

# 贾汉吉尔图的萨格勒布多项式和重新定义的萨格勒布指数

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**摘要:** 在化学图论、分子拓扑学和数学化学领域, 拓扑指数(称为连通性指数)是一种基于化学化合物的分子图计算的分子描述符。萨格勒布指数是最早被定义的指数之一, 对预测化合物熔点、沸点、毒性等有重要的应用价值。随后, 为了扩展萨格勒布指数的应用, 又重新定义了该指数。基于此目的, 计算了贾汉吉尔图的萨格勒布多项式及贾汉吉尔图重新定义的萨格勒布指数。

**关键词:** 贾汉吉尔图; 萨格勒布指数; 拓扑指数; 多项式; 度; 分子图

中图分类号: O157.6 文献标识码: A 文章编号: 1674-5639 (2019) 03-0065-04

DOI: 10.14091/j.cnki.kmxyxb.2019.03.014

## Zagreb Polynomials and Redefined Zagreb Indices of Jahangir Graph

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**Abstract:** In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index, known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. The Zagreb index is one of the earliest defined indexes and has important application value for predicting the melting point, boiling point and toxicity of compounds. Subsequently, in order to extend the application of the Zagreb index, the index was redefined so as to compute Zagreb polynomials of Jahangir graph and redefined Zagreb indices of Jahangir graph.

**Key words:** Jahangir graph; Zagreb index; topological index; polynomial; degree; molecular graph

## 1 Background Knowledge

The study of topological indices, based on distance in a graph, was effectively introduced in 1947 in chemistry by Weiner<sup>[1]</sup>. He introduced a distance-based topological index called the “Wiener index” to correlate properties of alkenes and the structures of their molecular graphs. These indices play a vital role in computational and theoretical aspects of chemistry in predicting material properties<sup>[2]</sup>. Several algebraic polynomials have useful applications in chemistry.

A graph  $G$  is an ordered pair  $(V, E)$ , where  $V$  and  $E$  are vertex and edge set respectively. A graph is connected if there is a connection between every pair of vertices of it. Graph theory is contributing a lion's share in many areas such as chemistry, physics, pharmacy, as well as in industry. We will start with some preliminary facts.

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收稿日期: 2019-03-09

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The first and the second Zagreb indices are defined as :

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v),$$

and

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

Considering the Zagreb indices , Fath-Tabar<sup>[3]</sup> defined first and the second Zagreb polynomials as :

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v},$$

and

$$M_2(G, x) = \sum_{uv \in E(G)} x^{d_u \times d_v}.$$

After that , in [4] the authors defined the third Zagreb index

$$M_3(G) = \sum_{uv \in E(G)} (d_u - d_v),$$

and the polynomial

$$M_3(G, x) = \sum_{uv \in E(G)} x^{d_u - d_v}.$$

In the year 2016<sup>[5]</sup> , following Zagreb type polynomials were defined

$$\begin{aligned} M_4(G, x) &= \sum_{uv \in E(G)} x^{d_u(d_u + d_v)}; \\ M_5(G, x) &= \sum_{uv \in E(G)} x^{d_v(d_u + d_v)}; \\ M_{a,b}(G, x) &= \sum_{uv \in E(G)} x^{ad_u + bd_v}; \\ M'_{a,b}(G, x) &= \sum_{uv \in E(G)} x^{(d_u + a)(d_v + b)}. \end{aligned}$$

Ranjini et al<sup>[6]</sup> redefined the Zagreb index , i. e. , the redefined first , second and third Zagreb indices of graph  $G$ . These indicators appear as :

$$\begin{aligned} \text{ReZG}_1(G) &= \sum_{uv \in E(PD_1)} \frac{d_u + d_v}{d_u \times d_v}; \\ \text{ReZG}_2(G) &= \sum_{uv \in E(PD_1)} \frac{d_u \times d_v}{d_u + d_v}; \\ \text{ReZG}_3(G) &= \sum_{uv \in E(PD_1)} (d_u \times d_v)(d_u + d_v). \end{aligned}$$

In this paper we compute other Zagreb polynomials and Redefined Zagreb indices of Jahangir graphs. The Jahangir graph  $J_{n,m}$  is a graph on  $(nm + 1)$  vertices and  $m(n + 1)$  edges for all  $n \geq 2$  and  $m \geq 3$ .  $J_{n,m}$  consists of a cycle  $C_{nm}$  with one additional vertex which is adjacent to  $m$  vertices of  $C_{nm}$  at distance to each other. Figure 1 shows some particular cases of  $J_{n,m}$ .

## 2 Computational Results

In this section , we present our computational results.

**Theorem 1** Let  $J_{n,m}$  be the Jahangir graph . Then ,

- 1)  $M_3(J_{n,m}, x) = m(n - 2) + 2mx + mx^{m-3};$
- 2)  $M_4(J_{n,m}, x) = m(n - 2)x^8 + 2mx^{10} + mx^{3(3+m)};$
- 3)  $M_5(J_{n,m}, x) = m(n - 2)x^8 + 2mx^{15} + mx^{m(3+m)};$
- 4)  $M_{a,b}(J_{n,m}, x) = mnx^{2a} + m(n - 2)x^{2b}$   
 $+ 2mx^{3b} + mx^{(3a+mb)};$
- 5)  $M'_{a,b}(J_{n,m}, x) = m(n - 2)x^{(2+a)(2+b)}$   
 $+ 2mx^{(2+a)(3+b)} + mx^{(3+a)(m+b)}.$

**Proof** Let  $G$  be the graph of  $J_{n,m}$ . It is clear that the total num-

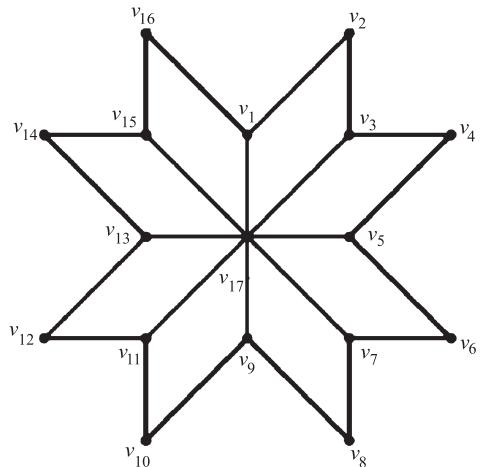


Figure 1 Janhangir Graph

ber of vertices in  $J_{n,m}$  are  $8n+2$  and the total number of edges are  $10n+1$ .

The edge set of  $J_{n,m}$  has the following three partitions,

$$E_1 = E_{\{2,2\}} = \{e = uv \in E(J_{n,m}) \mid d_u = 2, d_v = 2\},$$

$$E_2 = E_{\{2,3\}} = \{e = uv \in E(J_{n,m}) \mid d_u = 2, d_v = 3\},$$

And

$$E_3 = E_{\{3,m\}} = \{e = uv \in E(J_{n,m}) \mid d_u = 3, d_v = m\},$$

Now

$$|E_1(J_{n,m})| = m(n-2), |E_2(J_{n,m})| = 2m,$$

And

$$|E_3(J_{n,m})| = m.$$

$$\begin{aligned} 1) M_3(J_{n,m}, x) &= \sum_{uv \in E(J_{n,m})} x^{d_v - d_u} \\ &= \sum_{uv \in E_1(J_{n,m})} x^{2-2} + \sum_{uv \in E_2(J_{n,m})} x^{3-2} + \sum_{uv \in E_3(J_{n,m})} x^{m-3} \\ &= |E_1(J_{n,m})| + |E_2(J_{n,m})|x + |E_3(J_{n,m})|x^{m-3} \\ &= m(n-2) + 2mx + mx^{m-3}. \end{aligned}$$

$$\begin{aligned} 2) M_4(J_{n,m}, x) &= \sum_{uv \in E(J_{n,m})} x^{d_u(d_u+d_v)} \\ &= \sum_{uv \in E_1(J_{n,m})} x^{2(2+2)} + \sum_{uv \in E_2(J_{n,m})} x^{2(2+3)} + \sum_{uv \in E_3(J_{n,m})} x^{3(3+m)} \\ &= |E_1(J_{n,m})|x^8 + |E_2(J_{n,m})|x^{10} + |E_3(J_{n,m})|x^{3(3+m)} \\ &= m(n-2)x^8 + 2mx^{10} + mx^{3(3+m)}. \end{aligned}$$

$$\begin{aligned} 3) M_5(J_{n,m}, x) &= \sum_{uv \in E(J_{n,m})} x^{d_v(d_u+d_v)} \\ &= \sum_{uv \in E_1(J_{n,m})} x^{2(2+2)} + \sum_{uv \in E_2(J_{n,m})} x^{3(2+3)} + \sum_{uv \in E_3(J_{n,m})} x^{m(3+m)} \\ &= |E_1(J_{n,m})|x^8 + |E_2(J_{n,m})|x^{15} + |E_3(J_{n,m})|x^{m(3+m)} \\ &= m(n-2)x^8 + 2mx^{15} + mx^{m(3+m)}. \end{aligned}$$

$$\begin{aligned} 4) M_{a,b}(J_{n,m}, x) &= \sum_{uv \in E(J_{n,m})} x^{(ad_u+bd_v)} \\ &= \sum_{uv \in E_1(J_{n,m})} x^{(2a+2b)} + \sum_{uv \in E_2(J_{n,m})} x^{(2a+3b)} + \sum_{uv \in E_3(J_{n,m})} x^{(3a+mb)} \\ &= |E_1(J_{n,m})|x^{(2a+2b)} + |E_2(J_{n,m})|x^{(2a+3b)} + |E_3(J_{n,m})|x^{(3a+mb)} \\ &= m(n-2)x^{(2a+2b)} + 2mx^{(2a+3b)} + mx^{(3a+mb)} \\ &= [m(n-2) + 2m]x^{2a} + m(n-2)x^{2b} + 2mx^{3b} + mx^{(3a+mb)} \\ &= mnx^{2a} + m(n-2)x^{2b} + 2mx^{3b} + mx^{(3a+mb)}. \end{aligned}$$

$$\begin{aligned} 5) M'_{a,b}(J_{n,m}, x) &= \sum_{uv \in E(J_{n,m})} x^{(d_u+a)(d_v+b)} \\ &= \sum_{uv \in E_1(J_{n,m})} x^{(2+a)(2+b)} + \sum_{uv \in E_2(J_{n,m})} x^{(2+a)(3+b)} + \sum_{uv \in E_3(J_{n,m})} x^{(3+a)(m+b)} \\ &= |E_1(J_{n,m})|x^{(2+a)(2+b)} + |E_2(J_{n,m})|x^{(2+a)(3+b)} + |E_3(J_{n,m})|x^{(3+a)(m+b)} \\ &= m(n-2)x^{(2+a)(2+b)} + 2mx^{(2+a)(3+b)} + mx^{(3+a)(m+b)}. \end{aligned}$$

**Theorem 2** Let  $J_{n,m}$  be the Jahangir's graph. Then,

$$1) \text{ReZG}_1(J_{n,m}) = m(n-2) + \frac{5}{3}m + \frac{3+m}{3};$$

$$2) \text{ReZG}_2(J_{n,m}) = m(n-2) + \frac{3}{5}m + \frac{3m^2}{3+m};$$

$$3) \text{ReZG}_3(J_{n,m}) = 16m(n-2) + 60m + 3m^2(m+3).$$

**Proof**

$$\begin{aligned} 1) \text{ReZG}_1(J_{n,m}) &= \sum_{uv \in E(J_{n,m})} \frac{d_u + d_v}{d_u \times d_v} \\ &= \sum_{uv \in E_1(J_{n,m})} \frac{2+2}{2 \times 2} + \sum_{uv \in E_2(J_{n,m})} \frac{2+3}{2 \times 3} + \sum_{uv \in E_3(J_{n,m})} \frac{3+m}{3 \times m} \end{aligned}$$

$$\begin{aligned}
&= |E_1(J_{n,m})| + |E_2(J_{n,m})| \frac{5}{6} + |E_3(J_{n,m})| \frac{3+m}{3m} \\
&= m(n-2) + (2m) \frac{5}{6} + (m) \frac{3+m}{3m} \\
&= m(n-2) + \frac{5}{3}m + \frac{3+m}{3}.
\end{aligned}$$

$$\begin{aligned}
2) \text{ ReZG}_2(J_{n,m}) &= \sum_{uv \in E(J_{n,m})} \frac{d_u \times d_v}{d_u + d_v} \\
&= \sum_{uv \in E_1(J_{n,m})} \frac{2 \times 2}{2+2} + \sum_{uv \in E_2(J_{n,m})} \frac{2 \times 3}{2+3} + \sum_{uv \in E_3(J_{n,m})} \frac{3 \times m}{3+m} \\
&= |E_1(J_{n,m})| + |E_2(J_{n,m})| \frac{6}{5} + |E_3(J_{n,m})| \frac{3m}{3+m} \\
&= m(n-2) + (2m) \frac{6}{5} + (m) \frac{3m}{3+m} \\
&= m(n-2) + \frac{3}{5}m + \frac{3m^2}{3+m}.
\end{aligned}$$

$$\begin{aligned}
3) \text{ ReZG}_3(J_{n,m}) &= \sum_{uv \in E(J_{n,m})} (d_u \times d_v)(d_u + d_v) \\
&= \sum_{uv \in E_1(J_{n,m})} (2 \times 2)(2+2) + \sum_{uv \in E_2(J_{n,m})} (2 \times 3)(2+3) + \sum_{uv \in E_3(J_{n,m})} (3m)(3+m) \\
&= |E_1(J_{n,m})|16 + |E_2(J_{n,m})|30 + |E_3(J_{n,m})|(3m^2 + 9m) \\
&= 16m(n-2) + 30(2m) + m(3m^2 + 9m) \\
&= 16m(n-2) + 60m + 3m^2(m+3).
\end{aligned}$$

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