Abstract: A numeric quantity that comprehend characteristics of molecular graph $\Gamma$ of chemical compound is known as topological index. This number is, in fact, invariant with respect to symmetry properties of molecular graph $\Gamma$. Many researchers have established, after diverse studies, a parallel between the physicochemical 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

MSC: 5C12, 05C90

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 utilisations 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-
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 \( \Gamma \). A network is simply a connected graph having no multiple edges and loops. For a graph \( \Gamma \), 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, \( \Gamma \) is considered to be connected, finite, undirected and simple network with \( V(\Gamma) = \text{Vertext set, } E(\Gamma) = \text{Edge set and } d_v = \text{degree of vertex where } v \in V(\Gamma) \).

1.1 Preliminaries

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

\[
M(\Gamma; x, y) = f(x, y) = \sum_{ij} m_{ij}(\Gamma)x^i y^j
\]

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 \( \Gamma \) is given by:

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

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 \( \Gamma \) 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:

\[
R_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{d_u d_v}} \tag{3}
\]

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, Böllbás and Erdős [24], extended the idea to all real numbers and the new index received the name random Randić index and is defined below:

\[
R_a(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{(d_u d_v)^a} \tag{4}
\]

Moreover, inverse Randić index is defined by formula,

\[
RR_a(\Gamma) = \sum_{uv \in E(\Gamma)} (d_u d_v)^a \tag{5}
\]

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 \( \pi \)– electron of molecular graph. First, second and modified Zagreb indices are defined as follows:

\[
M_1(\Gamma) = \sum_{uv \in E} (d_u + d_v) \tag{6}
\]

\[
M_2(\Gamma) = \sum_{uv \in E} (d_u d_v) \tag{7}
\]

\[
^\ast M_2(\Gamma) = \sum_{uv \in E} \frac{1}{d_u d_v} \tag{8}
\]

**Definition 1. Generalized Zagreb Index**

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

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

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):

\[
HI(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2}{d_u d_v} \tag{10}
\]
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 be useful for computing the total $\pi$-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 Ko- vats 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 $\Gamma_1$ are given by $|V(\Gamma_1)| = 9n^2 - 15n + 7$ and total number of edges are $|E(\Gamma_1)| = 27n^2 - 51n + 24$. In $\Gamma_1$, 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 $\Gamma_1$ as follows:

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

\[
\begin{align*}
\text{ISI}(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{d_u d_v}{d_{uv}} \\
\text{AZI}(\Gamma) &= \sum_{uv \in E(\Gamma)} \left( \frac{d_u d_v}{d_{uv}} \right)^3 \\
\text{FI}(\Gamma) &= \sum_{uv \in E(\Gamma)} \left( d_u^2 + d_v^2 \right)
\end{align*}
\]
### 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 ($M_2$) | $(D_xD_y)f(x, y)$             |
| Modified 2nd Zagreb index ($^mM_2$) | $(S_xS_y)f(x, y)$         |
| General Randić index $R_\alpha$ | $D_\alpha^xD_\alpha^yf(x, y)$ |
| Inverse Randić index $RR_\alpha$ | $S_\alpha^xS_\alpha^yf(x, y)$ |
| Symmetric Division Index (SDD) | $(D_xS_y + S_xD_y)f(x, y)$ |
| Harmonic Index (HI) | $2S_xf(x, y)$ |
| Inverse sum Index (ISI) | $S_xJf(x, y)$ |
| Augmented Zagreb Index (AG) | $S_\alpha^Q_\alpha^1D_\alpha^xf(x, y)$ |
| Forgotten Index (FI) | $D_x[f(G;x)], x = 1$ |

where $D_xf = x\frac{df}{dx}$, $D_yf = y\frac{df}{dy}$, $S_xf = \int_0^x \frac{f(t,y)}{t}dt$, $S_yf = \int_0^y \frac{f(x,t)}{t}dt$, $Jf(x, y) = f(x, x)$, $Q_\alpha f = x^\alpha f$.

### Table 2: Vertex degree based edge partitioning of a graph $\Gamma_1$.

| $(d_u, d_v)$ | $(3,5)$ | $(3,7)$ | $(3,12)$ | $(5,7)$ | $(5,12)$ | $(7,7)$ | $(7,12)$ | $(12,12)$ |
|-------------|---------|---------|---------|---------|---------|---------|---------|---------|
| $uv \in E(\Gamma_1)$ |         |         |         |         |         |         |         |         |
| Number of edges | 12      | $18n-36$ | $18n^2 - 54n + 42$ | 12      | 6       | $6n-18$ | $12n-24$ | $9n^2 - 33n + 30$ |
| Set of edges   | $E_1$   | $E_2$   | $E_3$   | $E_4$   | $E_5$   | $E_6$   | $E_7$   | $E_8$   |
Following Figure 2 depicts graphs of $M$-polynomial of hex-derive network $HDN1(4)$.

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

\[
F(\Gamma_1, x) = \sum_{uv \in E(G)} x^{[(d_u)^2+(d_v)^2]}
\]

\[
= \sum_{uv \in E_1} m_{35}x^{34} + \sum_{uv \in E_2} m_{37}x^{58} + \sum_{uv \in E_3} m_{312}x^{153} + \sum_{uv \in E_4} m_{57}x^{74}
\]

\[
+ \sum_{uv \in E_5} m_{512}x^{169} + \sum_{uv \in E_6} m_{77}x^{98} + \sum_{uv \in E_7} m_{712}x^{193} + \sum_{uv \in E_8} m_{1212}x^{288}
\]

\[
= 12x^{34} + (18n - 36)x^{58} + (18n^2 - 54n + 42)x^{153} + 12x^{74} + 6x^{169}
\]

\[
+ (6n - 18)x^{98} + (12n - 24)x^{193} + (9n^2 - 33n + 30)x^{288}
\]

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 $\Gamma_1$, 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:

\[
(D_4 + D_y)f(x, y) = 10(18n - 36)x^3y^7 + 15(18n^2 - 54n + 42)x^3y^{12} + 96x^3y^5 + 144x^5y^7 + 102x^5y^{12}
\]

\[
+ 14(6n - 18)x^7y^7 + 19(12n - 24)x^7y^{12} + 24(9n^2 - 33n + 30)x^{12}y^{12}
\]

\[
D^a_4D^b_yf(x, y) = 21^a(18n - 36)x^3y^7 + 36^a(18n^2 - 54n + 42)x^3y^{12} + 15^a(12x^3y^5)
\]

\[
+ 35^a(12x^5y^7) + 60^a(6x^5y^{12}) + 84^a(12n - 24)x^7y^{12}
\]

\[
+ 7^a(6n - 18)x^7y^7 + 12^a(9n^2 - 33n + 30)x^{12}y^{12}
\]
Figure 1: A 4-dimensional hex-derive network $HDN_1(4)$

Figure 2: Graphical Representation of M-polynomial of hex-derive network $HDN_1(n)$

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

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

\[
Jf(x, y) = f(x, x) = 12x^8 + (18n - 36)x^{10} + (18n^2 - 54n + 42)x^{15} \\
+ 12x^{12} + 6x^{17} + (6n - 18)x^{14} + (12n - 24)x^{19} + (9n^2 - 33n + 30)x^{24}
\]
Figure 3: Graphical Representation of Forgotten polynomial of hex-derive network $HDN1(n)$

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

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

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

**First Zagreb Index** $M_1(\Gamma)$  

\[
= (D_x + D_y)f(x,y)|_{x=y=1}
= 486n^2 - 1110n + 624,
\]

**Second Zagreb Index** $M_2(\Gamma)$  

\[
= D_yJf(x,y)|_{x=y=1}
= 1944n^2 - 5016n - 750
\]

**Modified Zagreb Index** $^mM_2(\Gamma)$  

\[
= S_xS_yf(x,y)|_{x=y=1}
= \frac{9}{16}n^2 - \frac{7475}{2352}n + \frac{491}{1960}
\]

**Generalized Randić Index** $R_\alpha(\Gamma)$  

\[
= D_x^\alpha D_y^\alpha f(x,y)|_{x=y=1}
= 12(15^n + 35^n) + 6(60^n) + 21^n(18n - 36)
+ 36^n(18n^2 - 54n + 42) + 7^n(6n - 18)
+ 84^n(12n - 24) + 12^n(9n^2 - 33n + 30)
\]
Inverse Randić Index = \( RR_a(\Gamma_1) = S_y^a S_y^a f(x, y)|_{x=y=1} \)
\[= 12(15^{-a} + 35^{-a}) + 6(60^{-a}) + 36^{-a}(18n^2 - 54n + 42) \]
\[+ 21^{-a}(18n - 36) + 7^{-2a}(6n - 18) + 84^{-a}(12n - 24) \]
\[+ 12^{-2a}(9n^2 - 33n + 30) \]

Symmetric Division Index = SSD(\(\Gamma_1\))
\[= (D_x S_y + S_x D_y)f(x, y)|_{x=y=1} \]
\[= \frac{189}{2} n^2 - \frac{2887}{14} n + \frac{587}{5} \]

Harmonic Index = HI(\(\Gamma_1\))
\[= 2S_y f(x, x)|_{x=1} \]
\[= \frac{63}{20} n^2 - \frac{11251}{2660} n + \frac{34099}{22610} \]

Inverse Sum Index = ISI(\(\Gamma_1\))
\[= S_x D_x D_y f(x, y)|_{x=y=1} \]
\[= \frac{486}{5} n^2 - \frac{648}{325} n + \frac{627043}{3230} \]

Augmented Zagreb Index = AZI(\(\Gamma_1\))
\[= S_y^3 Q_{-2} J D_y^3 f(x, y)|_{x=y=1} \]
\[= 2906n^2 - 8219n + 5619 \]

Forgotten Index = F(\(\Gamma_1\))
\[= D_x F(\Gamma_1, x)|_{x=1} = 5346n^2 - 13818n + 8892. \]

### 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 \(\Gamma_2\) are given by \(|V(\Gamma_2)| = 9n^2 - 15n + 7\) and total number of edges are \(|E(\Gamma_2)| = 36n^2 - 72n + 36\). In \(\Gamma_2\), 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 \(\Gamma_2\).

| \((d_u, d_v) : uv \in E(\Gamma_2)\) | 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)          | 6\(n\)         | \(E_4\) | (7,12)          | 12\((n-2)\)   | \(E_9\) |
| (6,6)           | 3\((3n^2 - 11n + 10)\) | \(E_5\) | (12,12)         | 3\((3n^2 - 11n + 10)\) | \(E_{10}\) |
• **M-Polynomial of hex-derive network** HDN2(n)

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

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 $HDN2(n)$**

$$F(\Gamma_2, x) = \sum_{uv \in E(G)} x^{(d_u) + (d_v)}$$

$$= \sum_{uv \in E_1} m_{55}x^{50} + \sum_{uv \in E_2} m_{56}x^{61} + \sum_{uv \in E_3} m_{57}x^{74} + \sum_{uv \in E_4} m_{512}x^{169} + \sum_{uv \in E_5} m_{66}x^{72}$$

$$+ \sum_{uv \in E_6} m_{67}x^{85} + \sum_{uv \in E_7} m_{612}x^{180} + \sum_{uv \in E_8} m_{77}x^{98} + \sum_{uv \in E_9} m_{712}x^{193} + \sum_{uv \in E_{10}} m_{1212}x^{288}$$

$$= 18x^{50} + 12(n - 2)x^{61} + 12(n - 1)x^{74} + 6nx^{169} + 3(3n^2 - 11n + 10)x^{72}$$

$$+ 6(n - 2)x^{85} + 6(3n^2 - 10n + 8)x^{180} + 6(n - 3)x^{98}$$

$$+ 12(n - 2)x^{193} + 3(3n^2 - 11n + 10)x^{288}$$

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

- **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 $\Gamma_2$, 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:

$$M(\Gamma_2; x, y) = f(x, y)$$

$$= 12x^3y^5 + (18n - 36)x^3y^7 + (18n^2 - 54n + 42)x^3y^{12}$$

$$+ 12x^7y^7 + 6x^7y^{12} + (6n - 18)x^7y^7 + (12n - 24)x^7y^{12}$$

$$+ (9n^2 - 33n + 30)x^{12}y^{12}$$
\[ (D_x + D_y)f(x, y) = 180x^5y^5 + 132(n - 2)x^5y^6 + 144(n - 1)x^5y^7 + 102nx^5y^{12} 
+ 36(3n^2 - 11n + 10)x^6y^6 + 78(n - 2)x^6y^7 + 108(3n^2 - 10n + 8)x^6y^{12} 
+ 84(n - 2)x^7y^{12} + 228(n - 2)x^7y^{12} + 72(3n^2 - 11n + 10)x^{12}y^{12} \]

\[ D_x^6 D_y^6 f(x, y) = 18(2a)^6x^5y^5 + 30a(12n - 24)x^5y^6 + 35a(12n - 12)x^5y^7 
+ 60a(6nx^5y^{12}) + 42a(6n - 12)x^6y^7 + 6^{2a}(9n^2 - 33n + 30)x^6y^6 
+ 6^{1+a}12a(3n^2 - 10n + 8)x^6y^{12} + 7^2a(6n - 18)x^7y^7 + 12^{1+a}7^a(n - 2)x^7y^{12} 
+ 3.12^{2a}(3n^2 - 11n + 10)x^{12}y^{12} \]

\[ S_x^a S_y^a f(x, y) = \left( \frac{1}{6\pi a} + \frac{x^6y^6}{12\pi a} \right)(9n^2 - 33n + 30)x^6y^6 + \frac{1}{72a}(18n^2 - 60n + 48)x^6y^{12} 
+ \frac{1}{35a}(12n - 12)x^5y^7 + \left( \frac{2}{30a} + \frac{xy}{42a} + \frac{2x^6y^6}{84a} \right)(6n - 12)x^7y^6 + \frac{18}{52a}x^7y^5 
+ \frac{6n}{60a}x^5y^{12} + 7^{-2a}(6n - 18)x^7y^7 \]

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

\[ S_x J D_x D_y f(x, y) = 45x^{10} + \frac{30}{11}(n - 2)x^{11} + 35(n - 1)x^{12} 
+ \left( 27n^2 - 99n + 90 \right)x^{12}(1 + 2x^{12}) + \frac{252}{13}(n - 2)x^{13} + \frac{360}{17}nx^{17} 
+ 24(3n^2 - 10n + 8)x^{18} + 21(n - 3)x^{14} + \frac{1008}{19}(n - 2)x^{19} \]
\[
S^2_1 Q_{-2} J D^2_1 D^2_3 f(x, y) = \frac{140625}{256} x^8 + \left(\frac{4000}{9} + \frac{444528x^2}{1331} + \frac{7112448x^4}{4913}\right)(n-2)x^9
+ \frac{1029}{2} x^{10} + \left(\frac{17496}{125} + \frac{4478976x^{12}}{5324}\right)(3n^2 - 11n + 10)x^{10}
+ \frac{117649}{288}(n-3)x^{12} + 384nx^{15} + \frac{2187}{4}(3n^2 - 10n + 8)x^{16}.
\]

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

**First Zagreb Index** = \( M_1(\Gamma_2) \) = \( (D_x + D_y)f(x, y)|_{x=y=1} \)
= 648n^2 - 1500n + 852,

**Second Zagreb Index** = \( M_2(\Gamma_2) \) = \( D_y D_y f(x, y)|_{x=y=1} \)
= 2916n^2 - 7566n + 4764,

**Modified Zagreb Index** = \( m M_2(\Gamma_2) \) = \( S_x S_y f(x, y)|_{x=y=1} \)
= \( \frac{9}{16} n^2 - \frac{8563}{11760} n + \frac{30597}{88200} \)

**Generalized Randić Index** = \( R_a(\Gamma_2) \) = \( D_x^a D_y^a f(x, y)|_{x=y=1} \)
= \( 6^{2a}(1 + 4^a)(9n^2 - 33n + 30) + 6^a(2.5^a + 60^a)(6n) \)
+ \( (6^{1+2a}2^a)(3n^2 - 10n + 8) + 7^a + 2^{1+a})(6n - 12) \)
+ \( 35^a(12n - 12) + 7^2a(6n - 18) + 18(5^2a) \)

**Inverse Randić Index** = \( RR_a(\Gamma_2) \) = \( S_x^a S_y^a f(x, y)|_{x=y=1} \)
= \( 12(5^{-a} + 35^{-a}) + 6(60^{-a}) + 21^{-a}(18n - 36) \)
+ \( 7^{-2a}(6n - 18) + 84^{-a}(12n - 24) + 12^{-2a}(9n^2 - 33n + 30) \)
+ \( 36^{-a}(18n^2 - 54n + 42) \)

**Symmetric Division Index** = \( SSD(\Gamma_2) \) = \( (D_x S_y + S_x D_y)f(x, y)|_{x=y=1} \)
= \( 81n^2 - \frac{11453}{70} n + \frac{432}{5} \)

**Harmonic Index** = \( HI(\Gamma_2) \) = \( 2S f f(x, x)|_{x=1} \)
= \( \frac{17}{4} n^2 - \frac{27103217}{3879876} n + \frac{15629}{5000} \)

**Inverse Sum Index** = \( ISI(\Gamma_2) \) = \( S_x D_y f(x, y)|_{x=y=1} \)
= \( 153n^2 - 385n - 101 \)

**Augmented Zagreb Index** = \( AZI(\Gamma_2) \) = \( S^2_1 Q_{-2} J D^2_1 D^2_3 f(x, y)|_{x=y=1} \)
= \( 4584n^2 - 13243n + 9573 \)

**Forgotten Index** = \( F(\Gamma_2) = D_y F(\Gamma_2, x)|_{x=1} = 3346n^2 - 23818n + 7892. \)
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 \( HDN1(n) \).

| \( n \) | \( M_1 \) | \( M_2 \) | \( M_2^m \) | \( R_a \) | \( R_{aa} \) | 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 \( HDN2(n) \).

| \( n \) | \( M_1 \) | \( M_2 \) | \( M_2^m \) | \( R_a \) | \( R_{aa} \) | 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).](image-url)
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.
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 $a \in \{-1, -1/2\}$ as compared to the Randić index for $a \in \{1, 1/2\}$ 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 $\pi$-electron energy of the molecules, in the case of $HDN1(n)$ and $HDN2(n)$, their values provide total $\pi$-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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