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# M-polynomial and related degree-based topological indices of the third type of chain Hex-derived network

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#### Abstract

In chemical graph theory, a topological index is a numerical descriptor that describes the various biological activities, physical properties and chemical reactivities of molecular graphs. Recent studies compute several degree-based topological indices of a graph network by deriving its M-polynomial. In this paper, we would like to find out a closed form of M-polynomial for the third type of chain Hex-derived network of dimension *n* and hence derive various degree-based topological indices. Further, we plot the M-polynomial and all the related degree-based topological indices of the above network for different dimensional values.

#### Keywords

Degree-based topological indices, M-polynomial, Chain Hex-derived network, Graph polynomial.

#### **AMS Subject Classification**

05C10, 05C07, 92E10, 05C31.

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#### 1. Introduction

Let an ordered pair G = (V, E) be an undirected simple connected graph, where V = V(G) denotes the vertex set and E = E(G) denotes the set of edges which are unordered pairs of vertices. The *degree* of a vertex  $u \in V(G)$  in a graph *G* is the number of vertices adjacent to the vertex *u* and is denoted by d(u) [1].

#### 1.1 A Brief Literature Survey of Topological Indices and M-polynomials

Chemical Graph Theory (CGT) is a branch of mathematical chemistry in which the mathematical aspect of chemical compounds and their characteristic is being studied. In CGT, vertices of the graph correspond to atoms of some chemical compounds and edges represent the chemical bonds between the atoms. In [2–5], chemical applications of graphs and relation of graph theory with chemistry has been discussed. In the graph-theoretical representation of a molecule, we can find physical, biological and other properties of chemical compounds. In the area of CGT, a *topological index*<sup>1</sup> specifies the properties of a molecular structure. Generally, it is a numerical representation of a molecule, which is used in the development of Quantitative Structure Activity Relationships (QSARs) and Quantitative Structure Property Relationships (QSPRs)<sup>2</sup>. For more details see [6, 7].

The topological indices are mainly classified into degreebased topological indices [8], distance-based topological indices [9], degree and distance-based topological indices [10]

<sup>&</sup>lt;sup>1</sup>A topological index is also known as a *graph-theoretic index* or *connectivity index*.

<sup>&</sup>lt;sup>2</sup>In the area of Cheminformatics, QSAR and QSPR are used to predict the chemical, physical and biological properties of a chemical compound.

and counting related topological indices [11]. These indices describe the physical, chemical and other properties of various structures. Usually, we use the definitions of the respective topological indices to compute their numeric values. Instead, one may find a general method to produce the different topological indices of a particular class. Keeping this problem in mind, the concept of polynomials [12] is introduced in graph theory. By constructing a general polynomial of a given structure, one can derive several topological indices by differentiating or integrating (or combination of both) the corresponding polynomial.

In literature, several such polynomials are reported, some of which are as follows: the matching polynomial [13], the Clar covering polynomial (also known as the Zhang-Zhang polynomial) [14], the Schultz polynomial [15], the Tutte polynomial [16], the Hosoya polynomial [17], etc. Among all of these polynomials, the Hosoya polynomial is used for calculating the distance-based topological indices such as the Wiener index [18].

The degree-based topological indices contribute a major role to understand the properties of a molecular structure. In the recent past, the M-polynomial is introduced by Deutsch and Klavžar [19] to calculate several degree-based topological indices. The M-polynomials corresponding to various chemical networks and their related degree-based topological indices are evaluated in [20–24].

**Definition 1.1** ([19]). *For a simple connected graph G, the expression* 

$$M(G;x,y) = \sum_{\delta \le i \le j \le \Delta} m_{i,j}(G) \ x^i y^j$$

is known as the M-polynomial of a graph G, where  $\delta = \min\{d(u)|u \in V(G)\}, \Delta = \max\{d(u)|u \in V(G)\}$  and  $m_{i,j}(G)$  is the number of edges  $uv \in E(G)$  such that d(u) = i, d(v) = j  $(i, j \ge 1)$ .

As mentioned in [25], a degree-based topological index of a graph G is a kind of graph invariant, which is denoted as I(G) and can be written as:

$$I(G) = \sum_{i \le j} m_{i,j}(G) f(i,j).$$

**Theorem 1.2** ([19], Theorems 2.1, 2.2). *Let G be a simple connected graph.* 

1. If 
$$I(G) = \sum_{e=uv \in E(G)} f(d(u), d(v))$$
, where  $f(x, y)$  is a polynomial in x and y, then

$$I(G) = f(D_x, D_y)(M(G; x, y))|_{x=y=1}.$$

2. If  $I(G) = \sum_{\substack{e=uv \in E(G)}} f(d(u), d(v))$ , where  $f(x, y) = \sum_{\substack{i,j \in \mathbb{Z} \\ M(G;x,y)}} \alpha_{i,j} x^i y^j$ , then I(G) can be obtained from M(G;x,y) using the operators  $D_x, D_y, S_x$ , and  $S_y$ .

3. If 
$$I(G) = \sum_{e=uv \in E(G)} f(d(u), d(v))$$
, where  $f(x, y) = \frac{x^r y^s}{(x+y+\alpha)^t}$ , where  $r, s \ge 0, t \ge 1$  and  $\alpha \in \mathbb{Z}$ , then  
 $I(G) = S_x^t Q_\alpha J D_x^r D_y^s (M(G; x, y))|_{x=1}.$ 

# 1.2 Related Degree-based Topological Indices

This section discusses a brief about some degree-based topological indices which are associated in the context of the interest of this paper. In 1972, Gutman and Trinajstić [26] introduced the Zagreb indices which are helpful to determine the total  $\pi$ -electron energy<sup>3</sup> of a molecule. The Zagreb indices pay higher weights to the inner edges and vertices rather than the outer edges and vertices. On the contrary, the modified Zagreb indices [27] are proposed, inspired by the idea of the Zagreb indices. Another very popular degree-based topological index is the Randić index which is introduced by Milan Randić [28] in 1975. It is also known as branching index or connectivity index. Randić index has huge applications in the field of drug design. After two decades, seeing the success of Randić index, the mathematicians Bollobás and Erdős [29], and Amić et al. [30] introduced the generalized version of the Randić index<sup>4</sup> (for an arbitrary real number  $\alpha$ ) in 1998, which is known as general Randić index. In recent studies, to determine the total surface area of polychlorobiphenyls, the symmetric division (deg) index is proposed around 2010 in [31]. Whereas, the inverse sum (indeg) index [31, 32] predicts the total surface area of octane isomers. For the study of the heat of formation of alkanes, the augmented Zagreb index [33] is beneficial. For a graph G, the formulas of different degree-based topological indices of our interest are listed in Table 1.

#### **1.3 Third Type of Chain Hex-derived Network of Di**mension *n*

In 2002, Nocetti et al. discussed the Hexagonal network and its properties in [34]. Henceforth in 2008, the Hex-derived network of type 1 (HDN1[n]) and Hex-derived network of type 2 (HDN2[n]) are constructed in [35]. These Hex-derived networks provide much more connections and processors than the Hexagonal network. Recently in 2017, Raj and George proposed some chemical networks which are derived from the Hexagonal network of dimension n [36].

The most attractive and complex class of minerals are silicates. Generally, the  $SiO_4$  tetrahedron is the basic chemical unit of silicates. Figure 1 shows a simplified representation of a  $SiO_4$  tetrahedron in two-dimension. In chemistry, the oxygen atoms are at the corner vertices and the silicon atom is at the center vertex of the  $SiO_4$  tetrahedron. Commonly in CGT, we use the term oxygen node for each of the corner vertices, silicon node for the center vertex and edges represent the bond between them.

<sup>&</sup>lt;sup>4</sup>For  $\alpha = -\frac{1}{2}$ ,  $R_{\alpha}$  becomes Randić [28] (or connectivity) index; for  $\alpha = 1$ ,  $R_{\alpha}$  becomes second Zagreb index; and for  $\alpha = -1$ ,  $R_{\alpha}$  becomes modified second Zagreb index.



<sup>&</sup>lt;sup>3</sup>The *total*  $\pi$ -*electron energy* is related to the thermodynamic stability of a molecule.

SI.	Topological Index	Notation	Formula of Topological Indices
No.			
1.	First Zagreb Index [26]	$M_1(G)$	$M_1(G) = \sum_{(u) \in U} (d(u) + d(v))$
			$uv \in E(G)$
2.	Second Zagreb Index [26]	$M_2(G)$	$M_2(G) = \sum_{uv \in E(G)} (d(u)d(v))$
3.	Modified Second Zagreb Index [27]	$^{m}M_{2}(G)$	${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$
4.	General Randić Index [29]	$R_{\alpha}(G)$	$R_{\alpha}(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}$
5.	Inverse Randić Index [30]	$RR_{\alpha}(G)$	$RR_{lpha}(G) = \sum_{uv \in E(G)} \frac{1}{(d(u)d(v))^{lpha}}$
6.	Symmetric Division (Deg) Index [31]	SDD(G)	$SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{\min(d(u), d(v))}{\max(d(u), d(v))} + \frac{\max(d(u), d(v))}{\min(d(u), d(v))} \right\}$
7.	Harmonic Index [37]	H(G)	$H(G) = \sum_{uv \in E(G)} rac{2}{d(u) + d(v)}$
8.	Inverse Sum (Indeg) Index [31]	ISI(G)	$ISI(G) = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$
9.	Augmented Zagreb Index [33]	AZ(G)	$AZ(G) = \sum_{uv \in E(G)} \left\{ rac{d(u)d(v)}{d(u)+d(v)-2}  ight\}^3$

**Table 1.** Formula for degree-based topological indices of a graph G.



Figure 1. 2-D graphical representation of *SiO*<sub>4</sub> Tetrahedron.

By linking or joining the  $SiO_4$  tetrahedrons one can create different types of silicate structures such as orthosilicates, pyrosilicates, chain silicates, cyclic silicates, sheet silicates, three-dimensional silicates, etc. Among all of these, the linear arrangement of  $SiO_4$  tetrahedrons gives us the chain silicate network. See Figure 2 for the chain silicate network of dimension 5.

A third type of chain Hex-derived network of dimension<sup>5</sup> n (which is denoted by *CHDN3*[n], where  $n \ge 2$ ) has been constructed by keeping in mind the construction of chain silicate network [38] and Hex-derived network of type 3 [36].

Its drawing algorithmic steps are mentioned below:

**Step-1**: Draw a chain silicate network of dimension *n*.

**Step-2**: Replace each tetrahedron in the chain silicate network by planer octahedron (POH)<sup>6</sup> network cell once.

The graph representation of the third type of chain Hexderived network of dimension 5 (that is, *CHDN3*[5]) is shown in Figure 3.

# 1.4 Our Contribution

In [40], several degree-based topological indices of CHDN3[n] are calculated directly by using formulas of topological indices mentioned in Table 1. Instead of calculating them (degree-based topological indices) separately, in this paper, we compute a closed form of M-polynomial for the CHDN3[n]. More recently, we have done the similar computation for the third type of Hex-derived network of dimension n (HDN3[n]) in [41]. In Section 2, we construct a M-Polynomial for the CHDN3[n] network and henceforth compute the nine related degree-based topological indices of CHDN3[n] for different value of n. Moreover, the pictorial representation of the M-polynomial and the related topological indices are drawn in Section 3 for different values of n and finally the conclusion in Section 4.

# 2. Computing a M-polynomial for *CHDN*3[*n*] Network

**Theorem 2.1.** Let CHDN3[n] be the third type of chain Hexderived network of dimension  $n (\geq 2)$ . Then a M-polynomial of CHDN3[n] is

$$M(CHDN3[n]; x, y) = (5n+6)x^4y^4 + (6n-4)x^4y^8 + (n-2)x^8y^8.$$

*Proof.* By observing the Figure 3 of *CHDN*3[5], we can enumerate the cardinality of the vertex set and the edge set of CHDN3[n] as:

|V(CHDN3[n])| = 5n + 1 and |E(CHDN3[n])| = 12n.

We divide the vertex set V of CHDN3[n] into two disjoint parts according to the degree of vertices, as:

$$V_1(CHDN3[n]) = \{ u \in V(CHDN3[n] : d(u) = 4 \}, \\ V_2(CHDN3[n]) = \{ u \in V(CHDN3[n]) : d(u) = 8 \},$$



<sup>&</sup>lt;sup>5</sup>In a chain Hex-derived network of dimension n of type three, n stands for the number of edges in a row line.

<sup>&</sup>lt;sup>6</sup>For the construction of a planer octahedron network (POH), please refer to [39].

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Figure 3. Type 3 Chain Hex-derived network of dimension 5 (CHDN3[5]).

and the number of such vertices are:

 $|V_1(CHDN3[n])| = 4n + 2$  and  $|V_2(CHDN3[n])| = n - 1$ .

Also, we divide the edge set E of CHDN3[n] into three disjoint parts based on the degrees of the end vertices of each edge, as follows:

$$E_{1}(CHDN3[n]) = E_{\{4,4\}} = \{e = uv \in E(CHDN3[n]) :$$
  

$$d(u) = 4, d(v) = 4\},$$
  

$$E_{2}(CHDN3[n]) = E_{\{4,8\}} = \{e = uv \in E(CHDN3[n]) :$$
  

$$d(u) = 4, d(v) = 8\},$$
  

$$E_{3}(CHDN3[n]) = E_{\{8,8\}} = \{e = uv \in E(CHDN3[n]) :$$
  

$$d(u) = 8, d(v) = 8\},$$

and the number of edges corresponding to these degrees of end vertices are:

$$|E_1(CHDN3[n])| = 5n + 6, |E_2(CHDN3[n])| = 6n - 4, |E_3(CHDN3[n])| = n - 2.$$

Thus, the M-polynomial of CHDN3[n] is

$$\begin{split} & \mathcal{M}(CHDN3[n];x,y) \\ &= \sum_{i \leq j} m_{i,j} x^{i} y^{j} \quad \text{where} \quad i,j \in \{4,8\} \\ &= \sum_{4 \leq 4} m_{4,4} x^{4} y^{4} + \sum_{4 \leq 8} m_{4,8} x^{4} y^{8} + \sum_{8 \leq 8} m_{8,8} x^{8} y^{8} \\ &= \sum_{uv \in E_{1}(CHDN3[n])} m_{4,4} x^{4} y^{4} + \sum_{uv \in E_{2}(CHDN3[n])} m_{4,8} x^{4} y^{8} \\ &+ \sum_{uv \in E_{3}(CHDN3[n])} m_{8,8} x^{8} y^{8} \\ &= |E_{1}(CHDN3[n])| x^{4} y^{4} + |E_{2}(CHDN3[n])| x^{4} y^{8} \\ &+ |E_{3}(CHDN3[n])| x^{8} y^{8} \\ &= (5n+6) x^{4} y^{4} + (6n-4) x^{4} y^{8} + (n-2) x^{8} y^{8}. \end{split}$$

To produce the degree-based topological indices of a given graph G mentioned in Table 1 from the M-polynomial M(G;x,y), the derivation formulas in terms of integral or derivative (or both integral and derivative) are given in Table 2 [19]. In the Table 2,

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Sl.	Topological Index	Notation	f(x,y)	<b>Derivation from</b> $M(G; x, y)$
No.				
1.	First Zagreb Index	$M_1(G)$	x + y	$(D_x + D_y)(M(G; x, y)) _{x=y=1}$
2.	Second Zagreb Index	$M_2(G)$	xy	$(D_x D_y)(M(G;x,y)) _{x=y=1}$
3.	Modified Second Zagreb Index	$^{m}M_{2}(G)$	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y)) _{x=y=1}$
4.	General Randić Index	$R_{\alpha}(G)$	$(xy)^{\alpha}$	$(D_x^{\alpha} D_y^{\alpha})(M(G;x,y)) _{x=y=1}$
5.	Inverse Randić Index	$RR_{\alpha}(G)$	$\frac{1}{(xy)^{\alpha}}$	$(S_x^{\alpha}S_y^{\alpha})(M(G;x,y)) _{x=y=1}$
6.	Symmetric Division (Deg) Index	SDD(G)	$\frac{x^2+y^2}{xy}$	$(D_x S_y + D_y S_x)(M(G; x, y)) _{x=y=1}$
7.	Harmonic Index	H(G)	$\frac{2}{x+y}$	$2S_x J(M(G;x,y)) _{x=1}$
8.	Inverse Sum (Indeg) Index	ISI(G)	$\frac{xy}{x+y}$	$S_x J D_x D_y (M(G; x, y)) _{x=1}$
9.	Augmented Zagreb Index	AZ(G)	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (M(G; x, y)) _{x=1}$

Table 2. Derivation formulas for related degree-based topological indices derived from the M-polynomial of a graph G.

$$\begin{split} D_x &= x \frac{\partial (f(x,y))}{\partial x}, \qquad D_y = y \frac{\partial (f(x,y))}{\partial y}, \\ S_x &= \int_0^x \frac{f(t,y)}{t} dt, \qquad S_y = \int_0^y \frac{f(x,t)}{t} dt, \\ J(f(x,y)) &= f(x,x), \qquad \mathcal{Q}_\alpha(f(x,y)) = x^\alpha f(x,y), \ \alpha \neq 0. \end{split}$$

From the M-polynomial produced in Theorem 2.1, below we derive the values of the related degree-based topological indices of the CHDN3[n] for variable n.

**Theorem 2.2.** Let CHDN3[n] be the third type of chain Hexderived network of dimension n. Then

- 1.  $M_1(CHDN3[n]) = 32(4n-1).$
- 2.  $M_2(CHDN3[n]) = 336n 160.$
- 3.  ${}^{m}M_2(CHDN3[n]) = \frac{33}{64}n + \frac{7}{32}.$
- 4.  $R_{\alpha}(CHDN3[n]) = 4^{2\alpha}(5n+6) + 32^{\alpha}(6n-4) + 8^{2\alpha}(n-2)$ .
- 5.  $RR_{\alpha}(CHDN3[n]) = \frac{1}{4^{2\alpha}}(5n+6) + \frac{1}{32^{\alpha}}(6n-4) + \frac{1}{8^{2\alpha}}(n-2).$
- 6. SDD(CHDN3[n]) = 27n 2.
- 7.  $H(CHDN3[n]) = \frac{19}{8}n + \frac{7}{12}$ .
- 8.  $ISI(CHDN3[n]) = 30n \frac{20}{3}$ .
- 9.  $AZ(CHDN3[n]) = \frac{1}{385875}(149316779n 80401408).$

*Proof.* As computed in the Theorem 2.1, the M-polynomial for CHDN3[n] is

 $M(CHDN3[n];x,y) = (5n+6)x^4y^4 + (6n-4)x^4y^8 + (n-2)x^8y^8$ . For notational simplicity, we write g(x,y) = M(CHDN3[n];x,y). Therefore,

$$\begin{split} D_x(g(x,y)) &= 4(5n+6)x^4y^4 + 4(6n-4)x^4y^8 + 8(n-2)x^8y^8, \\ D_y(g(x,y)) &= 4(5n+6)x^4y^4 + 8(6n-4)x^4y^8 + 8(n-2)x^8y^8, \\ D_yD_x(g(x,y)) &= 16(5n+6)x^4y^4 + 32(6n-4)x^4y^8 + 64(n-2)x^8y^8, \\ S_x(g(x,y)) &= \frac{1}{4}(5n+6)x^4y^4 + \frac{1}{4}(6n-4)x^4y^8 + \frac{1}{8}(n-2)x^8y^8, \\ S_y(g(x,y)) &= \frac{1}{4}(5n+6)x^4y^4 + \frac{1}{8}(6n-4)x^4y^8 + \frac{1}{8}(n-2)x^8y^8, \end{split}$$

$$\begin{split} S_x S_y(g(x,y)) &= \frac{1}{16} (5n+6) x^4 y^4 + \frac{1}{32} (6n-4) x^4 y^8 + \frac{1}{64} (n-2) x^8 y^8, \\ D_x^\alpha D_y^\alpha(g(x,y)) &= 4^{2\alpha} (5n+6) x^4 y^4 + 32^\alpha (6n-4) x^4 y^8 + 8^{2\alpha} (n-2) x^8 y^8, \\ S_y D_x(g(x,y)) &= (5n+6) x^4 y^4 + \frac{1}{2} (6n-4) x^4 y^8 + (n-2) x^8 y^8, \\ S_x D_y(g(x,y)) &= (5n+6) x^4 y^4 + 2(6n-4) x^4 y^8 + (n-2) x^8 y^8, \\ S_x^\alpha S_y^\alpha(g(x,y)) &= \frac{1}{4^{2\alpha}} (5n+6) x^4 y^4 + \frac{1}{32^\alpha} (6n-4) x^4 y^8 + \frac{1}{8^{2\alpha}} (n-2) x^8 y^8, \\ S_x J(g(x,y)) &= \frac{1}{8} (5n+6) x^8 + \frac{1}{12} (6n-4) x^{12} + \frac{1}{16} (n-2) x^{16}, \\ S_x JD_x D_y(g(x,y)) &= 2 (5n+6) x^8 + \frac{8}{3} (6n-4) x^{12} + 4 (n-2) x^{16}, \\ S_x^3 Q_{-2} J D_x^3 D_y^3(g(x,y)) &= \frac{4^6}{6^3} (5n+6) x^6 + \frac{32^3}{10^3} (6n-4) x^{10} + \frac{8^6}{14^3} (n-2) x^{14}. \end{split}$$

Hence, the degree-based topological indices of the CHDN3[n] based on the derivation formulas mentioned in Table 2 are as follows.

1. First Zagreb Index:

$$M_1(CHDN3[n]) = (D_x + D_y)(g(x, y))|_{x=y=1} = 32(4n-1).$$

2. Second Zagreb Index:

 $M_2(CHDN3[n]) = D_x D_y(g(x,y))|_{x=y=1} = 336n - 160.$ 

3. Modified Second Zagreb Index:

$${}^{m}M_{2}(CHDN3[n]) = S_{x}S_{y}(g(x,y))|_{x=y=1} = \frac{33}{64}n + \frac{7}{32}.$$

4. General Randić Index:

$$R_{\alpha}(CHDN3[n]) = D_{x}^{\alpha}D_{y}^{\alpha}(g(x,y))|_{x=y=1}$$
  
= 4<sup>2\alpha</sup>(5n+6) + 32<sup>\alpha</sup>(6n-4) + 8<sup>2\alpha</sup>(n-2).

5. Inverse Randić Index:

=

$$RR_{\alpha}(CHDN3[n]) = S_{x}^{\alpha}S_{y}^{\alpha}(g(x,y))|_{x=y=1}$$
$$= \frac{1}{4^{2\alpha}}(5n+6) + \frac{1}{32^{\alpha}}(6n-4) + \frac{1}{8^{2\alpha}}(n-2).$$

6. Symmetric Division (Deg) Index:

$$SDD(CHDN3[n]) = (S_y D_x + S_x D_y)(g(x, y))|_{x=y=1}$$
  
= 27n - 2.

7. Harmonic Index:

$$H(CHDN3[n]) = 2S_x J(g(x,y))|_{x=1} = \frac{19}{8}n + \frac{7}{12}.$$

8. Inverse Sum (Indeg) Index:

$$ISI(CHDN3[n]) = S_x JD_x D_y(g(x,y))|_{x=1} = 30n - \frac{20}{3}.$$

9. Augmented Zagreb Index:

$$AZ(CHDN3[n]) = S_x^3 Q_{-2}JD_x^3 D_y^3 (g(x,y))|_{x=1}$$
$$= \frac{1}{385875} (149316779n - 80401408).$$

### 3. Plotting the M-polynomial and Associated Indices

For different dimensions of the *CHDN3*[*n*], the respective M-polynomials and several related degree-based topological indices are tabulated in Table 3. To see the nature of the M-polynomials and the related topological indices, we have varies the dimension of the *CHDN3*[*n*] from n = 2 to n = 8. The dimension in the table may be extended as and when required based on the Theorem 2.1. From the table we can observe, the values of each of the topological indices are increasing with the dimension increasing.



(*a*) The plot of the M-polynomial of *CHDN*3[2], where  $-0.5 \le x, y \le 0.5$ .

We have drawn the M-polynomial in Maple-13 software. Figure 4 gives the graphical representations of the M-polynomial (as proposed in Theorem 2.1) of the chain Hex-derived network of type 3 of dimension 2 (*CHDN3*[2]) in different ranges of x and y. The domains of x and y are:  $-0.5 \le x, y \le 0.5$ 



(c) The plot of the M-polynomial of *CHDN*3[2], where  $-2 \le x, y \le 2$ . **Figure 4.** The plot of the M-polynomial of *CHDN*3[2] in different regions of x and y.

in the Figure 4(*a*),  $-1 \le x, y \le 1$  in the Figure 4(*b*), and  $-2 \le x, y \le 2$  in the Figure 4(*c*).

Moreover, observing the wide range of values (in Table 3) of the different degree-based topological indices of *CHDN3*[*n*] for different values of *n* ( $2 \le n \le 8$ ), we have plotted the values of first Zagreb, second Zagreb, general Randić ( $\alpha = 1/2$ ) and augmented Zagreb indices in Figure 5, and the values of modified second Zagreb, inverse Randić ( $\alpha = 1/2$ ), symmetric division (deg), Harmonic and inverse sum (indeg) indices in Figure 6. In both the figures, the equation of each plotted line corresponding to each of the topological indices is also specified along the respective lines. Observe that the lines plotted for the inverse Randić index ( $\alpha = 1/2$ ) and harmonic index are almost overlapping in Figure 6.

SI	Dimension	n = 2	<i>n</i> = 3	n=4	<i>n</i> = 5	n = 6	<i>n</i> = 7	n = 8
51.	M-polynomial Topological Index	$\frac{16x^4y^4}{8x^4y^8}$ +	$ \begin{array}{r} 21x^4y^4 + \\ 14x^4y^8 + \\ x^8y^8 \end{array} $	$ \begin{array}{r} 26x^4y^4 + \\ 20x^4y^8 + \\ 2x^8y^8 \end{array} $	$ \begin{array}{r} 31x^4y^4 + \\ 26x^4y^8 + \\ 3x^8y^8 \end{array} $	$ \frac{36x^4y^4}{32x^4y^8} + \\ \frac{4x^8y^8}{4x^8y^8} + \\ $	$ \begin{array}{r} 41x^4y^4 + \\ 38x^4y^8 + \\ 5x^8y^8 \end{array} $	$ \begin{array}{r} 46x^4y^4 + \\ 44x^4y^8 + \\ 6x^8y^8 \end{array} $
1	First Zagreb Index	224	352	480	608	736	864	992
2	Second Zagreb Index	512	848	1184	1520	1856	2192	2528
3	Modified Second Zagreb Index	1.25	1.7656	2.2813	2.7969	3.3125	3.8281	4.3438
4	General Randić Index ( $\alpha = 1/2$ )	109.2548	171.1960	233.1371	295.0782	357.0193	418.9605	480.9016
5	Inverse Randić Index ( $\alpha = 1/2$ )	5.4142	7.8499	10.2855	12.7212	15.1569	17.5925	20.0282
6	Symmetric Division (Deg) Index	52	79	106	133	160	187	214
7	Harmonic Index	5.3333	7.7083	10.0833	12.4583	14.8333	17.2083	19.5833
8	Inverse Sum (Indeg) Index	53.3333	83.3333	113.3333	143.3333	173.3333	203.3333	233.3333
9	Augmented Zagreb Index	565.5514	952.5078	1339.4641	1726.4204	2113.3767	2500.3331	2887.2895

<b>Table 3.</b> Computation of degree-based topological indices of the $CHDN3[n]$ at different values of n and the respecti	ve
M-polyno	



**Figure 5.** Plot of first Zagreb, second Zagreb, general Randić ( $\alpha = 1/2$ ) and augmented Zagreb indices of *CHDN3*[*n*] for different values of *n* ( $2 \le n \le 8$ ).

# 4. Conclusion

In this paper, we have considered a new graph network which is the third type of chain Hex-derived network of dimension n (*CHDN*3[n]). Instead of calculating the various degree-based topological indices separately, we have derived a general form of M-polynomial to calculate directly nine related degree-based topological indices for different dimension n which are helpful in the study of the physical, chemical and other properties of the network. In addition, we have plotted the M-polynomial in different regions and all the topological indices for various n.

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**Figure 6.** Plot of modified second Zagreb, inverse Randić ( $\alpha = 1/2$ ), symmetric division (deg), harmonic and inverse sum (indeg) indices of *CHDN*3[*n*] for different values of *n* ( $2 \le n \le 8$ ).

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