Research Article

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On the Zagreb polynomials of benzenoid systems

Abstract: Topological indices play significant role in determining properties of chemical compound. Algebraic polynomials help to compute topological indices of studied chemical compounds. Benzenoid systems are used mainly as an intermediate to make other chemicals. In this report we aim to compute Zagreb polynomials of zigzag, rhombic, triangular, hourglass and jagged-rectangle benzenoid systems.

Keywords: topological index, Zagreb polynomial, benzenoid system

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1 Introduction

Chemical reaction network theory deals with an attempt to model the behavior of real world chemical systems. From the very beginning of its foundation, it is crucial for research community; especially due to its importance in two branches *i.e.* biochemistry and theoretical chemistry. It also has a significant place in pure mathematics particularly due to its mathematical structures.

Cheminformatics is an upcoming and progressive area that deals with the relationships of quantitative structure activity (QSAR), structure property (QSPR) and also predicts the biochemical activities and properties of chemical compounds (see [1, 2]). In these studies, for the prediction of bioactivity of the chemical compounds, some physicochemical properties and topological indices are used [3, 4].

Mathematical chemistry is a branch, which discusses the chemical structures with the aid of mathematical tools. Molecular graph is a simple graph in chemical graph theory. Such a graph consists of atoms and chemical bonds, which are represented by vertices and edges, respectively. For the connection of vertex set $V(G)$ and edge set $E(G)$ of a graph, there must be an existence of linking between any pair of vertices in G. The distance between two vertices u and v is represented as $d(u,v)$ and it is the shortest length between u and v in graph G. The degree of vertex is basically the number of vertices of G, adjacent to given vertex v and will be represented by $d(v)$.

Many algebraic polynomials have fruitful exercises in chemistry such as Hosoya polynomial, which helps to compute some important distance based topological indices. Degree based topological indices are determined from M-polynomial, which was introduced in 2015. This polynomial has been on the basic areas of interest in computational aspects of substances. Many topological indices can be calculated by using M-polynomial [5, 8]. The topological index of a molecule can be used to quantify the molecular structure and its branches design in many ways. To be simple, the topological index can be considered as a function that assigns each molecular structure to real number [9, 10]. Boiling point, heat of evaporation, heat of formation, chromatographic retention times, surface tension, vapor pressure, etc. can be predicted by using topological indices. The first and the second Zagreb indices are degree based graph invariants, which have been studied extensively since the 1970's. In 1998, Bollobás and Erdős introduced the general Randić index, which is the generalization of Randić index and has been widely studied by both mathematicians and theoretical chemists. Another variant of Randić index is the harmonic index and

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its usefulness for computing the heatof formation of alkanes [11, 12]. The graphs considered in this paper are simply connected.

In 1972, the quantities M_1 and M_2 were found to occur within certain approximate expressions for the total π-electron energy [13]. In 1975, these graph invariants were proposed to be the measures of branching of the carbon-atom skeleton [14]. The name "Zagreb index" (or more precisely, "Zagreb group index") seems to be used in the review article for the first time [15]. For details of the mathematical theory and chemical applications of the Zagreb indices, see surveys [16–19] and papers [20–28].

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

and

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

Considering the Zagreb indices, Fath-Tabar [22] defined the first and the second Zagreb polynomials as

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

and

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

The properties of the first and the second Zagreb polynomials for some chemical structures have been studied in the literature [29, 30].

The third Zagreb index is defined as:

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

This graph invariant is also known as irregularity of G, see Ref. [31–33].

The third Zagreb polynomial is defined as:

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

In the year 2016 [34], following Zagreb type polynomials were defined

$$M_4(G, x) = \sum_{uv \in E(G)} x^{d_u(d_u + d_v)}$$

$$M_5(G, x) = \sum_{uv \in E(G)} x^{d_v(d_u + d_v)}$$

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

$$M'_{a,b}(G, x) = \sum_{uv \in E(G)} x^{(d_u + a)(d_v + b)}.$$

For more details about topological indices and polynomials, we refer to Ref. [35–44].

Benzenoid hydrocarbons play a vital role in our environment, in the food and chemical industries. Benzenoid molecular graphs are systems with deleted hydrogens. It is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge.

This figure divides the plane into one infinite (external) region and a number of finite (internal) regions. All internal regions must be regular hexagons. Benzenoid systems are of considerable importance in theoretical chemistry, because they are the natural graph representation of benzenoid hydrocarbons. A vertex of a hexagonal system belongs to three hexagons, at most. A vertex shared by three hexagons is called an internal vertex [45].

In this paper we study five benzenoid systems. These are zigzag, rhombic, triangular, hourglass and jagged-rectangle benzenoid systems.

2 Main results

2.1 Zagreb polynomials of triangular benzenoid system

In this section, we present our computational results. In terms of chemical graph theory and mathematical chemistry, we associate a graph with the molecular structure, where vertices correspond to atoms and edges to bonds. Triangular benzenoid system is shown in Figure 1. In the following theorem we compute M-polynomial of triangular benzenoid system.

Theorem 1

Let T_p be a triangular benzenoid system where p shows the number of hexagons in the base graph and total number of hexagons in T_p is $\frac{1}{2}p(p + 1)$. Then

1. $M_3(T_p, x) = 6 + \frac{3}{2}p(p - 1) + 6(p - 1)x.$
2. $M_4(T_p, x) = 6x^8 + 6(p - 1)x^{10} + \frac{3}{2}p(p - 1)x^{18}.$
3. $M_5(T_p, x) = 6x^8 + 6(p - 1)x^{15} + \frac{3}{2}p(p - 1)x^{18}.$
4. $M_{a,b}(T_p, x) = 6px^{2a} + 6x^{2b} + \frac{3}{2}p(p - 1)x^{3a} + 3(p - 1)\left(6 + \frac{3}{2}p\right)x^{3b}.$
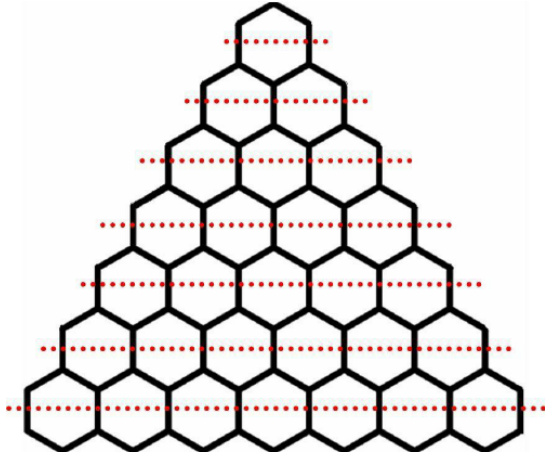
Figure 1: Triangular benzenoid.

5. $M'_{a,b}(T_p, x) = 6x^{(2+a)(2+b)} + 6(p-1)x^{(2+a)(3+b)} + \frac{3}{2}p(p-1)x^{(3+a)(3+b)}$.

Proof. Let T_p be a triangular benzenoid system as shown in Figure 1. Then we have,

$$|V(T_p)| = p^2 + 4p + 1.$$

$$|E(T_p)| = \frac{3}{2}p(p+3).$$

The edge set of T_p has following three partitions,

$$E_{\{2,2\}} = \left\{ e = uv \in E(T_p) \,|\, d_{T_p}(u) = 2, \ d_{T_p}(v) = 2 \right\},$$
$$E_{\{2,3\}} = \left\{ e = uv \in E(T_p) \,|\, d_{T_p}(u) = 2, d_{T_p}(v) = 3 \right\},$$
$$E_{\{3,3\}} = \left\{ e = uv \in E(T_p) \,|\, d_{T_p}(u) = 3, d_{T_p}(v) = 3 \right\},$$

Now

$$|E_{\{2,2\}}| = 6,$$
$$|E_{\{2,3\}}| = 6(p-1),$$

And
$|E_{\{3,3\}}| = \frac{3}{2}p(p-1),$
Now

1. $M_3(T_p, x) = \sum\limits_{uv \in E(T_p)} x^{d_u - d_v} = \sum\limits_{uv \in E_{\{2,2\}}(T_p)} x^{2-2} + \sum\limits_{uv \in E_{\{2,3\}}(T_p)} x^{3-2} + \sum\limits_{uv \in E_{\{3,3\}}(T_p)} x^{3-3} = |E_{\{2,2\}}(T_p)| + |E_{\{2,3\}}(T_p)|x + |E_{\{3,3\}}(T_p)| = 6 + 6(p-1)x + \frac{3}{2}p(p-1) = 6(p-1)x + \left(\frac{3}{2}p^2 - \frac{3}{2}p + 6\right)$.

2. $M_4(T_p, x) = \sum\limits_{uv \in E(T_p)} x^{d_u(d_u + d_v)} = \sum\limits_{uv \in E_{\{2,2\}}(T_p)} x^{2(2+2)} + \sum\limits_{uv \in E_{\{2,3\}}(T_p)} x^{2(2+3)} + \sum\limits_{uv \in E_{\{3,3\}}(T_p)} x^{3(3+3)} = |E_{\{2,2\}}(T_p)|x^8 + |E_{\{2,3\}}(T_p)|x^{10} + |E_{\{3,3\}}(T_p)|x^{18} = 6x^8 + 6(p-1)x^{10} + \frac{3}{2}p(p-1)x^{18}$.

3. $M_5(T_p, x) = \sum\limits_{uv \in E(T_p)} x^{d_v(d_u + d_v)} = \sum\limits_{uv \in E_{\{2,2\}}(T_p)} x^{2(2+2)} + \sum\limits_{uv \in E_{\{2,3\}}(T_p)} x^{3(2+3)} + \sum\limits_{uv \in E_{\{3,3\}}(T_p)} x^{3(3+3)} = |E_{\{2,2\}}(T_p)|x^8 + |E_{\{2,3\}}(T_p)|x^{15} + |E_{\{3,3\}}(T_p)|x^{18} = 6x^8 + 6(p-1)x^{15} + \frac{3}{2}p(p-1)x^{18}$.

4. $M_{a,b}(T_p, x) = \sum\limits_{uv \in E(T_p)} x^{(ad_u + bd_v)} = \sum\limits_{uv \in E_{\{2,2\}}(T_p)} x^{2a+2b} + \sum\limits_{uv \in E_{\{2,3\}}(T_p)} x^{2a+3b} + \sum\limits_{uv \in E_{\{3,3\}}(T_p)} x^{3a+3b} = |E_{\{2,2\}}(T_p)|x^{2a+2b} + |E_{\{2,3\}}(T_p)|x^{2a+3b} + |E_{\{3,3\}}(T_p)|x^{3a+3b} = 6x^{2a+2b} + 6(p-1)x^{2a+3b} + \frac{3}{2}p(p-1)x^{3a+3b} = 6px^{2a} + 6x^{2b} + \frac{3}{2}p(p-1)x^{3a} + (p-1)\left(6 + \frac{3}{2}p\right)x^{3b}$.

5. $M'_{a,b}(T_p, x) = \sum\limits_{uv \in E(T_p)} x^{(d_u + a)(d_v + b)} = \sum\limits_{uv \in E_{\{2,2\}}(T_p)} x^{(2+a)(2+b)} + \sum\limits_{uv \in E_{\{2,3\}}(T_p)} x^{(2+a)(3+b)} + \sum\limits_{uv \in E_{\{3,3\}}(T_p)} x^{(3+a)(3+b)} = |E_{\{2,2\}}(T_p)|x^{(2+a)(2+b)} + |E_{\{2,3\}}(T_p)|x^{(2+a)(3+b)} + |E_{\{3,3\}}(T_p)|x^{(3+a)(3+b)} = 6x^{(2+a)(2+b)} + 6(p-1)x^{(2+a)(3+b)} + \frac{3}{2}p(p-1)x^{(3+a)(3+b)}$.
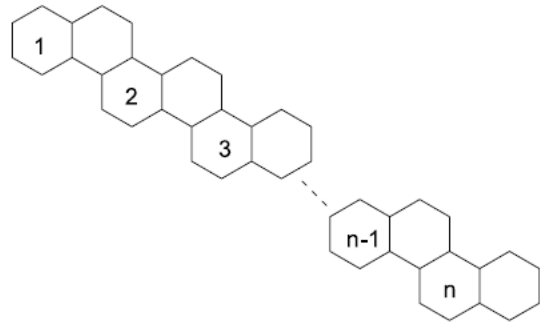
3 Zigzag benzenoid system

Zigzag benzenoid system is denoted by Z_n, where n is the number of rows in graph of Z_n and each row consists of two hexagons as shown in Figure 2.

Zigzag benzenoid system has the following three partitions,

$$E_{\{2,2\}} = \left\{ e = uv \in E(Z_n) \,|\, d_{Z_n}(u) = 2, \ d_{Z_n}(v) = 2 \right\},$$
$$E_{\{2,3\}} = \left\{ e = uv \in E(Z_n) \,|\, d_{Z_n}(u) = 2, d_{Z_n}(v) = 3 \right\},$$
$$E_{\{3,3\}} = \left\{ e = uv \in E(Z_n) \,|\, d_{Z_n}(u) = 3, d_{Z_n}(v) = 3 \right\},$$

Figure 2: Graph of zigzag benzenoid system Z_n.

Now

$$\left|E_{\{2,2\}}(Z_n)\right| = 2n + 4,$$
$$\left|E_{\{2,3\}}(Z_n)\right| = 4n,$$

And $\left|E_{\{3,3\}}(Z_n)\right| = 4n - 3$,
So we have following results.

Theorem 2

Consider a zigzag benzenoid system Z_n, then

1. $M_3(Z_n, x) = 4nx + (6n + 1)$.
2. $M_4(Z_n, x) = 2(n + 2)x^8 + 4nx^{10} + (4n - 3)x^{18}$.
3. $M_5(Z_n, x) = 2(n + 2)x^8 + 4nx^{15} + (4n - 3)x^{18}$.
4. $M_{a,b}(Z_n, x) = 2(3n + 2)x^{2a} + 2(n + 2)x^{2b} + (4n - 3)x^{3a} + (8n - 3)x^{3b}$.
5. $M'_{a,b}(Z_n, x) = 2(n + 2)x^{(2+a)(2+b)} + 4nx^{(2+a)(3+b)} + (4n - 3)x^{(3+a)(3+b)}$.

4 Rhombic benzenoid aystem

Take another benzenoid system in which hexagons are arranged to form a rhombic shape R_n, with n rows of n hexagons as given in Figure 3. Then, it has $2n(n + 2)$ vertices and $3n^2 + 4n - 1$ edges.

A graph of R_n has following three partitions,

$$E_{\{2,2\}} = \left\{e = uv \in E(R_n) \,|\, d_{R_n}(u) = 2,\ d_{R_n}(v) = 2\right\},$$
$$E_{\{2,3\}} = \left\{e = uv \in E(R_n) \,|\, d_{R_n}(u) = 2,\ d_{R_n}(v) = 3\right\},$$
$$E_{\{3,3\}} = \left\{e = uv \in E(R_n) \,|\, d_{R_n}(u) = 3,\ d_{R_n}(v) = 3\right\},$$

Now

$$\left|E_{\{2,2\}}(R_n)\right| = 6,$$
$$\left|E_{\{2,3\}}(R_n)\right| = 8(n - 1),$$

And
$$\left|E_{\{3,3\}}(R_n)\right| = 3n^2 - 4n + 1.$$
The following theorem follows immediately.

Theorem 3

Consider the rhombic bezenoid system R_n, then

1. $M_3(R_n, x) = 8(n - 1)x + (3n^2 - 4n + 7)$.
2. $M_4(R_n, x) = 6x^8 + 8(n - 1)x^{10} + (3n^2 - 4n + 1)x^{18}$.
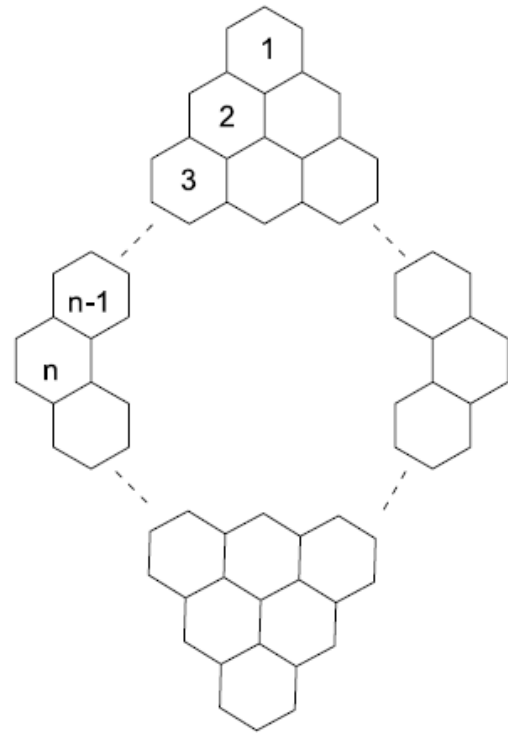3. $M_5(R_n, x) = 6x^8 + 8(n - 1)x^{15} + 4(3n^2 - 4n + 1)x^{18}$.

Figure 3: Graph of rhombic benzenoid system with n rows of n hexagons.

4. $M_{a,b}(R_n, x) = 2(4n - 1)x^{2a} + 6x^{2b} + (3n^2 - 4n + 1)x^{3a} + (3n^2 - 4n + 7)x^{3b}$.
5. $M'_{a,b}(R_n, x) = 6x^{(2+a)(2+b)} + 8(n - 1)x^{(2+a)(3+b)} + (3n^2 - 4n + 1)x^{(3+a)(3+b)}$.

5 Hourglass benzenoid system

Let X_p denotes the benzenoid hourglass, which is obtained from two copies of a triangular benzenoid T_p by overlapping their external hexagons. Then we have,

$$|V(X_p)| = 2(p^2 + 4p - 2)$$
$$|E(X_p)| = 3p^2 + 9p - 4$$

The edge set of X_p has following three partitions,

$$E_{\{2,2\}} = \left\{e = uv \in E(X_p) \,|\, d_{X_p}(u) = 2,\ d_{X_p}(v) = 2\right\},$$
$$E_{\{2,3\}} = \left\{e = uv \in E(X_p) \,|\, d_{X_p}(u) = 2,\ d_{X_p}(v) = 3\right\},$$

And

$$E_{\{3,3\}} = \left\{e = uv \in E(X_p) \,|\, d_{X_p}(u) = 3,\ d_{X_p}(v) = 3\right\}.$$

Now

$$\left|E_{\{2,2\}}(X_p)\right| = 8$$

$$\left|E_{\{2,3\}}\left(X_p\right)\right| = 4\left(3p - 4\right)$$

And

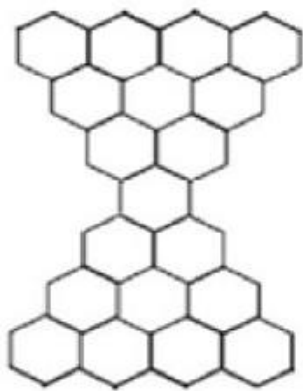$$\left|E_{\{3,3\}}\left(X_p\right)\right| = 3p^2 - 3p + 4$$

Figure 4: Benzenoid hourglass system.

Theorem 4

Consider the bezenoid hourglass X_p, then

1. $M_3(X_p, x) = 4\left(3p - 4\right)x + 3\left(p^2 - p + 4\right).$
2. $M_4(X_p, x) = 8x^8 + 4\left(3p - 4\right)x^{10} + \left(3p^2 - 3p + 4\right)x^{18}.$
3. $M_5(X_p, x) = 8x^8 + 4\left(3p - 4\right)x^{15} + \left(3p^2 - 3p + 4\right)x^{18}.$
4. $M_{a,b}(X_p, x) = 4\left(3p - 2\right)x^{2a} + 8x^{2b} + \left(3p^2 - 3p + 4\right)x^{3a} + 3\left(p^2 + 3p - 4\right)x^{3b}.$
5. $M'_{a,b}(X_p, x) = 8x^{(2+a)(2+b)} + 4\left(3p - 4\right)x^{(2+a)(3+b)} + \left(3p^2 - 3p + 4\right)x^{(3+a)(3+b)}.$

6 Benzenoid jagged-rectangle

Now we study the benzenoid jagged-rectangle shown in Figure 5.

Let $B_{p,q}$ denotes a benzenoid system jagged-rectangle for all $p, q \in N - 1$. A Benzenoid jagged-rectangle forms a rectangle and the number of benzenoids called in each chain alternate p and $p-1$. The edge set of $B_{p,q}$ has following three partitions,

$$E_{\{2,2\}} = \left\{e = uv \in E\left(B_{p,q}\right) | d_{B_{p,q}}\left(u\right) = 2, \ d_{B_{p,q}}\left(v\right) = 2\right\},$$

$$E_{\{2,3\}} = \left\{e = uv \in E\left(B_{p,q}\right) | d_{B_{p,q}}\left(u\right) = 2, \ d_{B_{p,q}}\left(v\right) = 3\right\},$$

$$E_{\{3,3\}} = \left\{e = uv \in E\left(B_{p,q}\right) | d_{B_{p,q}}\left(u\right) = 3, \ d_{B_{p,q}}\left(v\right) = 3\right\},$$
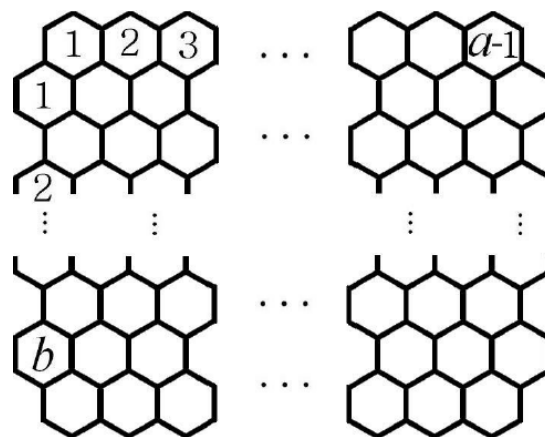
Figure 5: Benzenoid jagged-rectangle system.

Now

$$\left|E_{\{2,2\}}\left(B_{p,q}\right)\right| = 2q + 4,$$
$$\left|E_{\{2,3\}}\left(B_{p,q}\right)\right| = 4p + 4q - 4$$

And

$$\left|E_{\{3,3\}}\left(B_{p,q}\right)\right| = 6pq + p - 5q - 4.$$

Hence we have the following theorem.

Theorem 5

Consider the bezenoid jagged-rectangle $B_{p,q}$, then

1. $M_3(B_{p,q}, x) = 4\left(p + q - 1\right)x + \left(6pq + p - 3q\right).$
2. $M_4(B_{p,q}, x) = 2\left(q + 2\right)x^8 + 4\left(p + q - 1\right)x^{10} + \left(6pq + p - 5q - 4\right)x^{18}.$
3. $M_5(B_{p,q}, x) = 2\left(q + 2\right)x^8 + 4\left(p + q - 1\right)x^{15} + \left(6pq + p - 5q - 4\right)x^{18}.$
4. $M_{a,b}(B_{p,q}, x) = 2\left(2p + 3q\right)x^{2a} + 2\left(q + 2\right)x^{2b} + 4\left(p + q - 1\right)x^{3a} + 3\left(6pq + 5p - q - 8\right)x^{3b}.$
5. $M'_{a,b}(B_{p,q}, x) = 2\left(q + 2\right)x^{(2+a)(2+b)} + 4\left(p + q - 1\right)x^{(2+a)(3+b)} + \left(6pq + p - 5q - 4\right)x^{(3+a)(3+b)}.$

7 Conclusion

Topological indices are numbers associated with graphs of chemical compound and help to predict many properties of understudy chemical compound. Polynomials associated with the graph of chemical compound help to compute topological indices, for example Hosaya polynomial help to compute Wiener index, Hyper Wiener index etc. M-polynomial can be used to compute Zagreb indices, Randić index, symmetric division index, harmonic

index, inverse sum index, augmented Zagreb index. Similarly first, second and third Zagreb polynomial help to compute first, second and third Zagreb index. These polynomials also help to understand molecular structure of understudy chemical compound.

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