_1+G_2}(u)+d_{G_1+G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1}(u)+n_2+d_{G_1}(v)+n_2} + \sum_{uv\in E(G_2)} x^{d_{G_2}(u)+n_1+d_{G_2}(v)+n_1} + \sum_{u\in V(G_1), u\in V(G_2)} x^{d_{G_1}(u)+n_2+d_{G_2}(v)+n_1}$$

$$= x^{2n_2} M_1(G_1, x) + x^{2n_1} M_1(G_2, x) + x^{n_1+n_2} M_0(G_1, x) M_0(G_2, x).$$

$$M_2(G_1 + G_2, x) = \sum_{uv\in E(G_1+G_2)} x^{d_{G_1+G_2}(u)\cdot d_{G_1+G_2}(v)}$$

$$= \sum_{uv\in E(G_1)} x^{d_{G_1+G_2}(u)\cdot d_{G_1+G_2}(v)} + \sum_{uv\in E(G_2)} x^{d_{G_1+G_2}(u)\cdot d_{G_1+G_2}(v)} + \sum_{u\in V(G_1)} \sum_{v\in V(G_2)} x^{d_{G_1+G_2}(u)\cdot d_{G_1+G_2}(v)}$$

Proposition 3.5. *[7] If* G_1 *is an* (n_1, m_1) *-graph and* G_2 *is an* (n_2, m_2) *-graph, then*

$$d_{G_1\times G_2}((u_1, u_2)) = d_{G_1}(u_1) + d_{G_2}(u_2).$$

We define the following polynomial.

Definition 1. *For two graphs* G_1 *and* G_2,

$$M''(G_1G_2,x)=\sum_{u_i\in V(G_1)} x^{d_{G_1}(u_i)^2} \sum_{v_iv_j\in E(G_2)} x^{d_{G_1}(u_i)\left(d_{G_2}(v_i)+d_{G_2}(v_j)\right)}.$$

Theorem 3.6. *If* G_1 *is an* (n_1,m_1) *-graph and* G_2 *is an* (n_2,m_2) *-graph, then*

$$M_1(G_1\times G_2,x)=M_0(G_1,x^2)M_1(G_2,x)+M_0(G_2,x^2)M_1(G_1,x),$$

and

$$M_2(G_1\times G_2,x)=M''(G_1G_2,x)M_2(G_2,x)+M''(G_2G_1,x)M_2(G_1,x).$$

Proof. Using the definitions of first and second Zagreb polynomials and Propositions 2.1, 2.2, 3.5 and Definition 1, we get

$$\begin{aligned}
M_1(G_1\times G_2,x) &= \sum_{(u_1,u_2)(v_1,v_2)\in E(G_1\times G_2)} x^{d_{G_1\times G_2}((u_1,u_2))+d_{G_1\times G_2}((v_1,v_2))}\\
&= \sum_{u_1\in V(G_1)}\sum_{u_2v_2\in E(G_2)} x^{d_{G_1}(u_1)+d_{G_2}(u_2)+d_{G_1}(u_1)+d_{G_2}(v_2)}\\
&\quad + \sum_{u_2\in V(G_2)}\sum_{u_1v_1\in E(G_1)} x^{d_{G_2}(u_2)+d_{G_1}(u_1)+d_{G_2}(u_2)+d_{G_1}(v_1)}\\
&= \sum_{u_1\in V(G_1)} x^{2d_{G_1}(u_1)} \sum_{u_2v_2\in E(G_2)} x^{d_{G_2}(u_2)+d_{G_2}(v_2)}\\
&\quad + \sum_{u_2\in V(G_2)} x^{2d_{G_2}(u_2)} \sum_{u_1v_1\in E(G_1)} x^{d_{G_1}(u_1)+d_{G_1}(v_1)}\\
&= M_0(G_1,x^2)M_1(G_2,x)+M_0(G_2,x^2)M_1(G_1,x).
\end{aligned}$$

$$\begin{aligned}
M_2(G_1\times G_2,x) &= \sum_{(u_1,u_2)(v_1,v_2)\in E(G_1\times G_2)} x^{d_{G_1\times G_2}((u_1,u_2))\cdot d_{G_1\times G_2}((v_1,v_2))}\\
&= \sum_{u_1\in V(G_1)}\sum_{u_2v_2\in E(G_2)} x^{(d_{G_1}(u_1)+d_{G_2}(u_2))\cdot(d_{G_1}(u_1)+d_{G_2}(v_2))}\\
&\quad + \sum_{u_2\in V(G_2)}\sum_{u_1v_1\in E(G_1)} x^{(d_{G_2}(u_2)+d_{G_1}(u_1))\cdot(d_{G_2}(u_2)+d_{G_1}(v_1))}\\
&= \sum_{u_1\in V(G_1)}\sum_{u_2v_2\in E(G_2)} x^{d_{G_1}(u_1)^2+d_{G_1}(u_1)((d_{G_2}(u_2)+d_{G_2}(v_2))+d_{G_2}(u_2)d_{G_2}(v_2)}\\
&\quad + \sum_{u_2\in V(G_2)}\sum_{u_1v_1\in E(G_1)} x^{d_{G_2}(u_2)^2+d_{G_2}(u_2)((d_{G_1}(u_1)+d_{G_1}(v_1))+d_{G_1}(u_1)d_{G_1}(v_1)}\\
&= \sum_{u_1\in V(G_1)} x^{d_{G_1}(u_1)^2} \sum_{u_2v_2\in E(G_2)} x^{d_{G_1}(u_1)((d_{G_2}(u_2)+d_{G_2}(v_2))+d_{G_2}(u_2)d_{G_2}(v_2)}\\
&\quad + \sum_{u_2\in V(G_2)} x^{d_{G_2}(u_2)^2} \sum_{u_1v_1\in E(G_1)} x^{d_{G_2}(u_2)((d_{G_1}(u_1)+d_{G_1}(v_1))+d_{G_1}(u_1)d_{G_1}(v_1)}\\
&= M''(G_1G_2,x)M_2(G_2,x)+M''(G_2G_1,x)M_2(G_1,x).
\end{aligned}$$

International Journal of Applied Engineering Research ISSN 0973-4562 Volume 15, Number 3 (2020) pp. 287-293
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Proposition 3.7. *[7] If G_1 is an (n_1, m_1) -graph and G_2 is an (n_2, m_2) -graph, then*

$$d_{G_1[G_2]}((u_1,u_2)) = n_2 d_{G_1}(u_1) + d_{G_2}(u_2).$$

Theorem 3.8. *If G_1 is an (n_1, m_1) -graph and G_2 is an (n_2, m_2) -graph, then*

$$M_1(G_1[G_2],x) = M_1(G_1, x^{n_2})(M_0(G_2,x))^2 + M_1(G_2,x)M_0(G_1, x^{2n_2})$$

and

$$M_2(G_1[G_2],x) = M^{''}(G_1G_2, x^{n_2^2})M_2(G_2,x)$$
$$+ \sum_{u_2 \in V(G_2)} \sum_{v_2 \in V(G_2)} \sum_{u_1 v \in E(G_1)} x^{n_2 d_{G_1}(u_1)(n_2 d_{G_1}(v_1)+d_{G_2}(v_2))+n_2 d_{G_1}(u_2)d_{G_2}(v_1)+d_{G_2}(u_2)d_{G_2}(v_2)}.$$

Proof. From Propositions 2.1, 2.2, 3.7 and Definition 1, we have

$$\begin{aligned}
M_1(G_1[G_2],x) &= \sum_{(u_1,u_2)(v_1,v_2) \in E(G_1[G_2])} x^{d_{G_1[G_2]}((u_1,u_2))+d_{G_1[G_2]}((v_1,v_2))} \\
&= \sum_{u_1 \in V(G_1)} \sum_{u_2 v_2 \in E(G_2)} x^{n_2 d_{G_1}(u_1)+d_{G_2}(u_2)+n_2 d_{G_1}(u_1)+d_{G_2}(v_2)} \\
&\quad + \sum_{u_2 \in V(G_2)} \sum_{v_2 \in V(G_2)} \sum_{u_1 v_1 \in E(G_1)} x^{n_2(d_{G_1}(u_1)+d_{G_1}(v_1))+d_{G_2}(u_2)+d_{G_2}(v_2)} \\
&= M_1(G_1, x^{n_2}) \sum_{u_2 \in V(G_2)} \sum_{v_2 \in V(G_2)} x^{d_{G_2}(u_2)+d_{G_2}(v_2)} \\
&\quad + M_1(G_2,x) \sum_{u_1 \in V(G_1)} x^{2n_2 d_{G_1}(u_1)} \\
&= M_1(G_1, x^{n_2})(M_0(G_2,x))^2 + M_1(G_2,x)M_0(G_1, x^{2n_2}).
\end{aligned}$$

$$\begin{aligned}
M_2(G_1[G_2],x) &= \sum_{(u_1,u_2)(v_1,v_2) \in E(G_1[G_2])} x^{d_{G_1[G_2]}((u_1,u_2)) \cdot d_{G_1[G_2]}((v_1,v_2))} \\
&= \sum_{u_1 \in V(G_1)} \sum_{u_2 v_2 \in E(G_2)} x^{(n_2 d_{G_1}(u_1)+d_{G_2}(u_2))(n_2 d_{G_1}(u_1)+d_{G_2}(v_2))} \\
&\quad + \sum_{u_2 \in V(G_2)} \sum_{v_2 \in V(G_2)} \sum_{u_1 v_1 \in E(G_1)} x^{(n_2 d_{G_1}(u_1)+d_{G_2}(u_2))(n_2 d_{G_1}(v_1)+d_{G_2}(v_2))} \\
&= \sum_{u_1 \in V(G_1)} \sum_{u_2 v_2 \in E(G_2)} x^{n_2^2 d_{G_1}(u_1)^2+n_2 d_{G_1}(u_1)d_{G_2}(d)+n_2 d_{G_1}(u_1)d_{G_2}(u_2)+d_{G_1}(u_2)d_{G_2}(v_2)}.
\end{aligned}$$

On simplification, we get the result.

Proposition 3.9 *[7] If G_1 is an (n_1, m_1)-graph and G_2 is an (n_2, m_2)-graph, then*

$$d_{G_1 \circ G_2}(v) = \begin{cases} d_{G_1}(v) + n_2, & \text{if } v \in V(G_1), \\ d_{G_2}(v) + n_1, & \text{if } v \in V(G_2, i),\ i = 1,2,3,\ldots,n_1. \end{cases}$$

Theorem 3.10. *If G_1 is an (n_1, m_1)-graph and G_2 is an (n_2, m_2)-graph, then*

$$M_1(G_1 \circ G_2, x) = x^{2n_2} M_1(G_1, x) + n_1 x^{2n_1} M_1(G_2, x) + x^{n_1+n_2} M_0(G_1, x) M_0(G_2, x)$$

and

$$M_2(G_1 \circ G_2, x) = M'_{n_2,n_2}(G_1, x) + n_1 M'_{n_1,n_1}(G_2, x) + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} x^{(d_{G_1}(u)+n_2)(d_{G_2}(v)+n_1)}$$

Proof. Using the definitions of first and second Zagreb polynomials and from Propositions 2.1, 2.2, 3.9, we get

$$\begin{aligned} M_1(G_1 \circ G_2, x) &= \sum_{uv \in E(G_1 \circ G_2)} x^{d_{G_1 \circ G_2}(u) + d_{G_1 \circ G_2}(v)} \\ &= \sum_{uv \in E(G_1)} x^{d_{G_1 \circ G_2}(u) + d_{G_1 \circ G_2}(v)} + \sum_{uv \in E(G_2)} \sum_{i=1}^{n_1} x^{d_{G_1 \circ G_2}(u) + d_{G_1 \circ G_2}(v)} \\ &\quad + \sum_{u \in V(G_1), v \in V(G_2)} x^{d_{G_1 \circ G_2}(u) + d_{G_1 \circ G_2}(v)} \\ &= \sum_{uv \in E(G_1)} x^{d_{G_1}(u)+n_2+d_{G_1}(v)+n_2} + \sum_{uv \in E(G_2)} \sum_{i=1}^{n_1} x^{d_{G_2}(u)+n_1+d_{G_2}(v)+n_1} \\ &\quad + \sum_{u \in V(G_1), v \in V(G_2)} x^{d_{G_1}(u)+n_2+d_{G_2}(v)+n_1} \\ &= x^{2n_2} M_1(G_1, x) + n_1 x^{2n_1} M_1(G_2, x) + x^{n_1+n_2} M_0(G_1, x) M_0(G_2, x). \end{aligned}$$

$$\begin{aligned} M_2(G_1 \circ G_2, x) &= \sum_{uv \in E(G_1 \circ G_2)} x^{d_{G_1 \circ G_2}(u) \cdot d_{G_1 \circ G_2}(v)} \\ &= \sum_{uv \in E(G_1)} x^{d_{G_1 \circ G_2}(u) \cdot d_{G_1 \circ G_2}(v)} + \sum_{u \in V(G_1), v \in V(G_2)} x^{d_{G_1 \circ G_2}(u) \cdot d_{G_1 \circ G_2}(v)} \\ &= \sum_{uv \in E(G_1)} x^{(d_{G_1}(u)+n_2)(d_{G_1}(v)+n_2)} + \sum_{uv \in E(G_2)} \sum_{i=1}^{n_1} x^{(d_{G_2}(u)+n_1)(d_{G_2}(v)+n_1)} \\ &= M'_{n_2,n_2}(G_1, x) + n_1 M'_{n_1,n_1}(G_2, x) + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} x^{(d_{G_1}(u)+n_2)(d_{G_2}(v)+n_1)} \end{aligned}$$

ACKNOWLEDGEMENT

*This work is partially supported by the University Grants Commission (UGC), New Delhi, through UGC-SAP DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I).

[1]This work is supported by Govt. of India's DST INSPIRE Fellowship 2017: No. DST/INSPIRE Fellowship/[IF170465].

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