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Molecular Properties of Symmetrical Networks Using Topological Polynomials

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Abstract: A numeric quantity that comprehend characteristics of molecular graph G of chemical compound is known as topological index. This number is, in fact, invariant with respect to symmetry properties of molecular graph G . Many researchers have established, after diverse studies, a parallel between the physico chemical properties like boiling point, stability, similarity, chirality and melting point of chemical species and corresponding chemical graph. These descriptors defined on chemical graphs are extremely helpful for researchers to conduct regression model like QSAR/QSPR and better understand the physical features, complexity of molecules, chemical and biological properties of underlying compound.

In this paper, several structure descriptors of vital importance, namely, first, second, modified and augmented Zagreb indices, inverse and general Randic indices, symmetric division, harmonic, inverse sum and forgotten indices of Hex-derived Meshes (networks) of two kinds, namely, $HDN1(n)$ and $HDN2(n)$ are computed and recovered using general approach of topological polynomials.

Keywords: Topological indices; M-Polynomial; Forgotten Polynomial; Molecular graphs; Hex-derive networks

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1 Introduction

Graph theory is a standout amongst the most extraordinary and one of a kind branch of mathematics by which the showing of any structure is made possible. As of late, it achieves much consideration among scientists on account of its extensive variety of utilizations in Computer science, electrical systems, interconnected systems, biological networks, and in chemistry, and so forth. The chemical graph theory is the quickly developing zone among scientists. It helps in comprehension about the basic properties of a molecular graph. There is a considerable measure of molecular compounds which have assortment of utilizations in the fields of business, commercial, industrial, pharmaceutical chemistry, every day life, and in research facility.

In recent years researchers got immense attraction toward an emerging field *Cheminformatics*, an interplay between Chemistry, Mathematics, Statistics and Information Science. In fact, one of the main reasons behind the significance of *Cheminformatics* is the interlacing of these core areas of science. *Graph Theory* attained exceptional place in *Mathematical Chemistry* and this novel branch got the name *Chemical graph theory* which became increasingly common among researchers and deals with molecular graph of a chemical compound to calculate various topological indices to understand and predict the physicochemical properties of chemical compounds [1]. During QSAR/ QSPR study, the regression analysis relies upon molecular descriptors and is responsible to understand and predict the chemical, biological and physical characteristics of compounds. This provides basis in designing new chemical compounds and drugs having features of our own interest.

In literature, numerous types of degree based, distance based as well as topological polynomials [2] related topo-

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logical indices of molecular graphs have been introduced and many of them turned out to be applicable in mathematical chemistry. For instance, among the most well-known and well read graph invariants are the Wiener index, Szeged index [3], the Randić indices, Zagreb indices [4, 5], atom-bond connectivity, geometric arithmetic and the Hosoya Z indices [6]. Although all above mentioned classes of indices have their own significance, however, degree based indices are well read and find real importance in chemical graph theory and therein biochemistry [7–11].

A graph $\Gamma(V, E)$ with vertex set V and edge set E is connected, if there exists a connection between any pair of vertices in Γ . A *network* is simply a connected graph having no multiple edges and loops. For a graph Γ , the degree of a vertex v is the number of edges incident with v and denoted by d_v .

Paul Manuel et al., [12] conjectured that the minimum metric dimension of hex-derived networks $HDN1(n)$ and $HDN2(n)$ lies between 3 and 5 and this open problem has partially been answered by Dacheng Xu and Jianxi Fan [13]. Furthermore, Imran et al., [14] discussed some topological properties such as atom-bond connectivity, geometric arithmetic and Randić indices of the network under discussion. We have studied and computed some new indices as well as recovered some indices presented in [15–19] by using entirely different and general approach.

In this article, throughout, Γ is considered to be connected, finite, undirected and simple network with $V(\Gamma) = \text{Vertex set}$, $E(\Gamma) = \text{Edge set}$ and $d_v = \text{degree of vertex}$ where $v \in V(\Gamma)$.

1.1 Preliminaries

Definition 1. Deutsch and Klavžar [20] introduced M-polynomial for graph $\Gamma = (V, E)$ as follows:

$$M(\Gamma; x, y) = f(x, y) = \sum_{i \leq j} m_{ij}(\Gamma) x^i y^j \quad (1)$$

where $m_{ij}(\Gamma)$ represent number of edges $uv \in E(\Gamma)$ such that $\{d_u(\Gamma), d_v(\Gamma)\} = \{i, j\}$.

Definition 2. The forgotten polynomial of Γ is given by:

$$F(\Gamma; x) = \sum_{uv \in E(\Gamma)} x^{[(d_u)^2 + (d_v)^2]} \quad (2)$$

In 1947, the idea of topological index was first conceived and originated by Harold Wiener [21] during the study on boiling point of paraffin (bi-product of petroleum) and he referred it as *path number* but afterward *path number* was

assigned the name of its inventor and entitled as *Wiener index/number* [22]. This pioneering, eminent and well studied index of chemical graph Γ is distance-based index. It deserves high rank in theoretical Chemistry and Chemical graph theory due to its theoretical as well as applicable nature. In 1975, Milan Randić [23] introduced a topological index with the name *branching index* and is defined as:

$$R_{-\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{d_u d_v}} \quad (3)$$

Randić observed and established the fact that there exists a relationship between Randić index and various properties (boiling point, enthalpy of formation, surface area) of alkanes.

Later on in 1998, two distinguished researchers, Böllöbás and Erdős [24], extended the idea to all real numbers and the new index received the name general Randić index and is defined below:

$$R_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{(d_u d_v)^\alpha} \quad (4)$$

Moreover, inverse Randić index is defined by formula,

$$RR_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} (d_u d_v)^\alpha \quad (5)$$

In 1972, Ivan Gutman and Trinajstić [25] proposed two topological indices named as the first and the second Zagreb indices and soon after, these indices were used to analyze the structure-dependency of total π - *electron* of molecular graph. First, second and modified Zagreb indices are defined as follows:

$$M_1(\Gamma) = \sum_{vw \in E} (d_v + d_w) \quad (6)$$

$$M_2(\Gamma) = \sum_{vw \in E} (d_v d_w) \quad (7)$$

$${}^m M_2(\Gamma) = \sum_{vw \in E} \frac{1}{(d_v d_w)} \quad (8)$$

Definition 1. Generalized Zagreb Index

The concept of generalized Zagreb index was established by Azari and Iranmanesh [26] and defined as

$$Z_{a,b}(\Gamma) = \sum_{uv \in E(\Gamma)} (d_u^a d_v^b + d_u^b d_v^a) \quad (9)$$

where $a, b \in \mathbb{Z}^+$. Few more topological indices of our interest having utmost importance are defined below which include harmonic index (HI), inverse sum index (ISI), augmented Zagreb index (AZI) [27] and forgotten index (FI):

$$HI(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2}{d_u + d_v} \quad (10)$$

$$ISI(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{d_u d_v}{d_u + d_v} \quad (11)$$

$$AZI(\Gamma) = \sum_{uv \in E(\Gamma)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3 \quad (12)$$

$$FI(\Gamma) = \sum_{uv \in E(\Gamma)} (d_u^2 + d_v^2) \quad (13)$$

1.2 Applications of Topological polynomials

Several topological polynomials were established in the literature and played vital role in mathematical chemistry. Among other graph polynomials like matching polynomial [28], the Zhang-Zhang polynomial (Clar covering polynomial) [29], the Schultz polynomial [30], the Tutte polynomial [31], the most significant polynomials are Hosoya polynomial [32] introduced in 1988 and *M-polynomial* established in 2015. We can efficiently determine exact formulae for various degree and distance-based topological indices with the help of *M-polynomial* and Hosoya polynomial, respectively. *M-polynomial* is the tool which conceals lot of facts regarding degree based graph invariants. Moreover, the *M-polynomial* provides a very good correlation for the stability of linear alkanes as well as the branched alkanes and for computing the strain energy of cyclo alkanes [33]. For a certain family of networks, we normally use different formula to calculate each individual topological index. *M-polynomial* got advantage over this approach as we only need to operate specific differential, integral or both operators on corresponding polynomial to get various vertex-based indices. Many closed form degree-based topological indices of Triangular Boron Nanotubes and Jahangir graph $J_{n,m}$ are computed using *M-polynomial* [34, 35]. The Zhang-Zhang polynomial (Clar covering polynomial), were found to occur for computation of the total π -electron energy of the molecules within specific approximate expressions. The Randic index is a topological descriptor that has correlated with a lot of chemical characteristics of the molecules and has been found to be parallel to compute the boiling point and Kovats constants of the molecules.

2 Materials and Methods

Our main results includes the formulation of algebraic structures of *M-polynomial* and *F-polynomial* of $HDN1(n)$ and $HDN2(n)$, respectively. Then, we computed as well as

recovered various topological indices of vital importance. In particular, first, second, modified and augmented Zagreb indices, general and inverse Randić indices, symmetric division, harmonic, inverse sum and forgotten indices of these networks via *topological polynomials*.

To compute our results, we used the method of combinatorial computing, vertex partition method, edge partition method, graph theoretical tools, analytic techniques, degree counting method, and sum of degrees of neighbor's method. Moreover, we used Maple for mathematical calculations, verifications, and plotting these mathematical results.

3 Main Results

3.1 Methodology and Construction of Hex-Derived Network $HDN1(n)$ Formulas

The construction of first kind of hex-derived network $HDN1(n)$ is fairly simple and is achieved by placing additional node in each triangular face of hexagonal mesh $HX(n)$ [36] and then joining this extra nodes with all nodes of triangular face. For an alternate version of construction of $HDN1(n)$ from $HX(n)$. There are $9n^2 - 15n + 7$ number of nodes (vertices) and $27n^2 - 51n + 24$ number of edges in $HDN1(n)$. This new network has many advantage over the one from which it is obtained, for instance, represent configuration similar to molecular lattice structures in chemistry. This network is also called mesh network and mostly used in networking of computers to minimize cost, to achieve high performance and reliability. Moreover, $HDN1(n)$ is planar and this property gets advantage over non-planar network as far as cost is concerned. Figure 1 depicts a hex-derived network of first kind with dimension 4.

For the sake of simplicity as well as with out loss of generality, we assume $HDN1(n) = \Gamma_1$. As we know total number of vertices of Γ_1 are given by $|V(\Gamma_1)| = 9n^2 - 15n + 7$ and total number of edges are $|E(\Gamma_1)| = 27n^2 - 51n + 24$. In Γ_1 , we observe eight categories of edges on the basis of degree of the vertices of each edge which lead to edge partition of graph and is depicted in the table below.

Now, using definition 1 and definition 2 to compute *M-Polynomial* and *Forgotten Polynomial*, respectively of Γ_1 as follows:

- ***M-Polynomial* of hex-derive network $HDN1(n)$**

Table 1: Formulae of some prominent topological descriptors depending on M-polynomial.

Topological Descriptors	Formulae based on M-polynomial
1st Zagreb index (M_1)	$(D_x + D_y)f(x, y)$
2nd Zagreb index (M_2)	$(D_x \cdot D_y)f(x, y)$
Modified 2nd Zagreb index (mM_2)	$(S_x \cdot S_y)f(x, y)$
General Randić index R_α	$D_x^\alpha \cdot D_y^\alpha f(x, y)$
Inverse Randić index RR_α	$S_x^\alpha \cdot S_y^\alpha f(x, y)$
Symmetric Division Index (SDD)	$(D_x S_y + S_x D_y)f(x, y)$
Harmonic Index (HI)	$2S_x Jf(x, y)$
Inverse sum Index (ISI)	$S_x J D_x D_y f(x, y)$
Augmented Zagreb Index (AG)	$S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)$
Forgotten Index (FI)	$D_x, [f(G; x)], x = 1$

where $D_x f = x \frac{\partial f}{\partial x}$, $D_y f = y \frac{\partial f}{\partial y}$, $S_x f = \int_0^x \frac{f(t, y)}{t} dt$, $S_y f = \int_0^y \frac{f(x, t)}{t} dt$, $J(f(x, y)) = f(x, x)$, $Q_\alpha f = x^\alpha f$.

Table 2: Vertex degree based edge partitioning of a graph Γ_1 .

(d_u, d_v)								
$uv \in E(\Gamma_1)$	(3,5)	(3,7)	(3,12)	(5,7)	(5,12)	(7,7)	(7,12)	(12,12)
Number of edges	12	$18n - 36$	$18n^2 - 54n + 42$	12	6	$6n - 18$	$12n - 24$	$9n^2 - 33n + 30$
Set of edges	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8

$$\begin{aligned}
M(\Gamma_1; x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\
&= \sum_{3 \leq 5} m_{35} x^3 y^5 + \sum_{3 \leq 7} m_{37} x^3 y^7 + \sum_{3 \leq 12} m_{312} x^3 y^{12} + \sum_{5 \leq 7} m_{57} x^5 y^7 \\
&+ \sum_{5 \leq 12} m_{512} x^5 y^{12} + \sum_{7 \leq 7} m_{77} x^7 y^7 + \sum_{7 \leq 12} m_{712} x^7 y^{12} + \sum_{12 \leq 12} m_{1212} x^{12} y^{12} \\
&= \sum_{uv \in E_1} m_{35} x^3 y^5 + \sum_{uv \in E_2} m_{37} x^3 y^7 + \sum_{uv \in E_3} m_{312} x^3 y^{12} + \sum_{uv \in E_4} m_{57} x^5 y^7 \\
&+ \sum_{uv \in E_5} m_{512} x^5 y^{12} + \sum_{uv \in E_6} m_{77} x^7 y^7 + \sum_{uv \in E_7} m_{712} x^7 y^{12} + \sum_{uv \in E_8} m_{1212} x^{12} y^{12} \\
&= |E_1| x^3 y^5 + |E_2| x^3 y^7 + |E_3| x^3 y^{12} + |E_4| x^5 y^7 \\
&+ |E_5| x^5 y^{12} + |E_6| x^7 y^7 + |E_7| x^7 y^{12} + |E_8| x^{12} y^{12} \\
&= 12x^3 y^5 + (18n - 36)x^3 y^7 + (18n^2 - 54n + 42)x^3 y^{12} + (6n - 18)x^7 y^7 \\
&+ 12x^5 y^7 + 6x^5 y^{12} + (12n - 24)x^7 y^{12} + (9n^2 - 33n + 30)x^{12} y^{12}
\end{aligned}$$

Following Figure 2 depicts graphs of *M-polynomial* of hex-derive network HDN1(4).

- **Forgotten Polynomial of hex-derive network HDN1(n)**

$$\begin{aligned}
F(\Gamma_1, x) &= \sum_{uv \in E(G)} x^{[(d_u)^2 + (d_v)^2]} \\
&= \sum_{uv \in E_1} m_{35} x^{34} + \sum_{uv \in E_2} m_{37} x^{58} + \sum_{uv \in E_3} m_{312} x^{153} + \sum_{uv \in E_4} m_{57} x^{74} \\
&+ \sum_{uv \in E_5} m_{512} x^{169} + \sum_{uv \in E_6} m_{77} x^{98} + \sum_{uv \in E_7} m_{712} x^{193} + \sum_{uv \in E_8} m_{1212} x^{288} \\
&= 12x^{34} + (18n - 36)x^{58} + (18n^2 - 54n + 42)x^{153} + 12x^{74} + 6x^{169} \\
&+ (6n - 18)x^{98} + (12n - 24)x^{193} + (9n^2 - 33n + 30)x^{288}
\end{aligned}$$

Following Figure 3 depicts graphs of *Forgotten polynomial* of hex-derive network HDN1(4).

- **Computing Topological Indices using *M-polynomial* and *Forgotten polynomial* for hex-derive network HDN1(n)**

Now we compute the topological indices for hex-derive network Γ_1 , namely first, second, modified and augmented Zagreb indices, Randić indices, SSD index, harmonic index, ISI index and forgotten index. By applying the operators given in derivation of Table 1 on *M-polynomial* and *Forgotten polynomials* as follows:

$$\begin{aligned}
(D_x + D_y)f(x, y) &= 10(18n - 36)x^3 y^7 + 15(18n^2 - 54n + 42)x^3 y^{12} + 96x^3 y^5 + 144x^5 y^7 + 102x^5 y^{12} \\
&+ 14(6n - 18)x^7 y^7 + 19(12n - 24)x^7 y^{12} + 24(9n^2 - 33n + 30)x^{12} y^{12} \\
D_x^\alpha D_y^\alpha f(x, y) &= 21^\alpha (18n - 36)x^3 y^7 + 36^\alpha (18n^2 - 54n + 42)x^3 y^{12} + 15^\alpha (12x^3 y^5) \\
&+ 35^\alpha (12x^5 y^7) + 60^\alpha (6x^5 y^{12}) + 84^\alpha (12n - 24)x^7 y^{12} \\
&+ 7^{2\alpha} (6n - 18)x^7 y^7 + 12^{2\alpha} (9n^2 - 33n + 30)x^{12} y^{12}
\end{aligned}$$

Figure 1: A 4-dimensional hex-derive network $HDN1(4)$

Figure 2: Graphical Representation of M-polynomial of hex-derive network $HDN1(n)$

$$\begin{aligned}
 S_x^\alpha S_y^\alpha f(x, y) &= \frac{1}{21^\alpha} (18n - 36)x^3y^7 + \frac{1}{36^\alpha} (18n^2 - 54n + 42)x^3y^{12} + \frac{12}{15^\alpha} x^3y^5 \\
 &+ \frac{12}{35^\alpha} x^5y^7 + \frac{6}{60^\alpha} x^5y^{12} + \frac{1}{72^\alpha} (6n - 18)x^7y^7 \\
 &+ \frac{1}{84^\alpha} (12n - 24)x^7y^{12} + \frac{1}{12^{2\alpha}} (9n^2 - 33n + 30)x^{12}y^{12}
 \end{aligned}$$

$$\begin{aligned}
 (S_y D_x + S_x D_y)f(x, y) &= \frac{58}{21} (18n - 36)x^3y^7 + \frac{17}{4} (18n^2 - 54n + 42)x^3y^{12} \\
 &+ \frac{888}{35} x^5y^7 + \frac{169}{10} x^5y^{12} + 2(6n - 18)x^7y^7 + \frac{193}{84} (12n - 24)x^7y^{12} \\
 &+ \frac{136}{5} x^3y^5 + 2(9n^2 - 33n + 30)x^{12}y^{12}
 \end{aligned}$$

$$\begin{aligned}
 Jf(x, y) = f(x, x) &= 12x^8 + (18n - 36)x^{10} + (18n^2 - 54n + 42)x^{15} \\
 &+ 12x^{12} + 6x^{17} + (6n - 18)x^{14} + (12n - 24)x^{19} + (9n^2 - 33n + 30)x^{24}
 \end{aligned}$$

Figure 3: Graphical Representation of Forgotten polynomial of hex-derive network $HDN1(n)$

$$S_x J D_x D_y f(x, y) = \frac{45}{2} x^8 + \frac{1}{5} (18n - 36) x^{10} + \frac{12}{5} (18n^2 - 54n + 42) x^{15} \\ + 35x^{12} + \frac{360}{17} x^{17} + \frac{7}{2} (6n - 18) x^{14} + \frac{84}{19} (12n - 24) x^{19} + 6(9n^2 - 33n + 30) x^{24}$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y) = \frac{375}{2} x^6 + \frac{46656}{2197} (18n^2 - 54n + 42) x^{13} \\ + \frac{9261}{512} (18n - 36) x^8 + \frac{1029}{2} x^{10} + 384x^{15} + \frac{117649}{1728} (6n - 18) x^{12} \\ + \frac{592704}{4913} (12n - 24) x^{17} + \frac{373248}{1331} (9n^2 - 33n + 30) x^{22}$$

Again using derivation formulae of topological indices over M -polynomial from Table 1, we get

$$\begin{aligned} \text{FirtsZagrebIndex} = M_1(\Gamma_1) &= (D_x + D_y)f(x, y)|_{x=y=1} \\ &= 486n^2 - 1110n + 624, \end{aligned}$$

$$\begin{aligned} \text{SecondZagrebIndex} = M_2(\Gamma_1) &= D_y D_x f(x, y)|_{x=y=1} \\ &= 1944n^2 - 5016n - 750 \end{aligned}$$

$$\begin{aligned} \text{ModifiedZagrebIndex} = {}^m M_2(\Gamma_1) &= S_x S_y f(x, y)|_{x=y=1} \\ &= \frac{9}{16} n^2 - \frac{7475}{2352} n + \frac{491}{1960} \end{aligned}$$

$$\begin{aligned} \text{Generalized Randić Index} = R_\alpha(\Gamma_1) &= D_x^\alpha D_y^\alpha f(x, y)|_{x=y=1} \\ &= 12(15^\alpha + 35^\alpha) + 6(60^\alpha) + 21^\alpha(18n - 36) \\ &\quad + 36^\alpha(18n^2 - 54n + 42) + 7^{2\alpha}(6n - 18) \\ &\quad + 84^\alpha(12n - 24) + 12^{2\alpha}(9n^2 - 33n + 30) \end{aligned}$$

$$\begin{aligned}
\text{Inverse Randić Index} = RR_\alpha(\Gamma_1) &= S_x^\alpha S_y^\alpha f(x, y)|_{x=y=1} \\
&= 12(15^{-\alpha} + 35^{-\alpha}) + 6(60^{-\alpha}) + 36^{-\alpha}(18n^2 - 54n + 42) \\
&\quad + 21^{-\alpha}(18n - 36) + 7^{-2\alpha}(6n - 18) + 84^{-\alpha}(12n - 24) \\
&\quad + 12^{-2\alpha}(9n^2 - 33n + 30) \\
\text{Symmetric Division Index} = SSD(\Gamma_1) &= (D_x S_y + S_x D_y) f(x, y)|_{x=y=1} \\
&= \frac{189}{2}n^2 - \frac{2887}{14}n + \frac{587}{5} \\
\text{Harmonic Index} = HI(\Gamma_1) &= 2S_x J f(x, x)|_{x=1} \\
&= \frac{63}{20}n^2 - \frac{11251}{2660}n + \frac{34099}{22610} \\
\text{Inverse Sum Index} = ISI(\Gamma_1) &= S_x J D_x D_y f(x, y)|_{x=y=1} \\
&= \frac{486}{5}n^2 - \frac{648}{323}n + \frac{627043}{3230} \\
\text{Augmented Zagreb Index} = AZI(\Gamma_1) &= S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)|_{x=y=1} \\
&= 2906n^2 - 8219n + 5619 \\
\text{Forgotten Index} = F(\Gamma_1) &= D_x F(\Gamma_1, x)|_{x=1} = 5346n^2 - 13818n + 8892.
\end{aligned}$$

3.2 Methodology and Construction of Hex-Derived Network $HDN2(n)$ Formulas

The architecture of second kind of hex-derived network $HDN2(n)$ is bit sophisticated as it is obtained from the merger of hexagonal network $HX(n)$ of dimension n with honeycomb network $HC(n-1)$ of dimension $n-1$. The construction of $HDN2(n)$ can be accomplished by taking union of $HX(n)$ with its bounded dual $HC(n-1)$ and then by joining each honeycomb vertex with the three vertices of the corresponding face of $HX(n)$. There are $9n^2 - 15n + 7$ number of nodes (vertices) and $36n^2 - 72n + 36$ number of edges in $HDN2(n)$. Figure 4 depicts a hex-derived network of second kind with dimension 4.

Again for the sake of simplicity, suppose $HDN2(n) = \Gamma_2$. We know total number of vertices of Γ_2 are given by $|V(\Gamma_2)| = 9n^2 - 15n + 7$ and total number of edges are $|E(\Gamma_2)| = 36n^2 - 72n + 36$. In Γ_2 , we observe eight categories of edges on the basis of degree of the vertices of each edge which lead to edge partition of graph and is depicted in the table below. Now, using definition 1 and definition 2 to compute M -Polynomial and *Forgotten Polynomial*, respectively

Table 3: Vertex degree based edge partitioning of a graph Γ_2 .

$(d_u, d_v) : uv \in E(\Gamma_2)$	Number of edges	Sets	$(d_u, d_v) : uv \in E(\Gamma_2)$	Number of edges	Sets
(5,5)	18	E_1	(6,7)	$6(n-2)$	E_6
(5,6)	$12(n-2)$	E_2	(6,12)	$6(3n^2 - 10n + 8)$	E_7
(5,7)	$12(n-1)$	E_3	(7,7)	$6(n-3)$	E_8
(5,12)	$6n$	E_4	(7,12)	$12(n-2)$	E_9
(6,6)	$3(3n^2 - 11n + 10)$	E_5	(12,12)	$3(3n^2 - 11n + 10)$	E_{10}

of Γ_2 as follows:

Figure 4: A 4-dimensional hex-derive network $HDN2(4)$

• ***M*-Polynomial of hex-derive network $HDN2(n)$**

$$\begin{aligned}
 M(\Gamma_2; x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\
 &= \sum_{5 \leq 5} m_{55} x^5 y^5 + \sum_{5 \leq 6} m_{56} x^5 y^6 + \sum_{5 \leq 7} m_{57} x^5 y^7 + \sum_{5 \leq 12} m_{512} x^5 y^{12} \\
 &+ \sum_{6 \leq 6} m_{66} x^6 y^6 + \sum_{6 \leq 7} m_{67} x^6 y^7 + \sum_{6 \leq 12} m_{612} x^6 y^{12} + \sum_{7 \leq 7} m_{77} x^7 y^7 \\
 &+ \sum_{7 \leq 12} m_{712} x^7 y^{12} + \sum_{12 \leq 12} m_{1212} x^{12} y^{12}
 \end{aligned}$$

$$\begin{aligned}
 M(\Gamma_2; x, y) &= \sum_{uv \in E_1} m_{55} x^5 y^5 + \sum_{uv \in E_2} m_{56} x^5 y^6 + \sum_{uv \in E_3} m_{57} x^5 y^7 + \sum_{uv \in E_4} m_{512} x^5 y^{12} \\
 &+ \sum_{uv \in E_5} m_{66} x^6 y^6 + \sum_{uv \in E_6} m_{67} x^6 y^7 + \sum_{uv \in E_7} m_{612} x^6 y^{12} + \sum_{uv \in E_8} m_{77} x^7 y^7 \\
 &+ \sum_{uv \in E_9} m_{712} x^7 y^{12} + \sum_{uv \in E_{10}} m_{1212} x^{12} y^{12} \\
 &= |E_1| x^5 y^5 + |E_2| x^5 y^6 + |E_3| x^5 y^7 + |E_4| x^5 y^{12} + |E_5| x^6 y^6 \\
 &+ |E_6| x^6 y^7 + |E_7| x^6 y^{12} + |E_8| x^7 y^7 + |E_9| x^7 y^{12} + |E_{10}| x^{12} y^{12} \\
 &= 18x^5 y^5 + 12(n-2)x^5 y^6 + 12(n-1)x^5 y^7 + 3(3n^2 \\
 &- 11n + 10)x^6 y^6 + 6nx^5 y^{12} + 6(n-2)x^6 y^7 + 6(3n^2 - 10n + 8)x^6 y^{12} \\
 &+ 6(n-3)x^7 y^7 + 12(n-2)x^7 y^{12} + 3(3n^2 - 11n + 10)x^{12} y^{12}
 \end{aligned}$$

Following Figure 5 depicts graphs of *M*-polynomial of hex-derive network $HDN2(4)$.

Figure 5: Graphical Representation of M-polynomial of hex-derive network $HDN2(n)$

• **Forgotten Polynomial of hex-derive network $HDN2(n)$**

$$\begin{aligned}
 F(\Gamma_2, x) &= \sum_{uv \in E(G)} x^{[(d_u)^2 + (d_v)^2]} \\
 &= \sum_{uv \in E_1} m_{55} x^{50} + \sum_{uv \in E_2} m_{56} x^{61} + \sum_{uv \in E_3} m_{57} x^{74} + \sum_{uv \in E_4} m_{512} x^{169} + \sum_{uv \in E_5} m_{66} x^{72} \\
 &\quad + \sum_{uv \in E_6} m_{67} x^{85} + \sum_{uv \in E_7} m_{612} x^{180} + \sum_{uv \in E_8} m_{77} x^{98} + \sum_{uv \in E_9} m_{712} x^{193} + \sum_{uv \in E_{10}} m_{1212} x^{288} \\
 &= 18x^{50} + 12(n-2)x^{61} + 12(n-1)x^{74} + 6nx^{169} + 3(3n^2 - 11n + 10)x^{72} \\
 &\quad + 6(n-2)x^{85} + 6(3n^2 - 10n + 8)x^{180} + 6(n-3)x^{98} \\
 &\quad + 12(n-2)x^{193} + 3(3n^2 - 11n + 10)x^{288}
 \end{aligned}$$

Following Figure 6 depicts graphs of *Forgotten polynomial* of hex-derive network $HDN2(4)$.

• **Computing Topological Indices using M-polynomial and Forgotten polynomial for hex-derive network $HDN2(n)$**

Now we compute the topological indices for hex-derive network Γ_2 , namely first, second, modified and augmented Zagreb indices, Randić indices, SSD index, harmonic index, ISI index and forgotten index. By applying the operators given in derivation of Table 1 on *M-polynomial* and *Forgotten polynomials* as follows:

$$\begin{aligned}
 M(\Gamma_2; x, y) &= f(x, y) \\
 &= 12x^3y^5 + (18n-36)x^3y^7 + (18n^2-54n+42)x^3y^{12} \\
 &\quad + 12x^5y^7 + 6x^5y^{12} + (6n-18)x^7y^7 + (12n-24)x^7y^{12} \\
 &\quad + (9n^2-33n+30)x^{12}y^{12}
 \end{aligned}$$

Figure 6: Graphical Representation of Forgotten polynomial of hex-derive network $HDN2(n)$

$$\begin{aligned}
 (D_x + D_y)f(x, y) &= 180x^5y^5 + 132(n-2)x^5y^6 + 144(n-1)x^5y^7 + 102nx^5y^{12} \\
 &+ 36(3n^2 - 11n + 10)x^6y^6 + 78(n-2)x^6y^7 + 108(3n^2 - 10n + 8)x^6y^{12} \\
 &+ 84(n-2)x^7y^{12} + 228(n-2)x^7y^{12} + 72(3n^2 - 11n + 10)x^{12}y^{12}
 \end{aligned}$$

$$\begin{aligned}
 D_x^\alpha D_y^\alpha f(x, y) &= 18(5^{2\alpha})x^5y^5 + 30^\alpha(12n-24)x^5y^6 + 35^\alpha(12n-12)x^5y^7 \\
 &+ 60^\alpha(6nx^5y^{12}) + 42^\alpha(6n-12)x^6y^7 + 6^{2\alpha}(9n^2-33n+30)x^6y^6 \\
 &+ 6^{1+\alpha}12^\alpha(3n^2-10n+8)x^6y^{12} + 7^{2\alpha}(6n-18)x^7y^7 + 12^{1+\alpha}7^\alpha(n-2)x^7y^{12} \\
 &+ 3 \cdot 12^{2\alpha}(3n^2-11n+10)x^{12}y^{12}
 \end{aligned}$$

$$\begin{aligned}
 S_x^\alpha S_y^\alpha f(x, y) &= \left(\frac{1}{6^{2\alpha}} + \frac{x^6y^6}{12^{2\alpha}}\right)(9n^2-33n+30)x^6y^6 + \frac{1}{72^\alpha}(18n^2-60n+48)x^6y^{12} \\
 &+ \frac{1}{35^\alpha}(12n-12)x^5y^7 + \left(\frac{2}{30^\alpha} + \frac{xy}{42^\alpha} + \frac{2x^6y^6}{84^\alpha}\right)(6n-12)x^5y^6 + \frac{18}{5^{2\alpha}}x^5y^5 \\
 &+ \frac{6n}{60^\alpha}x^5y^{12} + 7^{-2\alpha}(6n-18)x^7y^7
 \end{aligned}$$

$$\begin{aligned}
 Jf = f(x, x) &= 18x^{10} + 12(n-2)x^{11} + 12(n-1)x^{12} + 6nx^{17} + 6(n-3)x^{14} \\
 &+ 3(3n^2-11n+10)x^{12} + 6(n-2)x^{13} + 6(3n^2-10n+8)x^{18} \\
 &+ 12(n-2)x^{19} + 3(3n^2-11n+10)x^{24}
 \end{aligned}$$

$$\begin{aligned}
 S_x J D_x D_y f(x, y) &= 45x^{10} + \frac{30}{11}(n-2)x^{11} + 35(n-1)x^{12} \\
 &+ (27n^2-99n+90)x^{12}(1+2x^{12}) + \frac{252}{13}(n-2)x^{13} + \frac{360}{17}nx^{17} \\
 &+ 24(3n^2-10n+8)x^{18} + 21(n-3)x^{14} + \frac{1008}{19}(n-2)x^{19}
 \end{aligned}$$

$$\begin{aligned}
S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y) &= \frac{140625}{256} x^8 + \left(\frac{4000}{9} + \frac{444528x^2}{1331} + \frac{7112448x^8}{4913} \right) (n-2)x^9 \\
&+ \frac{1029}{2} x^{10} + \left(\frac{17496}{125} + \frac{4478976x^{12}}{5324} \right) (3n^2 - 11n + 10)x^{10} \\
&+ \frac{117649}{288} (n-3)x^{12} + 384nx^{15} + \frac{2187}{4} (3n^2 - 10n + 8)x^{16}.
\end{aligned}$$

Again using derivation formulae of topological indices over *M-polynomial* from table 1, we get

$$\begin{aligned}
\text{First Zagreb Index} = M_1(\Gamma_2) &= (D_x + D_y)f(x, y)|_{x=y=1} \\
&= 648n^2 - 1500n + 852, \\
\text{Secondnd Zagreb Index} = M_2(\Gamma_2) &= D_y D_x f(x, y)|_{x=y=1} \\
&= 2916n^2 - 7566n + 4764, \\
\text{Modified Zagreb Index} = {}^m M_2(\Gamma_2) &= S_x S_y f(x, y)|_{x=y=1} \\
&= \frac{9}{16} n^2 - \frac{8563}{11760} n + \frac{30597}{88200} \\
\text{Generalized Randić Index} = R_\alpha(\Gamma_2) &= D_x^\alpha D_y^\alpha f(x, y)|_{x=y=1} \\
&= 6^{2\alpha} (1 + 4^\alpha) (9n^2 - 33n + 30) + 6^\alpha (2 \cdot 5^\alpha + 60^\alpha) (6n) \\
&+ (6^{1+2\alpha} \cdot 2^\alpha) (3n^2 - 10n + 8) + 7^\alpha + 2^{1+\alpha} (6n - 12) \\
&+ 35^\alpha (12n - 12) + 7^{2\alpha} (6n - 18) + 18(5^{2\alpha}) \\
\text{Inverse Randić Index} = RR_\alpha(\Gamma_2) &= S_x^\alpha S_y^\alpha f(x, y)|_{x=y=1} \\
&= 12(15^{-\alpha} + 35^{-\alpha}) + 6(60^{-\alpha}) + 21^{-\alpha} (18n - 36) \\
&+ 7^{-2\alpha} (6n - 18) + 84^{-\alpha} (12n - 24) + 12^{-2\alpha} (9n^2 - 33n + 30) \\
&+ 36^{-\alpha} (18n^2 - 54n + 42) \\
\text{Symmetric Division Index} = SSD(\Gamma_2) &= (D_x S_y + S_x D_y)f(x, y)|_{x=y=1} \\
&= 81n^2 - \frac{11453}{70} n + \frac{432}{5} \\
\text{Harmonic Index} = HI(\Gamma_2) &= 2S_x f(x, x)|_{x=1} \\
&= \frac{17}{4} n^2 - \frac{27103217}{3879876} n + \frac{15629}{5000} \\
\text{Inverse Sum Index} = ISI(\Gamma_2) &= S_x J D_x D_y f(x, y)|_{x=y=1} \\
&= 153n^2 - 385n - 101 \\
\text{Augmented Zagreb Index} = AZI(\Gamma_2) &= S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)|_{x=y=1} \\
&= 4584n^2 - 13243n + 9573 \\
\text{Forgotten Index} &= F(\Gamma_2) = D_x F(\Gamma_2, x)|_{x=1} = 3346n^2 - 23818n + 7892.
\end{aligned}$$

4 Comparisons and Discussion

In this section, we have computed all indices for different values of n for both structures $HDN1(n)$ and $HDN2(n)$. In addition, we construct Tables 4 and 5 for small values of n for these topological indices to the structure $HDN1(n)$ and $HDN2(n)$ respectively. Now, from Tables 4 and 5, we can easily see that all indices are in increasing order as the values of n are increases. In addition, on the other hand, indices showed higher values for $HDN2(n)$ as compared to those of $HDN1(n)$.

Table 4: Comparison of all indices for $HDN1(n)$.

n	M_1	M_2	M_2^m	R_α	$R_{\alpha\alpha}$	SSD	HI	ISI	AZI	FI
1	0	-3822	1.4	48.2	56.3	96.8	4.5	98.6	306	420
2	348	-3006	3.4	512.4	617.8	415.6	8.3	187.2	805	2640
3	1668	1698	6.3	1021.1	1108.4	918.2	13.6	415.3	7116	15552
4	3960	10290	9.7	1826.3	1936.5	1562.4	18.2	916.4	19239	39156
5	7224	22770	12.8	2445.1	2916.4	2113.5	25.6	1023.6	37174	73452

Table 5: Comparison of all indices for $HDN2(n)$.

n	M_1	M_2	M_2^m	R_α	$R_{\alpha\alpha}$	SSD	HI	ISI	AZI	FI
1	0	114	3.4	54.3	51.4	99.2	6.6	102	914	445
2	444	1296	5.4	615.6	827.8	635.4	9.6	235	1423	2740
3	2184	8310	9.3	1321.9	1508.2	1102.3	16.5	615	11100	16552
4	5220	21156	13.7	1926.5	2136.4	1862.3	21.3	1002	29945	40156
5	9552	39834	16.8	2645.2	3216.3	2313.6	29.3	1124	57959	75452

Now, we presented the comparison of all topological indices using Table 4, for $HDN1(n)$ in Figure 7 and using Table 5, for $HDN2(n)$ in Figure 8.

Figure 7: The comparison of all topological indices for $HDN1(n)$.

5 Conclusions

In this paper, we provide M-polynomials of two interesting networks $HDN1(n)$ and $HDN2(n)$. In addition, we offer closed form formulae of several degree-based topological indices of vital importance such as first, second, modified and augmented Zagreb indices, general and inverse Randić indices, SSD, HI, ISI and forgotten index of $HDN1(n)$ and $HDN2(n)$ are computed and recovered using topological polynomials attained in previous step.

Since the Randić index is a topological descriptor that has correlated with a lot of chemical characteristics of the molecules. Thus, it has been found that the boiling point of $HDN1(n)$ and $HDN2(n)$ is varying in increasing order for $\alpha \in \{1, -1, 1/2, -1/2\}$.

Since the SSD index and HI index provides a very good correlation for computing the strain energy of molecules, one can easily be seen that the strain energy of $HDN1(n)$ and $HDN2(n)$ is high as the values of n increases.

Figure 8: The comparison of all topological indices for $HDN2(n)$.

In addition, ISI index and forgotten index has much better predictive power than the predictive power of the Randić index, so the ISI index and forgotten index is more useful than the Randić index for $\alpha \in \{-1, -1/2\}$ as compared to the Randić index for $\alpha \in \{1, 1/2\}$ in the case of $HDN1(n)$ and $HDN2(n)$.

Since the first and second Zagreb indexes were found to occur for computation of the total π -electron energy of the molecules, in the case of $HDN1(n)$ and $HDN2(n)$, their values provide total π -electron energy in increasing order for higher values of n .

For future work we propose investigation of some new type of chemical graphs and networks to compute certain degree based topological indices using polynomials.

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