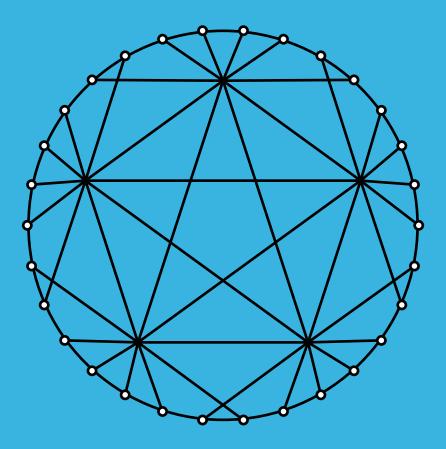
Volume 95

BULLETIN of The June 2022 INSTITUTE of **COMBINATORICS** and its **APPLICATIONS**

Editors-in-Chief:

Marco Buratti, Donald Kreher, Ortrud Oellermann, Tran van Trung



Duluth, Minnesota, U.S.A.

ISSN: 2689-0674 (Online) ISSN: 1183-1278 (Print)

Degree-based topological descriptors of type 3 rectangular hex-derived networks

Shibsankar Das*1 and Shikha Rai¹

¹Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India shib.iitm@gmail.com and shikharai48@gmail.com

Abstract. Topological indices are numeric values in the field of chemical graph theory that encode information about the chemical structure such as molecular shape, size, branching, and so on. A modern idea is to calculate degree-based topological indices using the M-polynomial. The hex-derived networks that are constructed by the hexagonal network of dimension n have various applications in networking, pharmacy, etc. In this paper, we are interested in deriving an expression of the M-polynomial for the type 3 rectangular hex-derived network of dimension n and thereafter all the associated degree-based topological indices. The acquired results can provide a foundation for further exploring rectangular hex-derived networks, their characteristics and applications.

1 Introduction

Let G be a graph that is simple and connected, defined by an ordered pair [V(G), E(G)], where V(G) denotes the vertex set and E(G) denotes the edge set, and consists of (distinct) unordered pairs of vertices. For any vertex u in a graph G, the degree is defined as the number of edges incident to the vertex u and is denoted by d(u) [36].

The topology segment of mathematical chemistry, which uses graphs to model chemical compounds, is Chemical Graph Theory (CGT). In the

Key words and phrases: type 3 rectangular hex-derived networks, degree-based topological indices, graph polynomial, M-polynomial

AMS (MOS) Subject Classifications: 05C10, 05C07, 92E10, 05C31

Received: 2 September 2021 Accepted: 1 Februrary 2022

^{*}Corresponding author.

Das and Rai

graphical representation of a chemical compound, the atoms are represented by the vertices and the chemical bonds between the atoms are represented by edges. In the field of CGT, there are several types of questions that have been studied in the last few decades. A topological index is an invariant for the molecular graph of chemical compounds in the area of CGT. Topological indices of interest are those that play a significant role in the analysis of Quantitative Structure-Activity Relationship (QSAR)/Quantitative Structure-Property Relationship (QSPR). The QSAR and QSPR are related to the prediction of bioactivity and physical-chemical properties of the chemical compounds. For chemical graphs, one of the most well-known topological indices is the Wiener index which is known to correlate closely with some of the physical properties of the chemical substance such as its boiling point (see [37]).

There are different classes of topological indices, for instance counting related topological indices [22], distance-based topological indices [2] and degree-based topological indices [17]. In order to predict the physicochemical properties of various chemical structures, all these topological indices of several classes are beneficial. The topological indices are generally calculated using their definitions. It would be beneficial to have a generic method that can provide several topological indices of a specific class. A well-recognized approach in this field, is the calculation of topological indices by constructing a general polynomial. Hence, if only the graph polynomial is known, various topological indices are determined by integrating or differentiating (or blending of both) the respective polynomial.

In the literature, many graph polynomials have evolved and played a significant role in mathematical chemistry. Some notable graph polynomials are the Hosoya polynomial [18], the matching polynomial [13], the Tutte polynomial [21], the Schultz polynomial [16], the Clar covering polynomial [38], and the M-polynomial [29]. In the evaluation of distance-based topological indices, the Hosoya polynomial is regarded as one of the most general polynomials and gives information on, for example, the Wiener index [37] and the hyper Wiener index [32]. In the same way, the M-polynomial is a recent and popular methodology that plays an important role in the evaluation of degree-based graph invariants.

The degree-based topological indices are most relevant in themselves because they are used to assess the medicinal activities, chemical reactivity, and physical properties of chemical compounds. In 2015, Deutsch and Klavžar [11] proposed the M-polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for degree-based topological indices is analogous with the Hosoya polynomial and reported that its importance for the following the followin

mial's importance for distance-based topological indices. The M-polynomial and their associated degree-based topological indices corresponding to different chemical networks are assessed in [26, 23, 20, 19, 39, 12, 6, 7, 5, 8, 28, 9].

Definition 1.1 (Deutsch and Klavžar [11]). 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 $(i, j \ge 1)$.

In [10], it is reported that for a graph G, a degree-based topological index is a type of graph invariant, denoted by I(G), and which is of the form

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

The following theorem uses the operators $D_x, D_y, S_x, S_y, J, Q_\alpha$ and they are defined as follows:

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

Theorem 1.1 (Deutsch and Klavžar [11], Theorems 2.1, 2.2). Let G be a simple connected graph.

(a) 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

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

- (b) 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 .
- (c) 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 $r, s \geq 0, t \geq 1$ and $\alpha \in \mathbb{Z}$, then

$$I(G) = S_x^t Q_\alpha J D_x^r D_y^s (M(G; x, y))|_{x=1}.$$

Gutman and Trinjastić [15] introduced the first and second Zagreb indices in 1972. Instead of the outer edges and vertices, the Zagreb indices give greater weight to the inner edges and vertices. The modified Zagreb indices are then introduced in [25], inspired by the idea of Zagreb indices. Furthermore, the *Randić index*, introduced by Milan Randić [31] in 1975, is a very prominent degree-based topological index. This index has diverse applications in the area of drug design. After seeing the effect of the Randić index, a generalized version of the Randić index, known as the general Randić index, is presented by Bollobás et al. [3] and Amić et al. [1] in 1998. In order to calculate the total surface area of polychlorobiphenyls, a symmetric division (deg) index [34] is introduced in 2010. It turns out that the inverse sum (indeq) index [34, 33] is a good indicator of the total surface area of octane isomers. Furtula et al. [14] presented the augmented Zagreb index, which is useful in analyzing the heat of formation of alkanes. For the mathematical expressions of the degree-based topological indices, please refer to [6].

Chen et al. [4] developed an addressing scheme as well as routing and broadcasting algorithms, for the hexagonal mesh multiprocessors. Hexagonal networks [27] are a type of network that is designed using planer graphs. Triangular plane tessellation, or the division of a plane into equilateral triangles, is the basis for these networks. Honeycomb networks and mesh networks are the nearest networks. Honeycomb networks are built on regular hexagons, while mesh networks are based on a regular square partition. A hexagonal network whose nodes are at the vertices of a regular triangular tessellation has up to six neighbours for each vertex. They are used to model benzenoid hydrocarbons in chemistry, as well as in image processing, computer graphics, and cellular and interconnectedness networks. Two hex-derived networks HDN1 and HDN2 are introduced in [24]. Afterwards, from the n dimensional hexagonal network, a new chemical network was introduced by Raj and George [30] in 2017 and named the type 3 rectangular hex-derived network (RHDN3[n]). Figure 1 shows a type 3 rectangular hex-derived network of dimension 4 (RHDN3[4]).

Outline of the work

Wei et al. [35] evaluated different degree-based topological indices for type 3 rectangular hex-derived networks of dimension n (RHDN3[n]) directly with the help of their degree dependent formulas. All these degree-based indices are helpful in understanding the properties of RHDN3[n]. In the present work, we calculate these degree-based topological indices by using

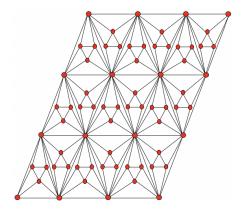


Figure 1: Type 3 rectangular hex-derived network of dimension 4 (RHDN3[4])

the M-polynomial. In Section 2, we obtain a general expression of the M-polynomial for the RHDN3[n] and hence we derive the associated degree-dependent topological indices and we conclude with Section 3.

2 Deriving M-polynomial for RHDN3[n] network

Below, we determine the M-polynomial of the type 3 rectangular hexderived network of dimension $n \ge 4$.

Theorem 2.1. Let RHDN3[n] be the type 3 rectangular hex-derived network of dimension $n \ge 4$. Then the M-polynomial of RHDN3[n] is $M(RHDN3[n]; x, y) = (6n^2 - 12n + 10)x^4y^4 + 8x^4y^7 + (24n - 44)x^4y^{10} + (12n^2 - 48n + 48)x^4y^{18} + 4x^7y^{10} + 2x^7y^{18} + (4n - 10)x^{10}y^{10} + (8n - 20)x^{10}y^{18} + (3n^2 - 16n + 21)x^{18}y^{18}.$

Proof. Consider the type 3 rectangular hex-derived network (RHDN3[n]) of dimension $n \geq 4$. It can be observed from Figure 1 of RHDN3[4] that the vertex set and edge set of RHDN3[n] have respective cardinalities

$$|V(RHDN3[n])| = 7n^2 - 12n + 6$$
 and $|E(RHDN3[n])| = 21n^2 - 40n + 19$.

Now, the vertex set V(RHDN3[n]) of RHDN3[n] can be partitioned into

four disjoint subsets that depend on the degree of end vertices, these are

$$\begin{split} V_1(RHDN3[n]) &= \{u \in V(RHDN3[n]) : d(u) = 4\}, \\ V_2(RHDN3[n]) &= \{u \in V(RHDN3[n]) : d(u) = 7\}, \\ V_3(RHDN3[n]) &= \{u \in V(RHDN3[n]) : d(u) = 10\}, \\ V_4(RHDN3[n]) &= \{u \in V(RHDN3[n]) : d(u) = 18\}, \end{split}$$

and counts the number of such vertices, they are

$$|V_1(RHDN3[n])| = (6n^2 - 12n + 8), |V_2(RHDN3[n])| = 2,$$

 $|V_3(RHDN3[n])| = 4(n - 2), |V_4(RHDN3[n])| = (n - 2)^2.$

Furthermore, depending on the degree of the end vertices, the edge set E(RHDN3[n]) of RHDN3[n] is partitioned into nine parts as follows.

$$\begin{split} E_{\{4,4\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 4, d(v) = 4\}, \\ E_{\{4,7\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 4, d(v) = 7\}, \\ E_{\{4,10\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 4, d(v) = 10\}, \\ E_{\{4,18\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 4, d(v) = 18\}, \\ E_{\{7,10\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 7, d(v) = 10\}, \\ E_{\{7,18\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 7, d(v) = 18\}, \\ E_{\{10,10\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 10, d(v) = 10\}, \\ E_{\{10,18\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 10, d(v) = 18\}, \\ E_{\{18,18\}} &= \{e = uv \in E(RHDN3[n]) : d(u) = 18, d(v) = 18\}. \end{split}$$

And their cardinalities are $|E_{\{4,4\}}|=6n^2-12n+10, |E_{\{4,7\}}|=8, |E_{\{4,10\}}|=24n-44, |E_{\{4,18\}}|=12n^2-48n+48, |E_{\{7,10\}}|=4, |E_{\{7,18\}}|=2, |E_{\{10,10\}}|=4n-10, |E_{\{10,18\}}|=8n-20, |E_{\{18,18\}}|=3n^2-16n+21.$ Thus, the M-polynomial of the RHDN3[n] network is given by

¹Note that, $|E_{\{7,7\}}| = 0$ because there is no edge uv in the type 3 rectangular hex-derived network of dimension n, such that d(u) = 7 = d(v).

$$\begin{split} &M(RHDN3[n];x,y)\\ &=\sum_{i\leq j}m_{i,j}x^iy^j, \quad \text{where} \quad i,j\in\{4,7,10,18\}\\ &=\sum_{uv\in E_{\{4,4\}}}m_{4,4}x^4y^4+\sum_{uv\in E_{\{4,7\}}}m_{4,7}x^4y^7+\sum_{uv\in E_{\{4,10\}}}m_{4,10}x^4y^{10}\\ &+\sum_{uv\in E_{\{4,18\}}}m_{4,18}x^4y^{18}+\sum_{uv\in E_{\{7,10\}}}m_{7,10}x^7y^{10}+\sum_{uv\in E_{\{7,18\}}}m_{7,18}x^7y^{18}\\ &+\sum_{uv\in E_{\{10,10\}}}m_{10,10}x^{10}y^{10}+\sum_{uv\in E_{\{10,18\}}}m_{10,18}x^{10}y^{18}\\ &+\sum_{uv\in E_{\{18,18\}}}m_{18,18}x^{18}y^{18}\\ &=(6n^2-12n+10)x^4y^4+8x^4y^7+(24n-44)x^4y^{10}\\ &+(12n^2-48n+48)x^4y^{18}+4x^7y^{10}+2x^7y^{18}+(4n-10)x^{10}y^{10}\\ &+(8n-20)x^{10}y^{18}+(3n^2-16n+21)x^{18}y^{18}. & \Box \end{split}$$

Table 1: Derived formulas [11] of degree-based topological indices of a graph G in the form of M-polynomial.

Sl. No.	Topological Index	Notation	f(x,y)	Derivation from $(M(G; x, y))$
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	$^mM_2(G)$	$\frac{1}{xy}$	$(S_x S_y)(M(G; x, y)) _{x=y=1}$
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)	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (M(G; x, y)) _{x=1}$

Note that, in Table 1,
$$D_x(f(x,y)) = x \frac{\partial (f(x,y))}{\partial x}, \qquad D_y(f(x,y)) = y \frac{\partial (f(x,y))}{\partial y}, \\ S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t} dt, \qquad S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t} dt, \\ J(f(x,y)) = f(x,x), \qquad Q_\alpha(f(x,y)) = x^\alpha f(x,y), \ \alpha \neq 0.$$

We now use the above expression of M-polynomial of the RHDN3[n] network to derive the associated degree-based topological indices in the following Theorem 2.2.

Theorem 2.2. Let RHDN3[n] be a type 3 rectangular hex-derived network of dimension $n \geq 4$. Then

1.
$$M_1(RHDN3[n]) = 2(210n^2 - 544n + 361).$$

2.
$$M_2(RHDN3[n]) = 4(483n^2 - 1508n + 1204).$$

3.
$${}^{m}M_{2}(RHDN3[n]) = \frac{119}{216}n^{2} - \frac{6331}{8100}n + \frac{611}{1512}.$$

4.
$$R_{\alpha}(RHDN3[n]) = 4^{2\alpha}(6n^2 - 12n + 10) + 8 \times 28^{\alpha} + 40^{\alpha}(24n - 44) + 72^{\alpha}(12n^2 - 48n + 48) + 4 \times 70^{\alpha} + 2 \times 126^{\alpha} + 10^{2\alpha}(4n - 10) + 180^{\alpha}(8n - 20) + 18^{2\alpha}(3n^2 - 16n + 21).$$

5.
$$RR_{\alpha}(RHDN3[n]) = \frac{1}{4^{2\alpha}}(6n^2 - 12n + 10) + \frac{8}{28^{\alpha}} + \frac{1}{40^{\alpha}}(24n - 44) + \frac{1}{72^{\alpha}}(12n^2 - 48n + 48) + \frac{4}{70^{\alpha}} + \frac{2}{126^{\alpha}} + \frac{1}{10^{2\alpha}}(4n - 10) + \frac{1}{180^{\alpha}}(8n - 20) + \frac{1}{18^{2\alpha}}(3n^2 - 16n + 21).$$

6.
$$SDD(RHDN3[n]) = \frac{224}{3}n^2 - \frac{1676}{9}n + \frac{13331}{105}$$
.

7.
$$H(RHDN3[n]) = \frac{91}{33}n^2 - \frac{1907}{495}n + \frac{137558}{98175}$$
.

8.
$$ISI(RHDN3[n]) = \frac{861}{11}n^2 - \frac{2036}{11}n + \frac{3557843}{32725}$$

9.
$$AZ(RHDN3[n]) = \frac{4^6}{6^3}(6n^2 - 12n + 10) + \frac{8 \times 28^3}{9^3} + \frac{40^3}{12^3}(24n - 44)$$

 $+ \frac{72^3}{20^3}(12n^2 - 48n + 48) + \frac{4 \times 70^3}{15^3} + \frac{2 \times 126^3}{23^3} + \frac{10^6}{18^3}(4n - 10)$
 $+ \frac{180^3}{26^3}(8n - 20) + \frac{18^6}{34^3}(3n^2 - 16n + 21)$
 $= \frac{18072253528}{5527125}n^2 - \frac{11885277153465184}{983590583625}n + \frac{5140351070639169064}{443235060406125}$

Proof. We assume that g(x,y)=M(RHDN3[n];x,y), for the sake of notational simplicity. Therefore, $g(x,y)=(6n^2-12n+10)x^4y^4+8x^4y^7+(24n-44)x^4y^{10}+(12n^2-48n+48)x^4y^{18}+4x^7y^{10}+2x^7y^{18}+(4n-10)x^{10}y^{10}+(8n-20)x^{10}y^{18}+(3n^2-16n+21)x^{18}y^{18}.$

Here, for calculating the degree-based topological indices, we will need the following terms:

$$\begin{split} D_x(g(x,y)) &= 4(6n^2 - 12n + 10)x^4y^4 + 32x^4y^7 + 4(24n - 44)x^4y^{10} \\ &\quad + 4(12n^2 - 48n + 48)x^4y^{18} + 28x^7y^{10} + 14x^7y^{18} \\ &\quad + 10(4n - 10)x^{10}y^{10} + 10(8n - 20)x^{10}y^{18} \\ &\quad + 18(3n^2 - 16n + 21)x^{18}y^{18}, \end{split}$$

$$\begin{split} D_y(g(x,y)) &= 4(6n^2 - 12n + 10)x^4y^4 + 56x^4y^7 + 10(24n - 44)x^4y^{10} \\ &\quad + 18(12n^2 - 48n + 48)x^4y^{18} + 40x^7y^{10} + 36x^7y^{18} \\ &\quad + 10(4n - 10)x^{10}y^{10} + 18(8n - 20)x^{10}y^{18} \\ &\quad + 18(3n^2 - 16n + 21)x^{18}y^{18}, \end{split}$$

$$D_y D_x(g(x,y)) = 16(6n^2 - 12n + 10)x^4y^4 + 224x^4y^7 + 40(24n - 44)x^4y^{10}$$

$$+ 72(12n^2 - 48n + 48)x^4y^{18} + 280x^7y^{10} + 252x^7y^{18}$$

$$+ 100(4n - 10)x^{10}y^{10} + 180(8n - 20)x^{10}y^{18}$$

$$+ 324(3n^2 - 16n + 21)x^{18}y^{18},$$

$$S_x(g(x,y)) = \frac{1}{4}(6n^2 - 12n + 10)x^4y^4 + 2x^4y^7 + \frac{1}{4}(24n - 44)x^4y^{10}$$

$$+ \frac{1}{4}(12n^2 - 48n + 48)x^4y^{18} + \frac{4}{7}x^7y^{10} + \frac{2}{7}x^7y^{18}$$

$$+ \frac{1}{10}(4n - 10)x^{10}y^{10} + \frac{1}{10}(8n - 20)x^{10}y^{18}$$

$$+ \frac{1}{18}(3n^2 - 16n + 21)x^{18}y^{18},$$

$$\begin{split} S_y(g(x,y)) &= \frac{1}{4}(6n^2 - 12n + 10)x^4y^4 + \frac{8}{7}x^4y^7 + \frac{1}{10}(24n - 44)x^4y^{10} \\ &+ \frac{1}{18}(12n^2 - 48n + 48)x^4y^{18} + \frac{4}{10}x^7y^{10} + \frac{2}{18}x^7y^{18} \\ &+ \frac{1}{10}(4n - 10)x^{10}y^{10} + \frac{1}{18}(8n - 20)x^{10}y^{18} \\ &+ \frac{1}{18}(3n^2 - 16n + 21)x^{18}y^{18}, \end{split}$$

$$\begin{split} S_x S_y(g(x,y)) &= \frac{1}{16} (6n^2 - 12n + 10) x^4 y^4 + \frac{2}{7} x^4 y^7 + \frac{1}{40} (24n - 44) x^4 y^{10} \\ &\quad + \frac{1}{72} (12n^2 - 48n + 48) x^4 y^{18} + \frac{4}{70} x^7 y^{10} + \frac{1}{63} x^7 y^{18} \\ &\quad + \frac{1}{100} (4n - 10) x^{10} y^{10} + \frac{1}{180} (8n - 20) x^{10} y^{18} \\ &\quad + \frac{1}{324} (3n^2 - 16n + 21) x^{18} y^{18}, \end{split}$$

$$\begin{split} D_x^\alpha D_y^\alpha(g(x,y)) &= 4^{2\alpha} (6n^2 - 12n + 10) x^4 y^4 + 8 \times 28^\alpha x^4 y^7 \\ &\quad + 40^\alpha (24n - 44) x^4 y^{10} + 72^\alpha (12n^2 - 48n + 48) x^4 y^{18} \\ &\quad + 4 \times 70^\alpha x^7 y^{10} + 2 \times 126^\alpha x^7 y^{18} + 10^{2\alpha} (4n - 10) x^{10} y^{10} \\ &\quad + 180^\alpha (8n - 20) x^{10} y^{18} + 18^{2\alpha} (3n^2 - 16n + 21) x^{18} y^{18}, \end{split}$$

$$S_y D_x(g(x,y)) = (6n^2 - 12n + 10)x^4y^4 + \frac{32}{7}x^4y^7 + \frac{4}{10}(24n - 44)x^4y^{10}$$

$$+ \frac{4}{18}(12n^2 - 48n + 48)x^4y^{18} + \frac{28}{10}x^7y^{10} + \frac{14}{18}x^7y^{18}$$

$$+ (4n - 10)x^{10}y^{10} + \frac{10}{18}(8n - 20)x^{10}y^{18}$$

$$+ (3n^2 - 16n + 21)x^{18}y^{18},$$

$$S_x D_y(g(x,y)) = (6n^2 - 12n + 10)x^4y^4 + 14x^4y^7 + \frac{10}{4}(24n - 44)x^4y^{10}$$

$$+ \frac{18}{4}(12n^2 - 48n + 48)x^4y^{18} + \frac{40}{7}x^7y^{10} + \frac{36}{7}x^7y^{18}$$

$$+ (4n - 10)x^{10}y^{10} + \frac{18}{10}(8n - 20)x^{10}y^{18}$$

$$+ (3n^2 - 16n + 21)x^{18}y^{18}.$$

$$\begin{split} S_x^\alpha S_y^\alpha(g(x,y)) &= \frac{1}{4^{2\alpha}} (6n^2 - 12n + 10) x^4 y^4 + \frac{8}{28^\alpha} x^4 y^7 \\ &\quad + \frac{1}{40^\alpha} (24n - 44) x^4 y^{10} + \frac{1}{72^\alpha} (12n^2 - 48n + 48) x^4 y^{18} \\ &\quad + \frac{4}{70^\alpha} x^7 y^{10} + \frac{2}{126^\alpha} x^7 y^{18} + \frac{1}{10^{2\alpha}} (4n - 10) x^{10} y^{10} \\ &\quad + \frac{1}{180^\alpha} (8n - 20) x^{10} y^{18} + \frac{1}{18^{2\alpha}} (3n^2 - 16n + 21) x^{18} y^{18}, \end{split}$$

$$\begin{split} S_x J(g(x,y)) &= \frac{1}{8} (6n^2 - 12n + 10) x^8 + \frac{8}{11} x^{11} + \frac{1}{14} (24n - 44) x^{14} \\ &+ \frac{1}{22} (12n^2 - 48n + 48) x^{22} + \frac{4}{17} x^{17} + \frac{2}{25} x^{25} \\ &+ \frac{1}{20} (4n - 10) x^{20} + \frac{1}{28} (8n - 20) x^{28} \\ &+ \frac{1}{36} (3n^2 - 16n + 21) x^{36}, \end{split}$$

$$S_x J D_x D_y(g(x,y)) = 2(6n^2 - 12n + 10)x^8 + \frac{224}{11}x^{11} + \frac{40}{14}(24n - 44)x^{14} + \frac{72}{22}(12n^2 - 48n + 48)x^{22} + \frac{280}{17}x^{17} + \frac{252}{25}x^{25} + 5(4n - 10)x^{20} + \frac{180}{28}(8n - 20)x^{28} + \frac{324}{36}(3n^2 - 16n + 21)x^{36},$$

$$\begin{split} S_x^3Q_{-2}JD_x^3D_y^3(g(x,y)) &= \frac{4^6}{6^3}(6n^2-12n+10)x^6 + \frac{8\times28^3}{9^3}x^9 \\ &\quad + \frac{40^3}{12^3}(24n-44)x^{12} + \frac{72^3}{20^3}(12n^2-48n+48)x^{20} \\ &\quad + \frac{4\times70^3}{15^3}x^{15} + \frac{2\times126^3}{23^3}x^{23} + \frac{10^6}{18^3}(4n-10)x^{18} \\ &\quad + \frac{180^3}{26^3}(8n-20)x^{26} + \frac{18^6}{34^3}(3n^2-16n+21)x^{34}. \end{split}$$

Thus, using the derivation formulas of topological indices mentioned in Table 1, the related degree-based topological indices of RHDN3[n] are:

1. First Zagreb Index:

$$M_1(RHDN3[n]) = (D_x + D_y)(g(x,y))|_{x=y=1} = 2(210n^2 - 544n + 361).$$

2. Second Zagreb Index:

$$M_2(RHDN3[n]) = D_x D_y(g(x,y))|_{x=y=1} = 4(483n^2 - 1508n + 1204).$$

3. Modified Second Zagreb Index:

$$^{m}M_{2}(RHDN3[n]) = S_{x}S_{y}(g(x,y))|_{x=y=1} = \frac{119}{216}n^{2} - \frac{6331}{8100}n + \frac{611}{1512}.$$

4. General Randić Index:

$$\begin{split} R_{\alpha}(RHDN3[n]) &= D_{x}^{\alpha}D_{y}^{\alpha}(g(x,y))|_{x=y=1} \\ &= 4^{2\alpha}(6n^{2} - 12n + 10) + 8 \times 28^{\alpha} + 40^{\alpha}(24n - 44) \\ &\quad + 72^{\alpha}(12n^{2} - 48n + 48) + 4 \times 70^{\alpha} + 2 \times 126^{\alpha} \\ &\quad + 10^{2\alpha}(4n - 10) + 180^{\alpha}(8n - 20) \\ &\quad + 18^{2\alpha}(3n^{2} - 16n + 21). \end{split}$$

5. Inverse Randić Index:

$$\begin{split} RR_{\alpha}(RHDN3[n]) &= S_{x}^{\alpha}S_{y}^{\alpha}(g(x,y))|_{x=y=1} \\ &= \frac{1}{4^{2\alpha}}(6n^{2} - 12n + 10) + \frac{8}{28^{\alpha}} + \frac{1}{40^{\alpha}}(24n - 44) \\ &\quad + \frac{1}{72^{\alpha}}(12n^{2} - 48n + 48) + \frac{4}{70^{\alpha}} + \frac{2}{126^{\alpha}} \\ &\quad + \frac{1}{10^{2\alpha}}(4n - 10) + \frac{1}{180^{\alpha}}(8n - 20) \\ &\quad + \frac{1}{18^{2\alpha}}(3n^{2} - 16n + 21). \end{split}$$

6. Symmetric Division (Deg) Index:

$$SDD(RHDN3[n]) = (S_yD_x + S_xD_y)(g(x,y))|_{x=y=1}$$
$$= \frac{224}{3}n^2 - \frac{1676}{9}n + \frac{13331}{105}.$$

7. Harmonic Index:

$$H(RHDN3[n]) = 2S_x J(g(x,y))|_{x=1} = \frac{91}{33}n^2 - \frac{1907}{495}n + \frac{137558}{98175}.$$

8. Inverse Sum (Indeg) Index:

$$ISI(RHDN3[n]) = S_x J D_x D_y(g(x,y))|_{x=1} = \frac{861}{11} n^2 - \frac{2036}{11} n + \frac{3557843}{32725}.$$

9. Augmented Zagreb Index:

$$\begin{split} AZ(RHDN3[n]) &= S_x^3 Q_{-2} J D_x^3 D_y^3(g(x,y))|_{x=1} \\ &= \frac{18072253528}{5527125} n^2 - \frac{11885277153465184}{983590583625} n \\ &+ \frac{5140351070639169064}{443235060406125}. \end{split}$$

3 Conclusion

In this present article, we have evaluated the degree-based topological indices for the RHDN3[n] networks with the help of the M-polynomial. At the very beginning, we have formulated the expression of the M-polynomial for the RHDN3[n] networks and using that expression we have computed nine associated standard degree-based topological indices. Observe that the M-polynomial method is very fast, compact and more appropriate to compute the degree-based topological indices of the network instead of calculating them using their degree-based formulas.

Acknowledgements

We thank the anonymous referee for the thorough review of this article and for the valuable suggestions which helped us to improve the quality of the article. Moreover, the second author is grateful to Banaras Hindu University (BHU), Varanasi for the financial support of BHU-fellowship.

References

- [1] D. Amić, D. Bešlo, B. Lučić, S. Nikolić, and N. Trinajstić, The vertex-connectivity index revisited, J. Chem. Inf. Comput. Sci., 38(5) (1998), 819–822. doi:10.1021/ci980039b.
- A.T. Balaban, Highly discriminating distance-based topological index, Chem. Phys. Lett., 89(5) (1982), 399-404. doi:10.1016/0009-2614(82)80009-2.
- [3] B. Bollobás and P. Erdős, Graphs of extremal weights, Ars Combin., 50 (1998), 225-233. https://www.semanticscholar.org/paper/Graphs-of-Extremal-Weights-Bollob%C3%A1s-Erd%C3%B6s/151f793cf967c7cff900a5bb1c2da9f5fba1efcf.
- [4] M.-S. Chen, K.G. Shin, and D.D. Kandlur, Addressing, routing, and broadcasting in hexagonal mesh multiprocessors, *IEEE Trans. Comput.*, **39(1)** (1990), 10–18. doi:10.1109/12.46277.

Das and Rai

- [5] S. Das and V. Kumar, On M-polynomial of the two-dimensional siliconcarbons, Palest. J. Math., 11(Special Issue II) (2022), 136–157. https://pjm.ppu.edu/paper/1035-m-polynomial-two-dimensionalsilicon-carbons.
- [6] S. Das and S. Rai, M-polynomial and related degree-based topological indices of the third type of hex-derived network, Nanosystems: Phys. Chem. Math., 11(3) (2020), 267–274. doi:10.17586/2220-8054-2020-11-3-267-274.
- [7] S. Das and S. Rai, M-polynomial and related degree-based topological indices of the third type of chain hex-derived network, *Malaya J. Mat.*, 8(4) (2020), 1842–1850. doi:10.26637/MJM0804/0085.
- [8] S. Das and S. Rai, Topological characterization of the third type of triangular hex-derived networks, Sci. Ann. Comput. Sci., 31(2) (2021), 145–161. doi:10.7561/SACS.2021.2.145.
- [9] S. Das and S. Rai, On M-polynomial and associated topological descriptors of subdivided Hex-derived network of type three, Comput. Technol., (2022), in press.
- [10] H. Deng, J. Yang, and F. Xia, A general modeling of some vertexdegree based topological indices in benzenoid systems and phenylenes, *Comput. Math. Appl.*, 61(10) (2011), 3017–3023. doi:10.1016/j. camwa.2011.03.089.
- [11] E. Deutsch and S. Klavžar, M-polynomial and degree-based topological indices, *Iranian J. Math. Chem.*, **6(2)** (2015), 93–102. doi:10.22052/ijmc.2015.10106.
- [12] E. Deutsch and S. Klavžar, On the M-polynomial of planar chemical graphs, *Iranian J. Math. Chem.*, **11(2)** (2020), 65–71. doi:10.22052/ijmc.2020.224280.1492.
- [13] E.J. Farrell, An introduction to matching polynomials, J. Combin. Theory Ser. B, **27(1)** (1979), 75–86. doi:10.1016/0095-8956(79) 90070-4.
- [14] B. Furtula, A. Graovac, and D. Vukičević, Augmented Zagreb index, J. Math. Chem., 48(2) (2010), 370–380. doi:10.1007/s10910-010-9677-3.
- [15] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17(4)** (1972), 535–538. doi:10.1016/0009-2614(72)85099-1.

Degree-based TDs of type 3 RHDNs

- [16] I. Gutman, Some relations between distance-based polynomials of trees, Bull. Cl. Sci. Math. Nat. Sci. Math., 131(30) (2005), 1–7. doi:10.2298/BMAT0530001G.
- [17] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta*, **86(4)** (2013), 351–361. doi:10.5562/cca2294.
- [18] H. Hosoya, On some counting polynomials in chemistry, *Discrete Appl. Math.*, **19(1-3)** (1988) 239–257. doi:10.1016/0166-218X(88) 90017-0.
- [19] M.N. Jahangeer Baig, C.Y. Jung, N. Ahmad, and S.M. Kang, On the M-polynomials and degree-based topological indices of an important class of graphs, J. Discret. Math. Sci. Cryptogr., 22(7) (2019), 1281– 1288. doi:10.1080/09720529.2019.1691327.
- [20] S.M. Kang, W. Nazeer, M.A. Zahid, A.R. Nizami, A. Aslam, and M. Munir, M-polynomials and topological indices of hex-derived networks, Open Phys., 16(1) (2018), 394–403. doi:10.1515/phys-2018-0054.
- [21] L.H. Kauffman, A Tutte polynomial for signed graphs, *Discrete Appl. Math.*, **25(1-2)** (1989), 105–127. doi:10.1016/0166-218X(89) 90049-8.
- [22] P.V. Khadikar, N.V. Deshpande, P.P. Kale, A. Dobrynin, I. Gutman, and G. Domotor, The Szeged index and an analogy with the Wiener index, J. Chem. Inf. Comput. Sci, 35(3) (1995), 547–550. doi:10.1021/ci00025a024.
- [23] Y.C. Kwun, M. Munir, W. Nazeer, S. Rafique, and S.M. Kang, M-polynomials and topological indices of V-phenylenic nanotubes and nanotori, *Sci. Rep.*, **7(1)** (2017), 1–9. doi:10.1038/s41598-017-08309-y.
- [24] P. Manuel, R. Bharati, I. Rajasingh, and C. Monica M, On minimum metric dimension of honeycomb networks, *J. Discrete Algorithms*, **6(1)** (2008), 20–27. doi:10.1016/j.jda.2006.09.002.
- [25] A. Miličević, S. Nikolić, and N. Trinajstić, On reformulated Zagreb indices, Mol. Divers., 8 (2004), 393–399. doi:10.1016/j.dam.2011. 09.021.
- [26] M. Munir, W. Nazeer, S. Rafique, and S.M. Kang, M-polynomial and degree-based topological indices of polyhex nanotubes, *Symmetry*, 8(12) (2016), Art. 149, 8 pp. doi:10.3390/sym8120149.

Das and Rai

- [27] F.G. Nocetti, I. Stojmenovic, and J. Zhang, Addressing and routing in hexagonal networks with applications for tracking mobile users and connection rerouting in cellular networks, *IEEE Trans. Parallel Distrib.* Syst., 13(9) (2002), 963–971. doi:10.1109/TPDS.2002.1036069.
- [28] S. Rai and S. Das, M-polynomial and degree-based topological indices of subdivided chain hex-derived network of type 3, Chapter 33 in "Advanced Network Technologies and Intelligent Computing", I. Woungang, S.K. Dhurandher, K.K. Pattanaik, A. Verma, P. Verma (Eds.), Springer International Publishing, Cham, 1534 (2022), 410–424. doi:10.1007/978-3-030-96040-7_33.
- [29] F.S. Raj and A. George, Network embedding on planar octahedron networks, in "2015 IEEE International Conference on Electrical, Computer and Communication Technologies (ICECCT)", (2015), 1–6. doi:10.1109/ICECCT.2015.7226174.
- [30] F.S. Raj and 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), 1333– 1336. doi:10.1109/ICPCSI.2017.8391927.
- [31] M. Randić, Characterization of molecular branching, J. Am. Chem. Soc., 97(23) (1975), 6609–6615. doi:10.1021/ja00856a001.
- [32] M. Randić, Novel molecular descriptor for structure property studies, Chem. Phys. Lett., 211(4-5) (1993), 478-483. doi:10.1016/0009-2614(93)87094-J.
- [33] J. Sedlar, D. Stevanović, and A. Vasilyev, On the inverse sum indeg index, Discrete Appl. Math., 184 (2015), 202–212. doi:10.1016/j.dam.2014.11.013.
- [34] D. Vukičević and M. Gašperov, Bond additive modeling 1. Adriatic indices, Croat. Chem. Acta, 83(3) (2010), 243-260. https://www.researchgate.net/publication/283150640.
- [35] C.-C. Wei, H. Ali, M.A. Binyamin, M.N. Naeem, and J.-B. Liu, Computing degree based topological properties of third type of hexderived networks, *Mathematics*, 7(4) (2019), 368. doi:10.3390/ math7040368.
- [36] D.B. West, Introduction to Graph Theory, 2nd Edition, Prentice Hall, 2000.
- [37] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69(1)** (1947), 17–20. doi:10.1021/ja01193a005.

Degree-based TDs of type 3 RHDNs

- [38] H. Zhang and F. Zhang, The Clar covering polynomial of hexagonal systems I, Discrete Appl. Math., **69(1-2)** (1996), 147–167. doi:10. 1016/0166-218X(95)00081-2.
- [39] X. Zuo, M. Numan, S.I. Butt, M.K. Siddiqui, R. Ullah, and U. Ali, Computing topological indices for molecules structure of polyphenylene via M-polynomials, *Polycycl. Aromat. Compd.*, (2020). doi: 10.1080/10406638.2020.1768413.