



# **FULL PAPER**

# M-polynomial and degree-based topological indices and line graph of hex board graph

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A topological index (TI) is a positive real number associated with the graph of molecule and remains invariant up to graph isomorphism. Until now, several TIs are defined and there are mainly three types: Degree depending, distance depending and spectrum depending. All these TIs found huge applications in pharmacy, theoretical chemistry and especially in QSPR/QSAR research. The aim of our study was to compute degree depending TIs for Hex board graph and its line graph. We firstly computed M-polynomial and by applying calculus, we computed several degree-based topological indices of Hex board graph and its line graph.

#### **KEYWORDS**

M-polynomial; topological index; Zagreb index; hex board; hexagonal network; line graph.

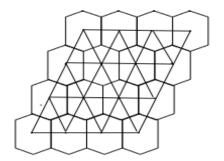
# Introduction

The branch of chemistry, in which we study chemical structures with the help mathematical logics, is known as mathematical chemistry. Chemical graph theory is a branch of mathematical chemistry in which we study molecular compounds graphically. We associate a graph to the molecular structure by taking atoms as dots or vertices and bounds as edges or lines, called molecular graph. A graph is connected if there is a connection between every two vertices of it and a graph is simple if there are no multiple edges or loops between any two vertices. All molecular graphs are simple and connected. The degree of a vertex is equal to the number of vertices attached with it. For basic notions of graph theory we refer the readers to the books [1,2].

To study topology of a molecular graph and make a hunch about some properties of concerned molecular compound, researchers

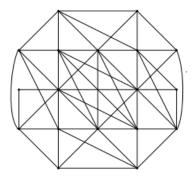
have defined TIs, which help us to know the properties of chemical compounds without performing experiments. In order to compute TIs, huge calculations are required, hence mathematician defined some polynomials that can help in computing TIs, for example Hosoya Polynomial [3] to compute distance depending TIs. Motivated by the Hosoya polynomial, recently M polynomial [4] has been defined to compute degree depending TIs. As stated earlier [4,5], many properties like boiling point of compounds, heat of evaporation of compounds, heat of formation of compounds, chromatographic retention times of compounds, surface tension of compounds, vapor pressure of compounds and many more can be predicted by with the help of TIs. Since its foundation, polynomial has attracted researchers, for example, M-polynomials of polyhex nanotubes [5], Nanostar dendrimers [6], titania nanotubes [7], circulant graphs [8], V-

Phenylenic Nanotubes and Nanotori [9]. For more results on M-polynomial, [10-12, 26-45] and references therein. In this study we aimed to compute M-polynomials of Hex board and line graph of Hex board graphs [13]. The honeycomb and hexagonal systems have additionally been perceived as critical developmental science, specifically for the advancement of cooperation, where the covering triangles are fundamental for the proliferation of participation in social difficulties. Figure 1 is the graph of Hex board graph.



**FIGURE 1** Hex board with center dots [23]

For a graph G, one can construct its line graph L(G) by associating a dot/vertex with each of its line/edge and joining two dots/vertices with an line/edge if and only if the corresponding lines/edges of graph G have a dot/vertex in common [13]. The line graph of Hex board network is shown in Figure 2.



**FIGURE 2** Line graph of hex board [13]

## Basic definitions and literature review

We fixed following notions in the remaining paper.

- *G*=simple connected graph
- V(G)=vertex set
- E(G)=edge set
- $d_{v}$ =degree of v

# M-polynomial

For *G*, the M-polynomial [4] is defined as:

$$M\left(G,x,y\right) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}\left(G\right) x^{i} y^{j}$$

where  $\delta$  is the minimum degree among all vertices and  $\Delta$  is maximum degree among all vertices. The  $m_{ij}(G)$  is the edge such that where

i≤j⁺

The first TI was defined by Wiener [14] which is today known as Wiener index and we have applied successfully in chemistry [15,16]. After the successful application of Wiener index in chemistry, Milan Randić defined first degree depending TIs, which is today known as Randić index,  $R_{-1/2}(G)$ . For the detail about this degree depending index and its application, one can see [17–21]. In literature we can find huge number of books and papers on this TI, for example [22–24]. For the definitions of other TIs and their literature review, we can refer to [4-10].

In Table 1 [4-10], we relate TIs with M-polynomial, where

$$D_{x} = x \frac{\partial (f(x,y))}{\partial x}, D_{y} = y \frac{\partial (f(x,y))}{\partial y},$$

$$S_{x} = \int_{0}^{x} \frac{f(t,y)}{t} dt, S_{y} = \int_{0}^{y} \frac{f(x,t)}{t} dt,$$

$$J(f(x,y)) = f(x,x),$$

$$Q_{\alpha}(f(x,y)) = x^{\alpha} f(x,y). \tag{1}$$

This paper aims to compute M-polynomial and degree depending TIs of hex board and line graph of hex board graphs.

# Methodology

To compute our results, firstly, we sketched hex board and constructed the line graph of hex board graph. Secondly, we counted the number of edges and vertices in hex board and line graph of hex board graphs. By means



of degrees, we divided the vertex set of both graphs in different classes. We also divided edge set of both graphs with respect to the degrees of end vertices into different classes. For the edge partition, we computed Mpolynomial of hex board and line graph of hex board graphs. At last, by using mathematical calculus, we obtained some degree depending TIs of under study graphs.

# **Motivation**

It is really important to compute topological indices of different families of graphs and graphs associated with different chemical compounds. The reality is we require lot of calculations to compute topological indices. In this work our aim was to provide an easy method to compute indices without huge calculations. We aimed to use a simple algebraic polynomial namely M-polynomials to calculate our main results. M-polynomial is important because of the information it contains about indices as almost all topological indices can be calculated from it.

# Applications of results in chemistry

TIs calculated in this study could help us in guessing many properties of compounds involving hex board and line graph of hex board graphs, for example, the Randić index demonstrates great relationship with every single physical property, aside from their liquefying focuses with correlation coefficient value r=0.219. Further, the value correlation coefficient, r lies between 0.881 to 0.995. Randić index has high connection with vaporization with coefficient, r=0.995. The foreseeing intensity of GA for the physical properties is similarly great as Randić index. The value of correlation coefficient lies between 0.889 to 0.987 aside from melting point, with r=0.235. Surprisingly, we could see that the connection of GA with heat of vaporization was extremely high with r=0.9871. The value of

correlation coefficient of sum-connectivity index with properties lies between 0.887 to 0.995 aside from the melting point, where r=0.240. From useful perspective, TI for which the absolute value of r is less than 0.8 can be portrayed as useless. While these degree based topological indices absolute value of r lies between 0.8 to 0.995 are useful.

# Main results

This section contains main computational results.

M-polynomial of hex board graph

The M-polynomial of Hex board graph is presented in the following theorem 1,

**Theorem 1.** Let H<sub>n</sub> be Hex board graph. Then 
$$M(H_n, x, y) = 4x^2y^4 + 4x^3y^4 + 2x^3y^6 + (4k-10)x^4y^4 + (8k-20)x^4y^6 + (3k^2-16k+21)x^6y^6$$
.

**Proof.** Let  $H_n$  be Hex board. The edge set of  $H_n$ has following six partitions [42]

$$E_{1} = \{uv \in E(H_{n}) | d_{u} = 2, d_{v} = 4\},$$

$$E_{2} = \{uv \in E(H_{n}) | d_{u} = 3, d_{v} = 4\},$$

$$E_{3} = \{uv \in E(H_{n}) | d_{u} = 3, d_{v} = 6\},$$

$$E_{4} = \{uv \in E(H_{n}) | d_{u} = 4, d_{v} = 4\},$$

$$E_{5} = \{uv \in E(H_{n}) | d_{u} = 4, d_{v} = 6\},$$

$$E_{6} = \{uv \in E(H_{n}) | d_{u} = 6, d_{v} = 6\}.$$

Such that

$$|E_1| = 4$$
,  $|E_2| = 4$ ,  $|E_3| = 2$ ,  $|E_4| = 4k - 10$ ,  
 $|E_5| = 8k - 20$  and  $|E_6| = 3k^2 - 16k + 21$ .

Now, by using definition of the M-Polynomial, we have

$$\begin{split} &M\left(H_{n};x,y\right) = \sum_{i \leq j} m_{ij} \left(H_{n}\right) x^{i} y^{j} \\ &= \sum_{2 \leq 4} m_{24} \left(H_{n}\right) x^{2} y^{4} + \sum_{3 \leq 4} m_{34} \left(H_{n}\right) x^{3} y^{4} + \sum_{3 \leq 6} m_{36} \left(H_{n}\right) x^{3} y^{6} \\ &+ \sum_{4 \leq 4} m_{44} \left(H_{n}\right) x^{4} y^{4} + \sum_{4 \leq 6} m_{46} \left(H_{n}\right) x^{4} y^{6} + \sum_{6 \leq 6} m_{66} \left(H_{n}\right) x^{6} y^{6} \\ &= \sum_{uv \in E_{1}} m_{24} \left(H_{n}\right) x^{2} y^{4} + \sum_{uv \in E_{2}} m_{34} \left(H_{n}\right) x^{3} y^{4} \\ &+ \sum_{uv \in E_{3}} m_{36} \left(H_{n}\right) x^{3} y^{6} + \sum_{uv \in E_{4}} m_{44} \left(H_{n}\right) x^{4} y^{4} \end{split}$$



$$+ \sum_{uv \in E_s} m_{46} (H_n) x^4 y^6 + \sum_{uv \in E_6} m_{66} (H_n) x^6 y^6$$

$$= 4x^2 y^4 + 4x^3 y^4 + 2x^3 y^6 + (4k - 10) x^4 y^4$$

$$+ (8k - 20) x^4 y^6 + (3k^2 - 16k + 21) x^6 y^6.$$

Now we derive formulae for nine degreedepending TIs by applying calculus on the using M-polynomial given in Theorem 1.

**Theorem 2.** Let  $H_n$  be the Hex board graph. Then

1. 
$$M_1(H_n) = 2(18k^2 - 40k + 21),$$

2. 
$$M_2(H_n) = 108k^2 - 320k + 232$$
,

3. 
$${}^{m}M_{2}(H_{n}) = \frac{1}{12}k^{2} + \frac{5}{36}k - \frac{7}{8},$$

4. 
$$R_{\alpha}(H_n) = 3 \times 6^{2\alpha} k^2 + (4^{2\alpha+1} + 2 \cdot 4^{\alpha+1} \cdot 6^{\alpha} - 16 \cdot 6^{2\alpha}) k$$
  
  $+4^{\alpha+1} (2^{\alpha} + 3^{\alpha} - 5 \cdot 6^{\alpha}) - 10 \cdot 4^{2\alpha} + 21 \cdot 6^{2\alpha},$ 

5. 
$$R_{\alpha}(H_n) = \frac{3}{6^{2\alpha}}k^2 + \left(\frac{1}{4^{2\alpha-1}} + \frac{8}{4^{\alpha} \cdot 6^{\alpha}} - \frac{16}{6^{2\alpha}}\right)k$$
  
  $+ \left(\frac{1}{2^{3\alpha-2}} + \frac{1}{3^{\alpha} \cdot 4^{\alpha-1}} + \frac{2}{3^{\alpha} \cdot 6^{\alpha}} - \frac{10}{4^{2\alpha}} - \frac{20}{4^{\alpha} \cdot 6^{\alpha}} + \frac{21}{6^{2\alpha}}\right)$ 

6. 
$$SSD(H_n) = 6k^2 - \frac{40}{3}k + \frac{56}{3}$$

7. 
$$H(H_n) = \frac{1}{2}k^2 - \frac{1}{15}k - \frac{5}{63}$$

8. 
$$I(H_n) = 9k^2 - \frac{104}{5}k - \frac{1088}{21}$$

9. 
$$A(H_n) = 3 \times 2^{n+3} + 21 \times 2^{n+2} + 369 \times 2^{n-2} - \frac{753}{8}$$
.

## Proof. Let

$$\begin{split} &M\left(H_{n},x,y\right)=f\left(x,y\right)=4x^{2}y^{4}+4x^{3}y^{4}+2x^{3}y^{6}\\ &+\left(4k-10\right)x^{4}y^{4}+\left(8k-20\right)x^{4}y^{6}+\left(3k^{2}-16k+21\right)x^{6}y^{6}.\\ &D_{x}f\left(x,y\right)=8x^{2}y^{4}+12x^{3}y^{4}+6x^{3}y^{6}+4\left(4k-10\right)x^{4}y^{4}\\ &+4\left(8k-20\right)x^{4}y^{6}+6\left(3k^{2}-16k+21\right)x^{6}y^{6},\\ &D_{y}f\left(x,y\right)=16x^{2}y^{4}+16x^{3}y^{4}+12x^{3}y^{6}+4\left(4k-10\right)x^{4}y^{4}\\ &+6\left(8k-20\right)x^{4}y^{6}+6\left(3k^{2}-16k+21\right)x^{6}y^{6},\\ &D_{y}D_{x}f\left(x,y\right)=32x^{2}y^{4}+48x^{3}y^{4}+36x^{3}y^{6}+16\left(4k-10\right)x^{4}y^{4}\\ &+24\left(8k-20\right)x^{4}y^{6}+36\left(3k^{2}-16k+21\right)x^{6}y^{6},\\ &S_{x}S_{y}\left(f\left(x,y\right)\right)=\frac{1}{2}x^{2}y^{4}+\frac{1}{3}x^{3}y^{4}+\frac{1}{9}x^{3}y^{6}+\frac{1}{16}\left(4k-10\right)x^{4}y^{4}\\ &+\frac{1}{24}\left(8k-20\right)x^{4}y^{6}+\frac{1}{36}\left(3k^{2}-16k+21\right)x^{6}y^{6},\\ &D_{x}^{\alpha}D_{y}^{\alpha}\left(f\left(x,y\right)\right)=2^{\alpha}\cdot4^{\alpha+1}x^{2}y^{4}+3^{\alpha}\cdot4^{\alpha+1}x^{3}y^{4}\\ &+2\cdot3^{\alpha}\cdot6^{\alpha}x^{3}y^{6}+4^{2\alpha}\left(4k-10\right)x^{4}y^{4} \end{split}$$

 $+4^{\alpha} \cdot 6^{\alpha} (8k-20) x^4 y^6 + 6^{2\alpha} (3k^2 - 16k + 21) x^6 y^6$ 

$$\begin{split} S_x{}^\alpha S_y{}^\alpha \left( f(x,y) = \frac{1}{2^\alpha \cdot 4^{\alpha-1}} \, x^2 \, y^4 + \frac{1}{3^\alpha \cdot 4^{\alpha-1}} \, x^3 \, y^4 \right. \\ &+ \frac{2}{3^\alpha \cdot 6^\alpha} \, x^3 \, y^6 + \frac{1}{4^{2\alpha}} \left( 4k - 10 \right) x^4 \, y^4 \\ &+ \frac{1}{4^\alpha \cdot 6^\alpha} \left( 8k - 20 \right) x^4 \, y^6 + \frac{1}{6^{2\alpha}} \left( 3k^2 - 16k + 21 \right) x^6 \, y^6 \,, \\ S_y D_x \left( f(x,y) \right) &= 2x^2 \, y^4 + 3x^3 \, y^4 + x^3 \, y^6 + \left( 4k - 10 \right) x^4 \, y^4 \\ &+ \frac{2}{3} \left( 8k - 20 \right) x^4 \, y^6 + \left( 3k^2 - 16k + 21 \right) x^6 \, y^6 \,, \\ S_x D_y \left( f(x,y) \right) &= 8x^2 \, y^4 + \frac{16}{3} \, x^3 \, y^4 + 4x^3 \, y^6 + \left( 4k - 10 \right) x^4 \, y^4 \\ &+ \frac{2}{3} \left( 8k - 20 \right) x^4 \, y^6 + \left( 3k^2 - 16k + 21 \right) x^6 \, y^6 \,, \\ S_x J f \left( x, \, y \right) &= \frac{2}{3} \, x^6 + \frac{4}{7} \, x^7 + \frac{2}{9} \, x^9 + \frac{1}{8} \left( 4k - 10 \right) x^8 \\ &+ \frac{1}{10} \left( 8k - 20 \right) x^{10} + \frac{1}{12} \left( 3k^2 - 16k + 21 \right) x^{12} \,\,, \\ S_x J D_x D_y f \left( x, \, y \right) &= \frac{16}{3} \, x^6 + \frac{48}{7} \, x^7 + 4x^9 + 2 \left( 4k - 10 \right) x^8 \\ &+ \frac{12}{5} \left( 8k - 20 \right) x^{10} + 3 \left( 3k^2 - 16k + 21 \right) x^{12} \,\,, \\ S_x \, ^3 Q_{-2} J D_x \, ^3 D_y \, ^3 f \left( x, \, y \right) &= 3 \times 2^{n+3} \, x \\ &+ \frac{369}{8} \left( 2^{n+1} - 1 \right) x^2 + 12 \left( 7 \times 2^n - 4 \right) x^3 \,\,. \end{split}$$

# 1. First Zagreb Index

$$M_1(H_n) = (D_x + D_y) f(x, y) \Big|_{x=y=1} = 2(18k^2 - 40k + 21).$$

2. Second Zagreb Index

$$M_2(H_n) = D_y D_x(f(x, y))\Big|_{x=y=1} = 108k^2 - 320k + 232.$$

4. Generalized Randić Index

$$\begin{split} R_{\alpha} \left( H_{n} \right) &= D_{x}^{\alpha} D_{y}^{\alpha} \left( f(x, y) \right) \Big|_{x = y = 1} \\ &= 3 \times 6^{2\alpha} k^{2} + \left( 4^{2\alpha + 1} + 2 \cdot 4^{\alpha + 1} \cdot 6^{\alpha} - 16 \cdot 6^{2\alpha} \right) k \\ &+ 4^{\alpha + 1} \left( 2^{\alpha} + 3^{\alpha} - 5 \cdot 6^{\alpha} \right) - 10 \cdot 4^{2\alpha} + 21 \cdot 6^{2\alpha}. \end{split}$$

5. Inverse Randić Index

$$\begin{split} RR_{\alpha}\left(H_{n}\right) &= S_{x}^{\alpha}S_{y}^{\alpha}\left(f(x,y)\right)\Big|_{x=y=1} \\ &= \frac{3}{6^{2\alpha}}k^{2} + \left(\frac{1}{4^{2\alpha-1}} + \frac{8}{4^{\alpha} \cdot 6^{\alpha}} - \frac{16}{6^{2\alpha}}\right)k \\ &+ \left(\frac{1}{2^{3\alpha-2}} + \frac{1}{3^{\alpha} \cdot 4^{\alpha-1}} + \frac{2}{3^{\alpha} \cdot 6^{\alpha}} - \frac{10}{4^{2\alpha}} - \frac{20}{4^{\alpha} \cdot 6^{\alpha}} + \frac{21}{6^{2\alpha}}\right). \end{split}$$

6. Symmetric Division Index

$$\begin{split} SSD(G) &= \Big( S_y D_x + S_x D_y \Big) \Big( f(x, y) \Big) \Big|_{x = y = 1} \\ &= 6k^2 - \frac{40}{3}k + \frac{56}{3}. \end{split}$$

7. Harmonic Index

$$H(G) = 2S_x J(f(x, y))|_{x=1} = \frac{1}{2}k^2 - \frac{1}{15}k - \frac{5}{63}.$$

8. Inverse Sum Index

$$I(G) = S_x J D_x D_y \left( f(x, y) \right)_{x=1} = 9k^2 - \frac{104}{5} k - \frac{1088}{21}.$$

M-polynomial of Line graph of hex board graph

Here, we will study line graph of Hex Board graph. In the next theorem we present the M-polynomial.

**Theorem 3.** Let G be the line graph of Hex board  $H_n$ . Then

$$M(G,x,y) = 2x^{4}y^{4} + 8x^{4}y^{6} + 4x^{4}y^{8} + 2x^{5}y^{5}$$

$$+4x^{5}y^{6} + 4x^{5}y^{7} + 8x^{5}y^{8} + (4k - 12)x^{6}y^{6}$$

$$+(16k - 48)x^{6}y^{8} + 4x^{7}y^{8} + 6x^{7}y^{10}$$

$$+(8k - 14)x^{8}y^{8} + (32k - 100)x^{8}y^{10}$$

$$+(15k^{2} - 96k + 152)x^{10}y^{10}.$$

**Proof.** Let  $_{G}$  be the line graph of Hex board graph. The edge set of  $_{G}$  has following 14 partitions.

partitions. 
$$E_{1} = \left\{uv \in E(G) | d_{u} = 4, d_{v} = 4\right\},$$

$$E_{2} = \left\{uv \in E(G) | d_{u} = 4, d_{v} = 6\right\},$$

$$E_{3} = \left\{uv \in E(G) | d_{u} = 4, d_{v} = 8\right\},$$

$$E_{4} = \left\{uv \in E(G) | d_{u} = 5, d_{v} = 5\right\},$$

$$E_{5} = \left\{uv \in E(G) | d_{u} = 5, d_{v} = 6\right\},$$

$$E_{6} = \left\{uv \in E(G) | d_{u} = 5, d_{v} = 7\right\},$$

$$E_{7} = \left\{uv \in E(G) | d_{u} = 5, d_{v} = 8\right\},$$

$$E_{8} = \left\{uv \in E(G) | d_{u} = 6, d_{v} = 6\right\},$$

$$E_{9} = \left\{uv \in E(G) | d_{u} = 6, d_{v} = 8\right\},$$

$$E_{10} = \left\{uv \in E(G) | d_{u} = 7, d_{v} = 8\right\},$$

$$E_{11} = \left\{uv \in E(G) | d_{u} = 7, d_{v} = 10\right\},$$

$$E_{12} = \left\{uv \in E(G) | d_{u} = 8, d_{v} = 8\right\},$$

$$E_{13} = \left\{uv \in E(G) | d_{u} = 8, d_{v} = 10\right\},$$

$$E_{14} = \left\{uv \in E(G) | d_{u} = 10, d_{v} = 10\right\},$$
Such that

$$|E_1| = 2$$
,  $|E_2| = 8$ ,  $|E_3| = 4$ ,  $|E_4| = 2$ ,  $|E_5| = 4$ ,  
 $|E_6| = 4$ ,  $|E_7| = 8$ ,  $|E_8| = 4k - 12$ ,  $|E_9| = 16k - 48$ ,  
 $|E_{10}| = 4$ ,  $|E_{11}| = 6$ ,  $|E_{12}| = 8k - 14$ ,  
 $|E_{13}| = 32k - 100$ ,  $|E_{14}| = 15k^2 - 96k + 152$ .

Now, by using the definition of the M-polynomial, we obtain

$$\begin{split} &M\left(G;x,y\right) = \sum_{i \leq j} m_{ij}\left(G\right)x^{i}y^{j} \\ &= \sum_{4 \leq 4} m_{44}\left(G\right)x^{4}y^{4} + \sum_{4 \leq 6} m_{46}\left(G\right)x^{4}y^{6} + \sum_{4 \leq 8} m_{48}\left(G\right)x^{4}y^{8} \\ &+ \sum_{5 \leq 5} m_{55}\left(G\right)x^{5}y^{5} + \sum_{5 \leq 6} m_{56}\left(G\right)x^{5}y^{6} + \sum_{5 \leq 7} m_{57}\left(G\right)x^{5}y^{7} \\ &+ \sum_{5 \leq 8} m_{58}\left(G\right)x^{5}y^{8} + \sum_{6 \leq 6} m_{66}\left(G\right)x^{6}y^{6} + \sum_{6 \leq 8} m_{68}\left(G\right)x^{6}y^{8} \\ &+ \sum_{7 \leq 8} m_{78}\left(G\right)x^{7}y^{8} + \sum_{7 \leq 10} m_{710}\left(G\right)x^{7}y^{10} + \sum_{8 \leq 8} m_{88}\left(G\right)x^{8}y^{8} \\ &+ \sum_{8 \leq 10} m_{810}\left(G\right)x^{8}y^{10} + \sum_{10 \leq 10} m_{1010}\left(G\right)x^{10}y^{10} \\ &= 2x^{4}y^{4} + 8x^{4}y^{6} + 4x^{4}y^{8} + 2x^{5}y^{5} + 4x^{5}y^{6} + 4x^{5}y^{7} \\ &+ 8x^{5}y^{8} + \left(4k - 12\right)x^{6}y^{6} + \left(16k - 48\right)x^{6}y^{8} + 4x^{7}y^{8} \\ &+ 6x^{7}y^{10} + \left(8k - 14\right)x^{8}y^{8} + \left(32k - 100\right)x^{8}y^{10} \\ &+ \left(15k^{2} - 96k + 152\right)x^{10}y^{10}. \end{split}$$

Now we derive formulae for nine degreedepending TIs by using calculus on the Mpolynomial given in the theorem 3.

**Theorem 4.** Let G be the line graph of Hex board graph. Then

1. 
$$M_1(G) = (300k^2 - 944k + 722),$$

2. 
$$M_2(G) = 1500k^2 - 5616k + 5194$$
,

3. 
$${}^{m}M_{2}(G) = \frac{3}{20}k^{2} + \frac{17}{1800}k + \frac{611}{420},$$

$$R_{\alpha}(G) = 15 \cdot 10^{2\alpha} k^2 + [2^{2\alpha+2} \cdot 3^{\alpha} + 2^{3\alpha+4} \cdot 6^{\alpha} + 8^{2\alpha+1}]$$

4. 
$$\begin{aligned} +2^{3\alpha+5} \cdot 10^{\alpha} \, ]k + & [2^{4\alpha+1} + 2^{3\alpha+3} \cdot 3^{\alpha} + 2^{5\alpha+2} + 2 \cdot 5^{2\alpha} \\ & +2^{\alpha+2} \cdot 3^{\alpha} \cdot 5^{\alpha} + 4 \cdot 5^{\alpha} \cdot 7^{\alpha} + 5^{\alpha} \cdot 8^{\alpha+1} - 12 \cdot 6^{2\alpha} \\ & -6^{\alpha+1} \cdot 8^{\alpha+1} + 2^{3\alpha+2} \cdot 7^{\alpha} + 3 \cdot 2^{\alpha+1} \cdot 5^{\alpha} \cdot 7^{\alpha} - 7 \cdot 2^{6\alpha+1} \\ & -10^{\alpha+2} \cdot 8^{\alpha} + 152 \cdot 10^{2\alpha} \, ], \end{aligned}$$

5. 
$$RR_{\alpha}(G) = \frac{15}{10^{2\alpha}} + \left[\frac{4}{6^{2\alpha}} + \frac{2}{6^{\alpha} \cdot 8^{\alpha - 1}} + \frac{1}{8^{2\alpha - 1}} + \frac{1}{2^{3\alpha - 5} \cdot 10^{\alpha}} - \frac{96}{10^{2\alpha}}\right]k + \left[\frac{1}{2^{4\alpha - 1}} + \frac{1}{6^{\alpha} \cdot 2^{2\alpha - 3}} + \frac{1}{2^{5\alpha - 2}} + \frac{2}{5^{2\alpha}} + \frac{4}{5^{\alpha} \cdot 7^{\alpha}} + \frac{1}{5^{\alpha} \cdot 8^{\alpha - 1}} - \frac{12}{6^{2\alpha}} - \frac{1}{6^{\alpha - 1} \cdot 8^{\alpha - 1}} + \frac{1}{7^{\alpha} \cdot 2^{3\alpha - 2}} + \frac{6}{7^{\alpha} \cdot 10^{\alpha}} - \frac{14}{8^{2\alpha}} - \frac{1}{8^{\alpha} \cdot 10^{\alpha - 2}} + \frac{152}{10^{2\alpha}}\right],$$

6. 
$$SSD(G) = 30k^2 - \frac{1036}{15}k + \frac{7889}{210}$$

7. 
$$H(G) = \frac{3}{2}k^2 - \frac{659}{315}k + \frac{1569319}{3063060}$$

8. 
$$I(G) = 75k^2 - \frac{15052}{63}k - \frac{440559038}{765765}$$

#### Proof. Let

$$\begin{split} M\left(G,x,y\right) &= f\left(x,y\right) = 2x^{4}y^{4} + 8x^{4}y^{6} + 4x^{4}y^{8} + 2x^{5}y^{5} \\ &+ 4x^{5}y^{6} + 4x^{5}y^{7} + 8x^{5}y^{8} + \left(4k - 12\right)x^{6}y^{6} + \left(16k - 48\right)x^{6}y^{8} \\ &+ 4x^{7}y^{8} + 6x^{7}y^{10} + \left(8k - 14\right)x^{8}y^{8} + \left(32k - 100\right)x^{8}y^{10} \\ &+ \left(15k^{2} - 96k + 152\right)x^{10}y^{10}. \end{split}$$

## Then

Then 
$$D_x f(x,y) = 8x^4 y^4 + 32x^4 y^6 + 16x^4 y^8 + 10x^5 y^5 + 20x^5 y^6 + 20x^5 y^7 + 40x^5 y^8 + 6(4k - 12)x^6 y^6 + 6(16k - 48)x^6 y^8 + 28x^7 y^8 + 42x^7 y^{10} + 8(8k - 14)x^8 y^8 + 8(32k - 100)x^8 y^{10} + 10(15k^2 - 96k + 152)x^{10}y^{10},$$

$$D_y f(x,y) = 8x^4 y^4 + 48x^4 y^6 + 32x^4 y^8 + 10x^5 y^5 + 24x^5 y^6 + 28x^5 y^7 + 64x^5 y^8 + 6(4k - 12)x^6 y^6 + 8(16k - 48)x^6 y^8 + 32x^7 y^8 + 60x^7 y^{10} + 8(8k - 14)x^8 y^8 + 10(32k - 100)x^8 y^{10} + 10(15k^2 - 96k + 152)x^{10}y^{10},$$

$$D_y D_x f(x,y) = 32x^4 y^4 + 192x^4 y^6 + 128x^4 y^8 + 50x^5 y^5 + 120x^5 y^6 + 140x^5 y^7 + 320x^5 y^8 + 36(4k - 12)x^6 y^6 + 48(16k - 48)x^6 y^8 + 224x^7 y^8 + 420x^7 y^{10} + 64(8k - 14)x^8 y^8 + 80(32k - 100)x^8 y^{10} + 100(15k^2 - 96k + 152)x^{10}y^{10},$$

$$S_x S_y (f(x,y)) = \frac{1}{8}x^4 y^4 + \frac{1}{3}x^4 y^6 + \frac{1}{8}x^4 y^8 + \frac{2}{25}x^5 y^5 + \frac{2}{15}x^5 y^6 + \frac{4}{35}x^5 y^7 + \frac{1}{5}x^5 y^8 + \frac{1}{36}(4k - 12)x^6 y^6 + \frac{1}{48}(16k - 48)x^6 y^8 + \frac{1}{14}x^7 y^8 + \frac{3}{35}x^7 y^{10} + \frac{1}{46}(8k - 14)x^8 y^8 + \frac{1}{80}(32k - 100)x^8 y^{10},$$

$$D_x a D_y a (f(x,y)) = 2^{4a+1}x^4 y^4 + 2^{3a+3} \cdot 3^a x^4 y^6 + 2^{5a+2}x^4 y^8 + 2 \cdot 5^{2a}x^5 y^5 + 2^{a+2} \cdot 3^a \cdot 5^a x^5 y^6 + 3x^5 y^7 + 5^a \cdot 8^{a+1}x^5 y^8 + 6^{2a}(4k - 12)x^6 y^6 + 6^a \cdot 8^a (16k - 48)x^6 y^8 + 2^{3a+2} \cdot 7^a x^7 y^8 + 3 \cdot 5^a \cdot 2^{a+1} \cdot 7^a x^7 y^{10} + 8^{2a}(8k - 14)x^8 y^8 + 3 \cdot 5^a \cdot 2^{a+1} \cdot 7^a x^7 y^{10} + 8^{2a}(8k - 14)x^8 y^8 + 3 \cdot 5^a \cdot 2^{a+1} \cdot 7^a x^7 y^{10} + 8^{2a}(8k - 14)x^8 y^8 + 3 \cdot 5^a \cdot 2^{a+1} \cdot 7^a x^7 y^{10} + 8^{2a}(8k - 14)x^8 y^8 + 3 \cdot 10^a (32k - 100)x^8 y^{10} + 10^{2a}(15k^2 - 96k + 152)x^{10}y^{10},$$

$$S_x a S_y a (f(x,y)) = \frac{1}{2^{4a-1}}x^4 y^4 + \frac{8}{8}x^4 x^4 y^6 + \frac{1}{12^{5a-2}}x^4 y^8 + \frac{2}{5^{2a}}x^5 y^5 + \frac{4}{6^a \cdot 5^a}x^5 y^6 + \frac{4}{5^a \cdot 7^a}x^5 y^7 + \frac{1}{5^a \cdot 8^{a-1}}x^5 y^8 + \frac{1}{6^a \cdot 8^a}(16k - 48)x^6 y^8 + \frac{1}{7^a \cdot 2^{3a-2}}x^7 y^8 + \frac{1}{6^a \cdot 8^a}(16k - 48)x^6 y^8 + \frac{1}{7^a \cdot 2^{3a-2}}x^7 y^8 + \frac{1}{6^a \cdot 8^a}(32k - 100)x^8 y^{10} + \frac{1}{10^{2a}}(15k^2 - 96k + 152)x^{10}y^{10},$$

$$S_x a$$

$$\begin{split} S_y D_x \Big( f(x,y) \Big) &= 2 x^4 y^4 + \frac{16}{3} x^4 y^6 + 2 x^4 y^8 + 2 x^5 y^5 \\ &+ \frac{10}{3} x^5 y^6 + \frac{20}{7} x^5 y^7 + 5 x^5 y^8 + (4k - 12) x^6 y^6 \\ &+ \frac{3}{4} (16k - 48) x^6 y^8 + \frac{28}{8} x^7 y^8 + \frac{21}{5} x^7 y^{10} + (8k - 14) x^8 y^8 \\ &+ \frac{4}{5} (32k - 100) x^8 y^{10} + \left(15k^2 - 96k + 152\right) x^{10} y^{10}, \\ S_x D_y \Big( f(x,y) \Big) &= 2 x^4 y^4 + 12 x^4 y^6 + 8 x^4 y^8 + 2 x^5 y^5 \\ &+ \frac{24}{5} x^5 y^6 + \frac{28}{5} x^5 y^7 + \frac{64}{5} x^5 y^8 + (4k - 12) x^6 y^6 \\ &+ \frac{4}{3} (16k - 48) x^6 y^8 + \frac{32}{7} x^7 y^8 + \frac{60}{7} x^7 y^{10} \\ &+ (8k - 14) x^8 y^8 + \frac{5}{4} (32k - 100) x^8 y^{10} \\ &+ \left(15k^2 - 96k + 152\right) x^{10} y^{10}, \\ S_x Jf(x,y) &= \frac{1}{4} x^8 + \frac{4}{5} x^{10} + \frac{1}{3} x^{12} + \frac{1}{5} x^{10} + \frac{4}{11} x^{11} \\ &+ \frac{1}{3} x^{12} + \frac{8}{13} x^{13} + \frac{1}{12} (4k - 12) x^{12} + \frac{1}{14} (16k - 48) x^{14} \\ &+ \frac{4}{15} x^{15} + \frac{6}{17} x^{17} + \frac{1}{16} (8k - 14) x^{16} \\ &+ \frac{1}{18} (32k - 100) x^{18} + \frac{1}{20} (15k^2 - 96k + 152) x^{20}, \\ S_x JD_x D_y f(x,y) &= 4 x^8 + \frac{192}{8} x^{10} + \frac{128}{12} x^{12} + 5 x^{10} + \frac{120}{11} x^{11} \\ &+ \frac{140}{12} x^{12} + \frac{320}{13} x^{13} + 3(4k - 12) x^{12} + \frac{48}{14} (16k - 48) x^{14} + \frac{224}{15} x^{15} \\ &+ \frac{420}{17} x^{17} + 4(8k - 14) x^{16} + \frac{80}{18} (32k - 100) x^{18} + 5 \left(15k^2 - 96k + 152\right) x^{20}, \\ S_x {}^3 Q_{-2} JD_x {}^3 D_y {}^3 f(x,y) &= 3 \times 2^{n+3} x \\ &+ \frac{369}{8} \Big( 2^{n+1} - 1 \Big) x^2 + 12 \Big( 7 \times 2^n - 4 \Big) x^3 \;. \end{split}$$

# 1. First Zagreb Index

$$M_1(G) = (D_x + D_y) f(x, y) \Big|_{x=y=1} = (300k^2 - 944k + 722).$$

# 2. Second Zagreb Index

$$M_2(G) = D_y D_x(f(x, y))\Big|_{x=y=1} = 1500k^2 - 5616k + 5194.$$

# 3. Modified Zagreb Index

$${}^{m}M_{2}(G) = S_{x}S_{y}(f(x,y))\Big|_{x=y=1} = \frac{3}{20}k^{2} + \frac{17}{1800}k + \frac{611}{420}$$

## 4. Generalized Randić Index

$$\begin{split} R_{\alpha}\left(G\right) &= D_{x}^{\alpha} D_{y}^{\alpha} \left(f(x,y)\right) \Big|_{x=y=1} \\ &= 15 \cdot 10^{2\alpha} \, k^{2} + \left[2^{2\alpha+2} \cdot 3^{\alpha} + 2^{3\alpha+4} \cdot 6^{\alpha} + 8^{2\alpha+1} + 2^{3\alpha+5} \cdot 10^{\alpha} \right] k + \left[2^{4\alpha+1} + 2^{3\alpha+3} \cdot 3^{\alpha} + 2^{5\alpha+2} + 2 \cdot 5^{2\alpha} + 2^{\alpha+2} \cdot 3^{\alpha} \cdot 5^{\alpha} + 4 \cdot 5^{\alpha} \cdot 7^{\alpha} + 5^{\alpha} \cdot 8^{\alpha+1} - 12 \cdot 6^{2\alpha} - 6^{\alpha+1} \cdot 8^{\alpha+1} + 2^{3\alpha+2} \cdot 7^{\alpha} + 3 \cdot 2^{\alpha+1} \cdot 5^{\alpha} \cdot 7^{\alpha} \\ &- 7 \cdot 2^{6\alpha+1} - 10^{\alpha+2} \cdot 8^{\alpha} + 152 \cdot 10^{2\alpha} \, \text{l}. \end{split}$$

#### 5. Inverse Randić Index

$$\begin{split} &RR_{\alpha}\left(G\right) = S_{x}^{\alpha}S_{y}^{\alpha}\left(f\left(x,y\right)\right)\Big|_{x=y=1} \\ &= \frac{15}{10^{2\alpha}} + \left(\frac{4}{6^{2\alpha}} + \frac{2}{6^{\alpha} \cdot 8^{\alpha-1}} + \frac{1}{8^{2\alpha-1}} + \frac{1}{2^{3\alpha-5} \cdot 10^{\alpha}} - \frac{96}{10^{2\alpha}}\right)k \\ &+ \frac{1}{2^{4\alpha-1}} + \frac{1}{6^{\alpha} \cdot 2^{2\alpha-3}} + \frac{1}{2^{5\alpha-2}} + \frac{2}{5^{2\alpha}} + \frac{4}{5^{\alpha} \cdot 7^{\alpha}} + \frac{1}{5^{\alpha} \cdot 8^{\alpha-1}} \\ &- \frac{12}{6^{2\alpha}} - \frac{1}{6^{\alpha-1} \cdot 8^{\alpha-1}} + \frac{1}{7^{\alpha} \cdot 2^{3\alpha-2}} \\ &+ \frac{6}{7^{\alpha} \cdot 10^{\alpha}} - \frac{14}{8^{2\alpha}} - \frac{1}{8^{\alpha} \cdot 10^{\alpha-2}} + \frac{152}{10^{2\alpha}} \,. \end{split}$$

# 6. Symmetric Division Index

$$SSD(G) = \left(S_y D_x + S_x D_y\right) \left(f(x, y)\right)\Big|_{x=y=1}$$
$$= 30k^2 - \frac{1036}{15}k + \frac{7889}{210}$$

7. Harmonic Index

$$H(G) = 2S_x J(f(x, y))|_{x=1} = \frac{3}{2}k^2 - \frac{659}{315}k + \frac{1569319}{3063060}.$$

8. Inverse Sum Index

$$I(G) = S_x J D_x D_y \left( f(x,y) \right)_{x=1} = 75 k^2 - \frac{15052}{63} k - \frac{440559038}{765765}.$$

## **Conclusion**

Graphs are a significant device that can be utilized to speak to and portray systems, calculations, social connection, data structures and streams of traffic, power and numerous different things. In this study we probed into Hex board graph and line graph of hex board graphs. We computed M-polynomials because, from the M-polynomial we can compute several degree-based topological indices like, Randić indices, Zagreb indices, symmetric division index, Harmonic index, etc.

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## References

- [1] D.B. West, *Introduction to graph theory*. 2, Upper Saddle River: Prentice hall. **2001**.
- [2] D. Bonchev, *Chemical graph theory:* introduction and fundamentals, 1. CRC Press. **1991**.
- [3] H. Hosoya, M. Murakami, M. Gotoh, *Nat. Sci. Rept. Ochanumizu Univ.*, **1973**, *24*, 27-34.
- [4] E. Deutsch, S. Klavžar, *arXiv preprint arXiv:* 1407.1592. **2014**.
- [5] M. Munir, W. Nazeer, S. Rafique, S.M. Kang, *Symmetry*, **2016**, *8*, 149-156.
- [6] M. Munir, W. Nazeer, S. Rafique, S.M. Kang, *Symmetry*, **2016**, *8*, 97-108.
- [7] M. Munir, W. Nazeer, A.R. Nizami, S. Rafique, S.M. Kang, *Symmetry*, **2016**, *8*, 117-125.
- [8] M. Munir, W. Nazeer, Z. Shahzadi, S.M. Kang, *Symmetry*, **2016**, *8*, 134-141
- [9] Y.C. Kwun, M. Munir, W. Nazeer, S. Rafique, S.M. Kang, *Scientific reports*, **2017**, *7*, 8756-8764.
- [10] A.R. Nizami, M. Idrees, N. Amin, *arXiv* preprint *arXiv*: 1708.08207. **2017**.
- [11] E. Deutsch, S. Klavžar, *arXiv preprint arXiv:* 1806.08183. **2018**.
- [12] M. Ahmad, M. Saeed, M. Arshad, I. Z. Cheema, M. Hussain, *J. Comput. Theor. Nanosci.*, **2018**, *15*, 1340-1347.
- [13] H.M. Rehman, R. Sardar, A. Raza, *Open J. Math. Sci.*, **2017**, *1*, 62-71.
- [14] H. Wiener, *J. Am. Chem. Soc.*, **1947**, 69, 17–20.
- [15] A.A. Dobrynin, I. Gutman, *Acta Appl. Math.*, **2001**, *66*, 211–249.
- [16] I. Gutman, O.E. Polansky, Springer: New York, NY, USA, **1986**.
- [17] M. Randić, *J. Am. Chem. Soc.*, **1975**, *97*, 6609–6615.
- [18] B. Bollobás, P. Erdös, *Ars Comb.*, **1998**, *50*, 225–233.



- [19] D. Amić, D. Bešlo, B. Lučić, S. Nikolić, N. Trinajstić, *J. Chem. Inf. Comput. Sci.*, **1998**, *38*, 819–822.
- [20] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, *MATCH Commun. Math. Comput. Chem.*, **2005**, *54*, 425–434.
- [21] G. Caporossi, I. Gutman, P. Hansen, L. Pavlovic, *Comput. Biol. Chem.*, **2003**, *27*, 85–90.
- [22] X. Li, I. Gutman, University of Kragujevac: Kragujevac, Serbia, **2006**.
- [23] L.B. Kier, L.H. Hall, Academic Press: New York, NY, USA, **1976**.
- [24] L.B. Kier, L.H. Hall, Wiley: New York, NY, USA, **1986**.
- [25] D. Dimitrov, *Appl. Math. Comput.*, **2017**, *313*, 418–430.
- [26] I. Gutman, B. Furtula, (Eds.) University of Kragujevac: Kragujevac, Serbia, **2008**.
- [27] M. Randić, On *MATCH Commun. Math. Comput. Chem.*, **2008**, *59*, 5–124.
- [28] M. Randić, *Mol. Graph. Model*, **2001**, *20*, 19–35.
- [29] X. Li, Y. Shi, *MATCH Commun. Math. Comput. Chem.*, **2008**, *59*, 127–156.
- [30] D. Dimitrov, D. Milosavljević, *MATCH Commun. Math. Comput. Chem.*, **2018**, *79*, 431–450.
- [31] S. Nikolić, G. Kovačević, G.A. Miličević, N. Trinajstić, *Croat. Chem. Acta.*, **2003**, *76*, 113–124.
- [32] I. Gutman, K.C. Das, *MATCH Commun. Math. Comput. Chem.*, **2004**, *50*, 83–92.
- [33] K.C. Das, I. Gutman, *MATCH Commun. Math. Comput. Chem.*, **2004**, *52*, 103–112.
- [34] N. Trinajstić, S. Nikolić, A. Miličević, *Kem. Ind.*, **2010**, *59*, 577–589. (In Croatian)

- [35] M. Knor, R. Skrekovski, A. Tepeh, *Appl. Math. Nonlinear Sci.*, **2018**, 3, 433-446.
- [36] M. Imran, S.A. Bokhary, S. Manzoor, M.K. Siddiqui. *Eurasian Chem. Communm.*, **2020**, 2, 680-687.
- [37] Z. Ahmad, M. Naseem, M.K. Jamil, Sh. Wang, M.F. Nadeem, *Eurasian Chem. Commun.*, **2020**, 2, 712-721.
- [38] Z. Ahmad, M. Naseem, M.K. Jamil, M.K. Siddiqui, M.F. Nadeem. *Eurasian Chem. Commun.*, **2020**, 2, 663-671.
- [39] M. Cancan, S. Ediz, M.R. Farahani, *Eurasian Chem. Commun.*, **2020**, 2, 641-645.
- [40] A.Q. Baig, M. Naeem, W. Gao, J.B. Liu, *Eurasian Chem. Commun.*, **2020**, 2, 634-640.
- [41] F. Afzal, M.A. Razaq, D. Afzal, S. Hameed, *Eurasian Chem. Commun.*, **2020**, 2, 652-662.
- [42] M.R. Farahani, *Acta Chim. Slov.*, **2012**, 59, 779–783.
- [43] W. Gao, M.K. Siddiqui, M. Imran, M.K. Jamil, M.R. Farahani, *Saudi Pharm. J.*, **2016**, 24, 258–264
- [44] W. Gao, Y. Wang, B. Basavanagoud, M.K. Jamil, *Saudi Pharm. J.*, **2017**, *25*, 580–586.
- [45] Y. Gao, M.R. Farahani, W. Nazeer, *Chem. Methodologies.*, **2018**, *3*, 39-45.

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