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

Shibsankar Das^{1*} and Shikha Rai²

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.

1,2*Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India.* ***Corresponding author**: ¹ shib.iitm@gmail.com; ² shikharai48@gmail.com **Article History**: Received **01** April **2020**; Accepted **06** October **2020** c 2020 MJM.

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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 $d(u)$ [\[1\]](#page-6-1).

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 [\[2](#page-6-2)[–5\]](#page-7-0), 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*[1](#page-0-2) 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 $(QSPRs)^2$ $(QSPRs)^2$. For more details see [\[6,](#page-7-1) [7\]](#page-7-2).

The topological indices are mainly classified into degreebased topological indices [\[8\]](#page-7-3), distance-based topological indices [\[9\]](#page-7-4), degree and distance-based topological indices [\[10\]](#page-7-5)

¹A topological index is also known as a *graph-theoretic index* or *connectivity index*.

²In 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 [\[11\]](#page-7-6). 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 [\[12\]](#page-7-7) 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 [\[13\]](#page-7-8), the Clar covering polynomial (also known as the Zhang-Zhang polynomial) [\[14\]](#page-7-9), the Schultz polynomial [\[15\]](#page-7-10), the Tutte polynomial [\[16\]](#page-7-11), the Hosoya polynomial [\[17\]](#page-7-12), etc. Among all of these polynomials, the Hosoya polynomial is used for calculating the distance-based topological indices such as the Wiener index [\[18\]](#page-7-13).

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\]](#page-7-14) 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 [\[20–](#page-7-15)[24\]](#page-8-1).

Definition 1.1 ([\[19\]](#page-7-14)). *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 δ = *min*{ $d(u) | u \in V(G)$ }, ∆ = *max*{ $d(u) | u \in V(G)$ } *and* $m_{i,i}(G)$ *is the number of edges* $uv \in E(G)$ *such that* $d(u) = i$, $d(v) =$ $j(i, j \geq 1)$.

As mentioned in [\[25\]](#page-8-2), 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:

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

Theorem 1.2 ([\[19\]](#page-7-14), Theorems 2.1, 2.2). *Let G be a simple connected graph.*

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

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\]](#page-8-3) introduced the *Zagreb indices* which are helpful to determine the total π -electron energy^{[3](#page-1-2)} 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* [\[27\]](#page-8-4) 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\]](#page-8-5) 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\]](#page-8-6), and Amić et al. [[30\]](#page-8-7) introduced the generalized version of the Randić index^{[4](#page-1-3)} (for an arbitrary real number α) 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 [\[31\]](#page-8-8). Whereas, the *inverse sum* (*indeg*) *index* [\[31,](#page-8-8) [32\]](#page-8-9) predicts the total surface area of octane isomers. For the study of the heat of formation of alkanes, the *augmented Zagreb index* [\[33\]](#page-8-10) is beneficial. For a graph *G*, the formulas of different degree-based topological indices of our interest are listed in Table [1.](#page-2-2)

1.3 Third Type of Chain Hex-derived Network of Dimension *n*

In 2002, Nocetti et al. discussed the Hexagonal network and its properties in [\[34\]](#page-8-11). Henceforth in 2008, the Hex-derived network of type 1 (*HDN*1[*n*]) and Hex-derived network of type 2 (*HDN*2[*n*]) are constructed in [\[35\]](#page-8-12). 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* [\[36\]](#page-8-13).

The most attractive and complex class of minerals are silicates. Generally, the $SiO₄$ tetrahedron is the basic chemical unit of silicates. Figure [1](#page-2-3) 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.

⁴For $\alpha = -\frac{1}{2}$, R_{α} becomes Randić [[28\]](#page-8-5) (or connectivity) index; for $\alpha = 1$, R_{α} becomes second Zagreb index; and for $\alpha = -1$, R_{α} becomes modified second Zagreb index.

³The *total* π*-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]	$M_1(G)$	$M_1(G) = \sum (d(u) + d(v))$	
			$uv \in E(G)$	
2.	Second Zagreb Index [26]	$M_2(G)$	$M_2(G) = \sum (d(u)d(v))$ $uv\varepsilon E(G)$	
3.	Modified Second Zagreb Index [27]	$^{m}M_{2}(G)$	$\overline{{}^m M_2(G)} = \overline{\sum_{uv \in E(G)} \frac{1}{d(u)d(v)}}$	
$\overline{4}$.	General Randić Index [29]	$R_{\alpha}(G)$	$R_{\alpha}(G) = \sum (d(u)d(v))^{\alpha}$ $uv \in E(G)$	
5.	Inverse Randić Index [30]	$RR_{\alpha}(G)$	$\overline{RR_{\alpha}(G)} = \sum_{uv \in E(G)} \frac{1}{(d(u)d(v))^{\alpha}}$	
6.	Symmetric Division (Deg) Index [31]	SDD(G)	$SDD(G) = \sum_{w \in E(G)} \left\{ \frac{\min(d(u), d(v))}{\max(d(u), d(v))} + \frac{\max(d(u), d(v))}{\min(d(u), d(v))} \right\}$ $uv \in E(G)$	
7.	Harmonic Index [37]	H(G)	$\overline{H}(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$	
8.	Inverse Sum (Indeg) Index [31]	ISI(G)	$\mathit{ISI}(G) = \sum_{uv \in E(G)} \overline{\frac{d(u)d(v)}{d(u)+d(v)}}$	
9.	Augmented Zagreb Index [33]	AZ(G)	$AZ(G) = \sum_{uv \in E(G)} \left\{ \frac{d(u)d(v)}{d(u)+d(v)-2} \right\}$	

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

Figure 1. 2-D graphical representation of *SiO*⁴ 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](#page-3-0) for the chain silicate network of dimension 5.

A third type of chain Hex-derived network of dimension^{[5](#page-2-4)} *n* (which is denoted by *CHDN*3[*n*], where $n \ge 2$) has been constructed by keeping in mind the construction of chain silicate network [\[38\]](#page-8-15) and Hex-derived network of type 3 [\[36\]](#page-8-13).

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)^{[6](#page-2-5)} network cell once.

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

in Figure [3.](#page-3-1)

1.4 Our Contribution

In [\[40\]](#page-8-17), several degree-based topological indices of *CHDN*3[*n*] are calculated directly by using formulas of topological indices mentioned in Table [1.](#page-2-2) Instead of calculating them (degree-based topological indices) separately, in this paper, we compute a closed form of M-polynomial for the *CHDN*3[*n*]. More recently, we have done the similar computation for the third type of Hex-derived network of dimension n (*HDN*3[*n*]) in [\[41\]](#page-8-18). In Section [2,](#page-2-1) we construct a M-Polynomial for the *CHDN*3[*n*] network and henceforth compute the nine related degree-based topological indices of *CHDN*3[*n*] for different value of *n*. Moreover, the pictorial representation of the Mpolynomial and the related topological indices are drawn in Section [3](#page-5-0) for different values of *n* and finally the conclusion in Section [4.](#page-5-1)

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

Theorem 2.1. *Let CHDN*3[*n*] *be the third type of chain Hexderived network of dimension* $n \geq 2$ *). Then a M-polynomial of CHDN*3[*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](#page-3-1) of *CHDN*3[5], we can enumerate the cardinality of the vertex set and the edge set of *CHDN*3[*n*] as:

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

We divide the vertex set *V* of *CHDN*3[n] into two disjoint parts according to the degree of vertices, as:

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

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

⁵ In a chain Hex-derived network of dimension *n* of type three, *n* stands for the number of edges in a row line.

⁶For the construction of a planer octahedron network (POH), please refer to [\[39\]](#page-8-16).

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Figure 3. Type 3 Chain Hex-derived network of dimension 5 (*CHDN*3[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:

$$
E_1(CHDN3[n]) = E_{\{4,4\}} = \{e = uv \in E(CHDN3[n]):
$$

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

\n
$$
E_2(CHDN3[n]) = E_{\{4,8\}} = \{e = uv \in E(CHDN3[n]):
$$

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

\n
$$
E_3(CHDN3[n]) = E_{\{8,8\}} = \{e = uv \in E(CHDN3[n]):
$$

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

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

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

Thus, the M-polynomial of *CHDN*3[*n*] is

$$
M(CHDN3[n]; x, y)
$$

= $\sum_{i \le j} m_{i,j}x^iy^j$ where $i, j \in \{4, 8\}$
= $\sum_{4 \le 4} m_{4,4}x^4y^4 + \sum_{4 \le 8} m_{4,8}x^4y^8 + \sum_{8 \le 8} m_{8,8}x^8y^8$
= $\sum_{uv \in E_1(CHDN3[n])} m_{4,4}x^4y^4 + \sum_{uv \in E_2(CHDN3[n])} m_{4,8}x^4y^8$
+ $\sum_{uv \in E_3(CHDN3[n])} m_{8,8}x^8y^8$
= $[E_1(CHDN3[n])| x^4y^4 + |E_2(CHDN3[n])| x^4y^8$
+ $[E_3(CHDN3[n])| x^8y^8$
= $(5n + 6)x^4y^4 + (6n - 4)x^4y^8 + (n - 2)x^8y^8$.

To produce the degree-based topological indices of a given graph *G* mentioned in Table [1](#page-2-2) 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](#page-4-0) [\[19\]](#page-7-14). In the Table [2,](#page-4-0)

M-polynomial and related degree-based topological indices of the third type of chain Hex-derived network — 1846[/1850](#page-8-0)

SI.	Topological Index	Notation	f(x,y)	Derivation from $M(G; x, y)$
No.				
1.	First Zagreb Index	$M_1(G)$	$x + y$	$\overline{(D_x+D_y)}\overline{(M(G;x,y))}\vert_{x=y=1}$
2.	Second Zagreb Index	$M_2(G)$	xy	$\overline{(D_xD_y)(M(G;x,y)) _{x=y=1}}$
3.	Modified Second Zagreb Index	${}^m M_2(G)$	xv	$\overline{(S_xS_y)}(M(G;x,y)) _{x=y=1}$
4.	General Randić Index	$R_{\alpha}(G)$	$(xy)^{\alpha}$	$\overline{(D_x^{\alpha}D_y^{\alpha})(M(G;x,y)) _{x=y=1}}$
5.	Inverse Randić Index	$RR_{\alpha}(G)$	$\overline{(xy)}^{\alpha}$	$\overline{(S_x^{\alpha}S_y^{\alpha})(M(G;x,y))} _{x=y=1}$
6.	Symmetric Division (Deg) Index	SDD(G)	$x^2 + y^2$ $\frac{xy}{2}$	$(D_xS_y + D_yS_x)(M(G; x, y)) _{x=y=1}$
7.	Harmonic Index	H(G)	$\overline{x+y}$	$2S_xJ(M(G;x,y)) _{x=1}$
8.	Inverse Sum (Indeg) Index	ISI(G)	$\frac{xy}{x+y}$	$\overline{S_xJD_xD_y(M(G;x,y))} _{x=1}$
9.	Augmented Zagreb Index	AZ(G)	$\frac{xy}{x+y-2}$	$\sqrt{S_x^3 Q_{-2} JD_x^3 D_y^3(M(G;x,y)) _{x=1}}$

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

$$
D_x = x \frac{\partial (f(x, y))}{\partial x}, \qquad D_y = y \frac{\partial (f(x, y))}{\partial y},
$$

\n
$$
S_x = \int_0^x \frac{f(t, y)}{t} dt, \qquad S_y = \int_0^y \frac{f(x, t)}{t} dt,
$$

\n
$$
J(f(x, y)) = f(x, x), \quad Q_\alpha(f(x, y)) = x^\alpha f(x, y), \ \alpha \neq 0.
$$

From the M-polynomial produced in Theorem [2.1,](#page-2-6) below we derive the values of the related degree-based topological indices of the *CHDN*3[*n*] for variable *n*.

Theorem 2.2. *Let CHDN*3[*n*] *be the third type of chain Hexderived network of dimension n. Then*

- *1.* M_1 (*CHDN*3[*n*]) = 32(4*n*−1).
- 2. $M_2(CHDN3[n]) = 336n 160$.
- 3. ${}^mM_2(CHDN3[n]) = \frac{33}{64}n + \frac{7}{32}$.
- 4. $R_{\alpha}(CHDN3[n]) = 4^{2\alpha}(5n+6) + 32^{\alpha}(6n-4) + 8^{2\alpha}(n-4)$ 2).
- 5. $RR_{\alpha}(CHDN3[n]) = \frac{1}{4^{2\alpha}}(5n+6) + \frac{1}{3^{2\alpha}}(6n-4) + \frac{1}{8^{2\alpha}}(n-4)$ 2).
- *6.* $SDD(CHDN3[n]) = 27n-2$.
- 7. $H(CHDN3[n]) = \frac{19}{8}n + \frac{7}{12}$.
- *8. ISI*(*CHDN*3[*n*]) = $30n \frac{20}{3}$.
- 9. $AZ(CHDN3[n]) = \frac{1}{385875} (149316779n 80401408).$

Proof. As computed in the Theorem [2.1,](#page-2-6) the M-polynomial for *CHDN*3[*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,

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

Hence, the degree-based topological indices of the *CHDN*3[*n*] based on the derivation formulas mentioned in Table [2](#page-4-0) 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:

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

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:

$$
R_{\alpha}(CHDN3[n]) = D_x^{\alpha} D_y^{\alpha}(g(x, y))|_{x=y=1}
$$

= $4^{2\alpha}(5n+6) + 32^{\alpha}(6n-4) + 8^{2\alpha}(n-2)$.

5. Inverse Randic 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:

$$
SDD(CHDN3[n]) = (S_yD_x + S_xD_y)(g(x, y))|_{x=y=1}
$$

= 27n - 2.

 \Box

7. Harmonic Index:

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

8. Inverse Sum (Indeg) Index:

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

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 *CHDN*3[*n*], the respective M-polynomials and several related degree-based topological indices are tabulated in Table [3.](#page-6-3) To see the nature of the M-polynomials and the related topological indices, we have varies the dimension of the *CHDN*3[*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.](#page-2-6) 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](#page-5-2) gives the graphical representations of the M-polynomial (as proposed in Theorem [2.1\)](#page-2-6) of the chain Hex-derived network of type 3 of dimension 2 (*CHDN*3[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 $-2 < x, y < 2$. **Figure 4.** The plot of the M-polynomial of *CHDN*3[2] in different regions of *x* and *y*.

in the Figure [4](#page-5-2)(*a*), −1 ≤ *x*, *y* ≤ 1 in the Figure 4(*b*), and $-2 \le x, y \le 2$ in the Figure [4](#page-5-2)(*c*).

Moreover, observing the wide range of values (in Table [3\)](#page-6-3) of the different degree-based topological indices of *CHDN*3[*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,](#page-6-4) and the values of modified second Zagreb, inverse Randić ($\alpha = 1/2$), symmetric division (deg), Harmonic and inverse sum (indeg) indices in Figure [6.](#page-7-16) 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 Randic index ($\alpha = 1/2$) and harmonic index are almost overlapping in Figure [6.](#page-7-16)

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*.

References

- [1] D. B. West, Introduction to Graph Theory, 2nd Edition, Prentice Hall, 2000.
- [2] R. Hammack, W. Imrich, S. Klavžar, Handbook of Product Graphs, 2nd Edition, CRC Press, Inc., Boca Raton, FL, USA, 2011.
- [3] E. Estrada, Randić index, irregularity and complex biomolecular networks, Acta Chimica Slovenica 57 (2010) 597 – 603.
- ^[4] R. García-Domenech, J. Gálvez, J. V. de Julián-Ortiz, L. Pogliani, Some new trends in chemical graph theory, Chemical Reviews 108 (3) (2008) 1127–1169.

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

- [5] A. T. Balaban, Chemical applications of graph theory, Mathematical Chemistry, Academic Press, 1976.
- [6] N. Trinajstić, Chemical Graph Theory, 2nd Edition, Mathematical Chemistry Series, CRC Press, 1992.
- [7] J. L. Gross, J. Yellen, P. Zhang, Handbook of Graph Theory, 2nd Edition, Discrete Mathematics and Its Applications, Chapman and Hall/CRC, 2013.
- [8] I. Gutman, Degree-based topological indices, Croatica Chemica Acta 86 (4) (2013) 351–361.
- [9] A. T. Balaban, Highly discriminating distance-based topological index, Chemical Physics Letters 89 (5) (1982) 399–404.
- [10] K. Pattabiraman, Degree and distance based topological indices of graphs, Electronic Notes in Discrete Mathematics 63 (2017) 145–159.
- [11] P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. Dobrynin, I. Gutman, G. Domotor, The szeged index and an analogy with the wiener index, Journal of Chemical Information and Computer Sciences 35 (3) (1995) 547–550.
- [12] I. Gutman, The acyclic polynomial of a graph, Publications de l'Institut Mathématique 22(36) (42) (1977) 63–69.
- [13] E. J. Farrell, An introduction to matching polynomials, Journal of Combinatorial Theory, Series B 27 (1) (1979) 75–86.
- [14] H. Zhang, F. Zhang, The clar covering polynomial of

hexagonal systems I, Discrete Applied Mathematics 69 (1-2) (1996) 147–167.

- [15] I. Gutman, Some relations between distance-based polynomials of trees, Bulletin (Academie serbe des sciences et ´ des arts. Classe des sciences mathématiques et naturelles. Sciences mathématiques) $131 (30) (2005)$ 1-7.
- 1 [16] L. H. Kauffman, A tutte polynomial for signed graphs, Discrete Applied Mathematics 25 (1-2) (1989) 105–127.
- [17] H. Hosoya, On some counting polynomials in chemistry, Discrete Applied Mathematics 19 (1-3) (1988) 239–257.
- [18] H. Wiener, Structural determination of paraffin boiling points, Journal of the American Chemical Society 69 (1) (1947) 17–20.
- [19] E. Deutsch, S. Klavžar, M-polynomial and degree-based topological indices, Iranian Journal of Mathematical Chemistry 6 (2) (2015) 93–102.
- [20] M. Munir, W. Nazeer, S. Rafique, S. M. Kang, Mpolynomial and degree-based topological indices of polyhex nanotubes, Symmetry 8 (12) (2016) 149.
- [21] M. Munir, W. Nazeer, S. Rafique, S. M. Kang, Mpolynomial and related topological indices of nanostar dendrimers, Symmetry 8 (9) (2016) 97.
- [22] M. Munir, W. Nazeer, A. R. Nizami, S. Rafique, S. M. Kang, M-polynomial and topological indices of titania nanotubes, Symmetry 8 (1-9) (2016) 117.
- [23] Y. C. Kwun, M. Munir, W. Nazeer, S. Rafique, S. M.

Kang, M-polynomials and topological indices of Vphenylenic nanotubes and nanotori, Scientific Reports 7 (1) (2017) 1–9.

- [24] S. M. Kang, W. Nazeer, M. A. Zahid, A. R. Nizami, A. Aslam, M. Munir, M-polynomials and topological indices of hex-derived networks, Open Physics 16 (1) (2018) 394–403.
- [25] H. Deng, J. Yang, F. Xia, A general modeling of some vertex-degree based topological indices in benzenoid systems and phenylenes, Computers & Mathematics with Applications 61 (10) (2011) 3017–3023.
- [26] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. total π -electron energy of alternant hydrocarbons, Chemical Physics Letters 17 (4) (1972) 535–538.
- ^[27] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated zagreb indices, Molecular Diversity 8 (2004) 393–399.
- [28] M. Randić, Characterization of molecular branching, Journal of the American Chemical Society 97 (23) (1975) 6609–6615.
- ^[29] B. Bollobás, P. Erdős, Graphs of extremal weights, Ars Combinatoria 50 (1998) 225–233.
- [30] D. Amić, D. Bešlo, B. Lučić, S. Nikolić, N. Trinajstić, The vertex-connectivity index revisited, Journal of Chemical Information and Computer Sciences 38 (5) (1998) 819–822.
- [31] D. Vukičević, M. Gašperov, Bond additive modeling 1. adriatic indices, Croatica Chemica Acta 83 (3) (2010) 243–260.
- [32] J. Sedlar, D. Stevanović, A. Vasilyev, On the inverse sum indeg index, Discrete Applied Mathematics 184 (2015) 202–212.
- [33] B. Furtula, A. Graovac, D. Vukičević, Augmented zagreb index, Journal of Mathematical Chemistry 48 (2) (2010) 370–380.
- [34] F. G. Nocetti, I. Stojmenovic, J. Zhang, Addressing and routing in hexagonal networks with applications for tracking mobile users and connection rerouting in cellular networks, IEEE Transactions on Parallel and Distributed Systems 13 (9) (2002) 963–971.
- [35] P. Manuel, R. Bharati, I. Rajasingh, C. Monica M, On minimum metric dimension of honeycomb networks, Journal of Discrete Algorithms 6 (1) (2008) 20–27.
- [36] F. S. Raj, A. George, On the metric dimension of *HDN* 3 and *PHDN* 3, in: 2017 IEEE International Conference on Power, Control, Signals and Instrumentation Engineering (ICPCSI), 2017, pp. 1333–1336.
- ^[37] O. Favaron, M. Mahéo, J.-F. Saclé, Some eigenvalue properties in graphs (conjectures of graffiti-II), Discrete Mathematics 111 (1-3) (1993) 197–220.
- [38] S. Hayat, M. Imran, Computation of topological indices of certain networks, Applied Mathematics and Computation 240 (2014) 213–228.
- [39] F. S. Raj, A. George, Network embedding on planar octahedron networks, in: 2015 IEEE International Conference on Electrical, Computer and Communication Technolo-

gies (ICECCT), IEEE, 2015, pp. 1–6.

- [40] C.-C. Wei, H. Ali, M. A. Binyamin, M. N. Naeem, J.-B. Liu, Computing degree based topological properties of third type of hex-derived networks, Mathematics 7 (4) (2019) 368.
- [41] S. Das, S. Rai, M-polynomial and related degree-based topological indices of the third type of hex-derived network, Nanosystems: Physics, Chemistry, Mathematics 11 (3) (2020) 267–274.

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