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On M-polynomial and associated topological descriptors of subdivided Hex-derived network of type three

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Topological indices have the numerical worth that usually describes the numerous properties of molecular graphs, such as physical, chemical, biological, etc. At the present time, it is very prevalent to calculate various degree-based topological indices by using the M-polynomial. Hex-derived networks are used extensively in the field of pharmaceutics, telecommunications networks, and electronics. In the current study, we construct the subdivided Hex-derived network of third type of dimension n and obtain its corresponding M-polynomial. Further, we calculate the degree-based topological indices of the above network by using their direct formulas and alternatively from the exact expression of the M-polynomial. In addition, we sketch the M-polynomial and the related topological indices for different values of n. The attained results can set a foundation to explore further into subdivided Hex-derived networks, their properties and appliances.

Keywords: M-polynomial, subdivided Hex-derived network of third type, degree-based topological indices, graph polynomial.

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Introduction

Let us assume $G = (V, E)$ be a simple, undirected and connected graph, with $V = V(G)$ denoting the vertex set and $E = E(G)$ denoting the edge set, which includes unordered pairs of vertices. The number of edges that are incident to a vertex $u \in V(G)$ in a graph G is known as the *degree* of a vertex u and is denoted by $d(u)$. A *subdivision* of a graph G is acquired by adding a new vertex to an edge of the graph G [1].

A brief discussion on topological indices and M-polynomial. In Chemical Graph Theory (CGT), to form a graph of a given chemical compound, the atoms are represented by vertices and the bonds between the atoms are represented by edges. The correlation between graph theory and chemistry and their various chemical applications have been discussed in [2]. In the field of CGT, a topological index describes the properties of the chemical structure. Basically, a topological index is a numerical parameter that characterizes the molecular structure and is used in quantitative structure-property relationships (QSPRs) and quantitative structure-activity relationships (QSARs). For more information, please refer to [3].

The topological indices are usually divided into distance-based topological indices, counting related topological indices, eigenvalue-based topological indices, degree-based topological indices, and degree and distance-based topological indices. The indices of different classes are useful in predicting the physico-chemical properties of several chemical structures. In general, we compute the topological indices of a molecular structure by using their corresponding mathematical formulas. Presently, the graphic polynomials [4] are used to calculate the topological indices of different classes. Here, the basic idea is to construct a polynomial of the given graph structure and then derive various topological indices by means of differentiating or integrating (or a distinct combination of both) the polynomial.

In the review of literature, various polynomials are discussed, which include: the M-polynomial [5], the matching polynomial [6], the Tutte polynomial [7], the Clar covering polynomial (also Zhang-Zhang polynomial) [8], the Hosoya polynomial [9], the Schultz polynomial [10], etc. Among all of the above-mentioned polynomials, the Hosoya polynomial is useful for calculating the topological indices depending on distance, for example, the Wiener index [11], the hyper-Wiener index [12], etc.

For the prediction of numerous properties of chemical structures, degree-based topological indices are crucial. In emerging trends, Deutsch and Klavžar [5] introduced the concept of M-polynomial to compute various degree-based topological indices. There are several papers in the literature in which the M-polynomials and their respective degree-based topological indices are calculated for different graph structures, such as the polyphenylene [13], planer chemical graphs [14], different families of Hex-derived networks [15–19], coronoid systems [20], Silicon-Carbons [21], etc.

Definition 1 (see [5])**.** *The expression*

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

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 $m_{i,j}(G)$ denotes the number of edges $uv\in E(G)$ such that $d(u)=i$, $d(v)=j (i,j\ge 1)$.

In the article [22], it is stated that a degree-based topological index for a graph G is a type of graph invariant, denoted as $T(G)$, and is defined as:

$$T(G)=\sum_{uv\in E(G)} f(d(u),d(v)),$$

where $f(x,y)$ is a non-negative real function of x and y related to topological indices. Table 2 depicts $f(x,y)$ in the context of our current research work. Hence, $T(G)$ can be expressed as follows:

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

Theorem 1 (see [5], Theorems 2.1, 2.2)**.** *Let G be a simple connected graph.*

1. *If $T(G)=\sum\limits_{e=uv\in E(G)} f(d(u),d(v))$, where $f(x,y)$ is a polynomial in x and y, then $T(G)=f(D_x,D_y)(M(G;x,y))|_{x=y=1}$.*

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

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

Some well-known degree-based topological indices. We now discuss briefly some standard degree-based topological indices of a graph G which can be derived from the M-polynomial $M(G;x,y)$ of G. The *Zagreb indices* have been proposed by Gutman and Trinajstić [23], which are useful in determining the total π-electron energy of a molecule. Influenced by the concept of Zagreb indices, the *modified Zagreb indices* are introduced in [24]. The *Randić index*, which is proposed by Milan Randić [25], is one of the most prevalent degree-based topological indices. This index has enormous applications in the area of drug design. After two decades, inspired by the success of Randić index, the mathematicians Bollobás and Erdős [26] and Amić et al. [27] proposed the idea of a generalized form of the Randić index (for an arbitrary real number α), termed as the *general Randić index*. In [28], the *symmetric division* (*deg*) *index* is introduced in predicting the total surface area of polychlorobiphenyls. Whereas the total surface area of octane isomers is predicted by the *inverse sum* (*indeg*) *index* [29]. Furtula et al. [30] introduced the *augmented Zagreb index*, helpful for the study of heat of formation of alkanes. The formulas of the above-discussed degree-based topological indices are listed in Table 1.

A framework of our plan. Very recently, the degree-based topological indices of subdivided Hex-derived network of type one ($SHDN1[n]$) and subdivided chain Hex-derived network of third type ($SCHDN3[n]$) are estimated in [17, 32]. In this paper, we first discuss the

T a b l e 1. Degree-based topological indices and their formulas for a graph G

Topological index	Notation and formula of topological indices
First Zagreb index [23]	$M_1(G) = \sum\limits_{uv\in E(G)} (d(u)+d(v))$
Second Zagreb index [23]	$M_2(G) = \sum\limits_{uv\in E(G)} (d(u)d(v))$
Modified second Zagreb index [24]	${}^mM_2(G) = \sum\limits_{uv\in E(G)} \dfrac{1}{d(u)d(v)}$
General Randić index [26]	$R_\alpha(G) = \sum\limits_{uv\in E(G)} (d(u)d(v))^\alpha$
Inverse Randić index [27]	$RR_\alpha(G) = \sum\limits_{uv\in E(G)} \dfrac{1}{(d(u)d(v))^\alpha}$
Symmetric division (deg) index [28]	$SDD(G) = \sum\limits_{uv\in E(G)} \left\{\dfrac{\min(d(u),d(v))}{\max(d(u),d(v))} + \dfrac{\max(d(u),d(v))}{\min(d(u),d(v))}\right\}$
Harmonic index [31]	$H(G) = \sum\limits_{uv\in E(G)} \dfrac{2}{d(u)+d(v)}$
Inverse sum (indeg) index [28]	$ISI(G) = \sum\limits_{uv\in E(G)} \dfrac{d(u)d(v)}{d(u)+d(v)}$
Augmented Zagreb index [30]	$AZ(G) = \sum\limits_{uv\in E(G)} \left\{\dfrac{d(u)d(v)}{d(u)+d(v)-2}\right\}^3$

construction of the n dimensional subdivided Hex-derived network of third type ($SHDN3[n]$) by elementary subdivision of Hex-derived network of third type ($HDN3[n]$) in Section 1. In Section 2, we compute the degree-based topological indices for $SHDN3[n]$ directly by using the standard formulas mentioned in Table 1. On the other hand, we figure out an exact expression of M-polynomial for the $SHDN3[n]$ network and derive the same associated degree-based topological indices with the help of the M-polynomial, in Section 3. Furthermore, in Section 4, we plot the M-polynomial and the indices for different values of n to observe their geometrical characteristics.

1. Subdivided Hex-derived network of third type of dimension n

The hexagonal network and its applications have been discussed in [33]. From the hexagonal network of dimension n, two new Hex-derived networks $HDN1$ and $HDN2$ were proposed in [34]. These networks confer a lot more processors and connections in comparison to the hexagonal network. Several years later in 2017, a new chemical network named the third type of Hex-derived network of dimension n ($HDN3[n]$) [35] has been derived from the hexagonal network.

We now derive a new graph from the existing one by incorporating the graph subdivision operation. By applying the elementary subdivision operation on $HDN3[n]$ network, we obtain a new chemical network of our interest and name it a *subdivided Hex-derived network* of third type of dimension n ($SHDN3[n]$). As an example, we graphically describe the $SHDN3[3]$ network of dimension 3 in Fig. 1.

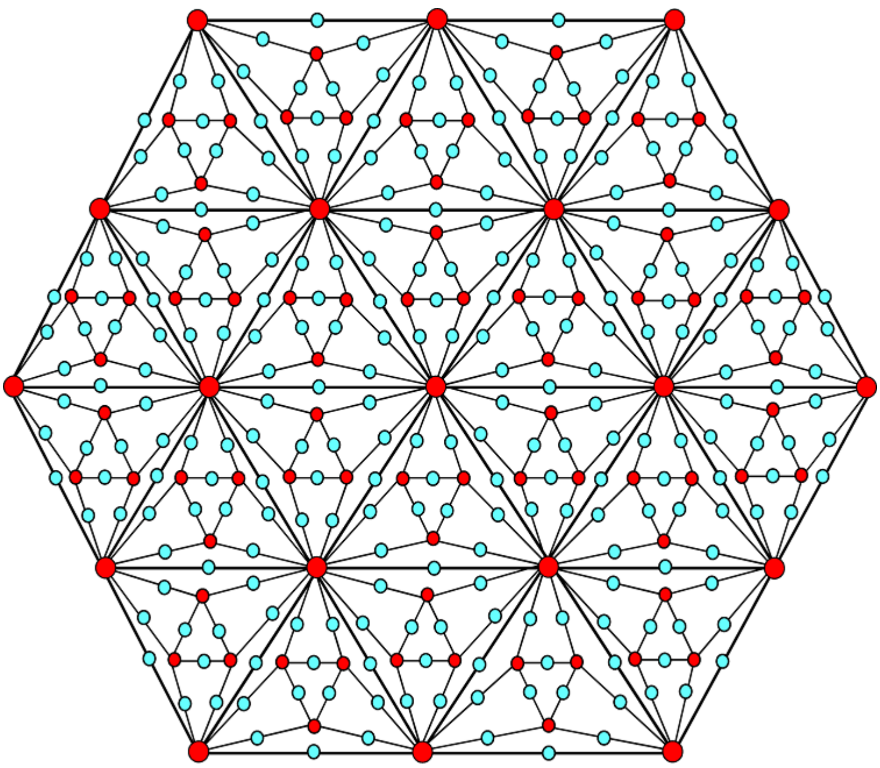

Fig. 1. Subdivided Hex-derived network of third type of dimension 3 ($SHDN3[3]$)

2. Evaluating the degree-based topological indices of $SHDN3[n]$ network

This section deals with the direct evaluation of the degree-based topological indices of the subdivided Hex-derived network of third type of dimension n ($n \geq 3$), by using the formulas mentioned in Table 1.

Theorem 2. *Let $SHDN3[n]$ be the subdivided Hex-derived network of third type of dimension n ($n \geq 3$). Then*

(i) $M_1(SHDN3[n]) = 18(84n^2 - 188n + 105)$,

(ii) $M_2(SHDN3[n]) = 12(210n^2 - 482n + 275)$,

(iii) ${}^mM_2(SHDN3[n]) = \frac{1}{2}(21n^2 - 39n + 19)$,

(iv) $R_\alpha(SHDN3[n]) = 72 \cdot 8^\alpha(n-1)^2 + 42 \cdot 14^\alpha + 60 \cdot 20^\alpha(n-2) + 18 \cdot 36^\alpha(3n^2 - 9n + 7)$,

(v) $RR_\alpha(SHDN3[n]) = \frac{72}{8^\alpha}(n-1)^2 + \frac{42}{14^\alpha} + \frac{60}{20^\alpha}(n-2) + \frac{18}{36^\alpha}(3n^2 - 9n + 7)$,

(vi) $SDD(SHDN3[n]) = 672n^2 - 1524n + 863$,

(vii) $H(SHDN3[n]) = \frac{147}{5}n^2 - \frac{271}{5}n + \frac{389}{15}$,

(viii) $ISI(SHDN3[n]) = \frac{966}{5}n^2 - \frac{1918}{5}n + \frac{2822}{15}$,

(ix) $AZ(SHDN3[n]) = 48(21n^2 - 41n + 20)$.

Proof. For any two arbitrary vertices u and v of the $SHDN3[n]$ network, below we calculate its degree-based topological indices by using their respective formulas (listed in Table 1).

First Zagreb index

$$M_1(SHDN3[n]) = \sum_{uv \in E(SHDN3[n])} (d(u) + d(v)) = 72(n-1)^2(2+4) + 42(2+7) +$$
$$+60(n-2)(2+10) + 18(3n^2 - 9n + 7)(2+18) =$$
$$= 432(n-1)^2 + 378 + 720(n-2) + 360(3n^2 - 9n + 7) = 18(84n^2 - 188n + 105).$$

Second Zagreb index

$$M_2(SHDN3[n]) = \sum_{uv \in E(SHDN3[n])} (d(u)d(v)) = 72(n-1)^2(2 \cdot 4) + 42(2 \cdot 7) +$$
$$+60(n-2)(2 \cdot 10) + 18(3n^2 - 9n + 7)(2 \cdot 18) =$$
$$= 576(n-1)^2 + 588 + 1200(n-2) + 648(3n^2 - 9n + 7) = 12(210n^2 - 482n + 275).$$

Modified second Zagreb index

$$^{m}M_2(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} \frac{1}{d(u)d(v)} = 72(n-1)^2\left(\frac{1}{2\cdot 4}\right) + 42\left(\frac{1}{2\cdot 7}\right) +$$

$$+60(n-2)\left(\frac{1}{2\cdot 10}\right) + 18(3n^2-9n+7)\left(\frac{1}{2\cdot 18}\right) =$$

$$= 9(n-1)^2 + 3 + 3(n-2) + \frac{1}{2}(3n^2-9n+7) = \frac{1}{2}(21n^2-39n+19).$$

General Randić index

$$R_\alpha(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} (d(u)d(v))^\alpha =$$

$$= 72\cdot 8^\alpha(n-1)^2 + 42\cdot 14^\alpha + 60\cdot 20^\alpha(n-2) + 18\cdot 36^\alpha(3n^2-9n+7).$$

Inverse Randić index

$$RR_\alpha(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} \frac{1}{(d(u)d(v))^\alpha} =$$

$$= \frac{72}{8^\alpha}(n-1)^2 + \frac{42}{14^\alpha} + \frac{60}{20^\alpha}(n-2) + \frac{18}{36^\alpha}(3n^2-9n+7).$$

Symmetric division (deg) index

$$SDD(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} \left\{\frac{\min(d(u),d(v))}{\max(d(u),d(v))} + \frac{\max(d(u),d(v))}{\min(d(u),d(v))}\right\} =$$

$$= 72(n-1)^2\left\{\frac{\min(2,4)}{\max(2,4)} + \frac{\max(2,4)}{\min(2,4)}\right\} + 42\left\{\frac{\min(2,7)}{\max(2,7)} + \frac{\max(2,7)}{\min(2,7)}\right\} +$$

$$+60(n-2)\left\{\frac{\min(2,10)}{\max(2,10)} + \frac{\max(2,10)}{\min(2,10)}\right\} + 18(3n^2-9n+7)\left\{\frac{\min(2,18)}{\max(2,18)} + \frac{\max(2,18)}{\min(2,18)}\right\} =$$

$$= 72(n-1)^2\left\{\frac{2}{4}+\frac{4}{2}\right\} + 42\left\{\frac{2}{7}+\frac{7}{2}\right\} + 60(n-2)\left\{\frac{2}{10}+\frac{10}{2}\right\} + 18(3n^2-9n+7)\left\{\frac{2}{18}+\frac{18}{2}\right\} =$$

$$= 180(n-1)^2 + 159 + 312(n-2) + 164(3n^2-9n+7) = 672n^2 - 1524n + 863.$$

Harmonic index

$$H(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} \frac{2}{d(u)+d(v)} =$$

$$= 72(n-1)^2\frac{2}{2+4} + 42\frac{2}{2+7} + 60(n-2)\frac{2}{2+10} + 18(3n^2-9n+7)\frac{2}{2+18} =$$

$$= 24(n-1)^2 + \frac{28}{3} + 10(n-2) + \frac{9}{5}(3n^2-9n+7) = \frac{147}{5}n^2 - \frac{271}{5}n + \frac{389}{15}.$$

Inverse sum (indeg) index

$$ISI(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} \frac{d(u)d(v)}{d(u)+d(v)} =$$

$$= 72(n-1)^2\frac{2\cdot 4}{2+4} + 42\frac{2\cdot 7}{2+7} + 60(n-2)\frac{2\cdot 10}{2+10} + 18(3n^2-9n+7)\frac{2\cdot 18}{2+18} =$$

$$= 96(n-1)^2 + \frac{196}{3} + 100(n-2) + \frac{162}{5}(3n^2-9n+7) = \frac{966}{5}n^2 - \frac{1918}{5}n + \frac{2822}{15}.$$

Augmented Zagreb index

$$AZ(SHDN3[n]) = \sum_{uv\in E(SHDN3[n])} \left\{\frac{d(u)d(v)}{d(u)+d(v)-2}\right\}^3 = 72(n-1)^2\left\{\frac{2\cdot 4}{2+4-2}\right\}^3 +$$
$$+42\left\{\frac{2\cdot 7}{2+7-2}\right\}^3 + 60(n-2)\left\{\frac{2\cdot 10}{2+10-2}\right\}^3 + 18(3n^2-9n+7)\left\{\frac{2\cdot 18}{2+18-2}\right\}^3 =$$
$$= 576(n-1)^2 + 336 + 480(n-2) + 144(3n^2-9n+7) = 48(21n^2-41n+20). \qquad \square$$

3. Determining M-polynomial of the $SHDN3[n]$ network

In this section, we obtain a closed expression of M-polynomial for the $SHDN3[n]$ network and hence derive the associated degree-based topological indices by using the derivation formulas (as mentioned in Table 2).

Theorem 3. *Let $SHDN3[n]$ be the subdivided Hex-derived network of third type of dimension n ($n \geq 3$). Then M-polynomial of the $SHDN3[n]$ network is $M(SHDN3[n];x,y) = 72(n-1)^2x^2y^4 + 42x^2y^7 + 60(n-2)x^2y^{10} + 18(3n^2-9n+7)x^2y^{18}$.*

Proof. As enumerated in [15], the cardinalities of the vertex set and the edge set of the third type of Hex-derived network of dimension n ($HDN3[n]$) are as follows:

$$|V(HDN3[n])| = 21n^2 - 39n + 19, \quad \text{and} \quad |E(HDN3[n])| = 63n^2 - 123n + 60.$$

Here, in our case, we can easily calculate the total number of vertices and edges of the $SHDN3[n]$ network. Since, the $SHDN3[n]$ network is obtained by performing the subdivision operation on $HDN3[n]$ network, i. e. by adding a new vertex between each edge of $HDN3[n]$ network. Therefore,

$$|V(SHDN3[n])| = |V(HDN3[n])| + |E(HDN[n])| = 84n^2 - 162n + 79,$$
$$\text{and} \quad |E(SHDN3[n])| = 2|E(HDN3[n])| = 126n^2 - 246n + 120.$$

Now, based on the degree of the vertices of the $SHDN3[n]$ network, below we partition the vertex set $V(SHDN3[n])$ into five disjoint sets, as

$$V_1(SHDN3[n]) = \{u \in V(SHDN3[n]) : d(u) = 2\},$$
$$V_2(SHDN3[n]) = \{u \in V(SHDN3[n]) : d(u) = 4\},$$
$$V_3(SHDN3[n]) = \{u \in V(SHDN3[n]) : d(u) = 7\},$$
$$V_4(SHDN3[n]) = \{u \in V(SHDN3[n]) : d(u) = 10\},$$
$$V_5(SHDN3[n]) = \{u \in V(SHDN3[n]) : d(u) = 18\},$$

and each of the above vertex set has the cardinality

$$|V_1(SHDN3[n])| = 3(21n^2-41n+20), \quad |V_2(SHDN3[n])| = 18(n-1)^2,$$
$$|V_3(SHDN3[n])| = 6, \quad |V_4(SHDN3[n])| = 6(n-2), \quad |V_5(SHDN3[n])| = 3n^2-9n+7.$$

Moreover, we divide the edge set $E(SHDN3[n])$ into four parts on the basis of degrees of the end vertices of each edge. Let us name them as

$$E_{\{i,j\}} = \{e = uv \in E(SHDN3[n]) : d(u) = i, d(v) = j\},$$

where $\{i,j\} = \{2,4\}$, $\{2,7\}$, $\{2,10\}$, and $\{2,18\}$. And the cardinalities of these edge sets are given by $|E_{\{2,4\}}| = 72(n-1)^2$, $|E_{\{2,7\}}| = 42$, $|E_{\{2,10\}}| = 60(n-2)$ and $|E_{\{2,18\}}| = 18(3n^2-9n+7)$. Thus, by using the definition 1, M-polynomial of the $SHDN3[n]$ network is given as

$$M(SHDN3[n];x,y) = \sum_{i\le j} m_{i,j}x^i y^j, \quad \text{where } i,j \in \{2,4,7,10,18\} =$$
$$= \sum_{2\le 4} m_{2,4}x^2y^4 + \sum_{2\le 7} m_{2,7}x^2y^7 + \sum_{2\le 10} m_{2,10}x^2y^{10} + \sum_{2\le 18} m_{2,18}x^2y^{18} =$$
$$= \sum_{uv\in E_{\{2,4\}}} m_{2,4}x^2y^4 + \sum_{uv\in E_{\{2,7\}}} m_{2,7}x^2y^7 + \sum_{uv\in E_{\{2,10\}}} m_{2,10}x^2y^{10} + \sum_{uv\in E_{\{2,18\}}} m_{2,18}x^2y^{18} =$$
$$= |E_{\{2,4\}}|x^2y^4 + |E_{\{2,7\}}|x^2y^7 + |E_{\{2,10\}}|x^2y^{10} + |E_{\{2,18\}}|x^2y^{18} =$$
$$= 72(n-1)^2x^2y^4 + 42x^2y^7 + 60(n-2)x^2y^{10} + 18(3n^2-9n+7)x^2y^{18}. \qquad \square$$

Table 2 gives the derivation formulas in terms of integral or derivative (or both integral and derivative) [5]. By applying them to our obtained M-polynomial of the $SHDN3[n]$ network, we now derive directly the associated degree-based topological indices (described in Table 1) of the $SHDN3[n]$ network. Essentially, we present below the M-polynomial based proof of Theorem 2 as directed above.

An alternate proof of the theorem 2 (M-polynomial based). For reasons of simplicity, let us assume $\eta(x,y) = M(SHDN3[n];x,y)$. Therefore, the M-polynomial for

T a b l e 2. Derivation formulas on the M-polynomial for deriving the degree-based topological indices of a graph G

Topological index	Notation	$f(x,y)$	Derivation from $(M(G;x,y))$
First Zagreb index	$M_1(G)$	$x+y$	$(D_x+D_y)(M(G;x,y))\|_{x=y=1}$
Second Zagreb index	$M_2(G)$	xy	$(D_xD_y)(M(G;x,y))\|_{x=y=1}$
Modified second Zagreb index	${}^mM_2(G)$	$\frac{1}{xy}$	$(S_xS_y)(M(G;x,y))\|_{x=y=1}$
General Randić index	$R_\alpha(G)$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\|_{x=y=1}$
Inverse Randić index	$RR_\alpha(G)$	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\|_{x=y=1}$
Symmetric division (deg) index	$SDD(G)$	$\frac{x^2+y^2}{xy}$	$(D_xS_y+D_yS_x)(M(G;x,y))\|_{x=y=1}$
Harmonic index	$H(G)$	$\frac{2}{x+y}$	$2S_xJ(M(G;x,y))\|_{x=1}$
Inverse sum (indeg) index	$ISI(G)$	$\frac{xy}{x+y}$	$S_xJD_xD_y(M(G;x,y))\|_{x=1}$
Augmented Zagreb index	$AZ(G)$	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3Q_{-2}JD_x^3D_y^3(M(G;x,y))\|_{x=1}$

Here, $D_x(f(x,y)) = x\frac{\partial(f(x,y))}{\partial x}$, $D_y(f(x,y)) = y\frac{\partial(f(x,y))}{\partial y}$, $S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt$, $S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t}dt$, $J(f(x,y)) = f(x,x)$, $Q_\alpha(f(x,y)) = x^\alpha f(x,y)$, $\alpha \ne 0$.

the $SHDN3[n]$ network (as obtained in theorem 3) is

$$\eta(x,y) = 72(n-1)^2x^2y^4 + 42x^2y^7 + 60(n-2)x^2y^{10} + 18(3n^2-9n+7)x^2y^{18}.$$

Now, we calculate the following terms which will be required for our further computation of various degree-based topological indices.

$$D_x(\eta(x,y)) = 144(n-1)^2x^2y^4 + 84x^2y^7 + 120(n-2)x^2y^{10} + 36(3n^2-9n+7)x^2y^{18},$$
$$D_y(\eta(x,y)) = 288(n-1)^2x^2y^4 + 294x^2y^7 + 600(n-2)x^2y^{10} + 324(3n^2-9n+7)x^2y^{18},$$
$$D_yD_x(\eta(x,y)) = 576(n-1)^2x^2y^4 + 588x^2y^7 + 1200(n-2)x^2y^{10} + 648(3n^2-9n+7)x^2y^{18},$$
$$S_x(\eta(x,y)) = 36(n-1)^2x^2y^4 + 21x^2y^7 + 30(n-2)x^2y^{10} + 9(3n^2-9n+7)x^2y^{18},$$
$$S_y(\eta(x,y)) = 18(n-1)^2x^2y^4 + 6x^2y^7 + 6(n-2)x^2y^{10} + (3n^2-9n+7)x^2y^{18},$$
$$S_xS_y(\eta(x,y)) = 9(n-1)^2x^2y^4 + 3x^2y^7 + 3(n-2)x^2y^{10} + \frac{1}{2}(3n^2-9n+7)x^2y^{18},$$
$$D_x^\alpha D_y^\alpha(\eta(x,y)) = 72\cdot 8^\alpha(n-1)^2x^2y^4 + 42\cdot 14^\alpha x^2y^7 + 60\cdot 20^\alpha(n-2)x^2y^{10} + \\ +18\cdot 36^\alpha(3n^2-9n+7)x^2y^{18},$$
$$S_yD_x(\eta(x,y)) = 36(n-1)^2x^2y^4 + 12x^2y^7 + 12(n-2)x^2y^{10} + 2(3n^2-9n+7)x^2y^{18},$$
$$S_xD_y(\eta(x,y)) = 144(n-1)^2x^2y^4 + 147x^2y^7 + 300(n-2)x^2y^{10} + 162(3n^2-9n+7)x^2y^{18},$$
$$S_x^\alpha S_y^\alpha(\eta(x,y)) = \frac{72}{8^\alpha}(n-1)^2x^2y^4 + \frac{42}{14^\alpha}x^2y^7 + \frac{60}{20^\alpha}(n-2)x^2y^{10} + \frac{18}{36^\alpha}(3n^2-9n+7)x^2y^{18},$$
$$S_xJ(\eta(x,y)) = 12(n-1)^2x^6 + \frac{14}{3}x^9 + 5(n-2)x^{12} + \frac{9}{10}(3n^2-9n+7)x^{20},$$
$$S_xJD_xD_y(\eta(x,y)) = 96(n-1)^2x^6 + \frac{196}{3}x^9 + 100(n-2)x^{12} + \frac{162}{5}(3n^2-9n+7)x^{20},$$
$$S_x^3Q_{-2}JD_x^3D_y^3(\eta(x,y)) = 576(n-1)^2x^4 + 336x^7 + 480(n-2)x^{10} + 144(3n^2-9n+7)x^{18}.$$

Thus, from the derivation formulas listed in Table 2, the degree-based topological indices of the $SHDN3[n]$ network are as follows:

First Zagreb index

$$M_1(SHDN3[n]) = (D_x + D_y)(\eta(x,y))|_{x=y=1} = 18(84n^2 - 188n + 105).$$

Second Zagreb index

$$M_2(SHDN3[n]) = D_xD_y(\eta(x,y))|_{x=y=1} = 12(210n^2 - 482n + 275).$$

Modified second Zagreb index

$${}^mM_2(SHDN3[n]) = S_xS_y(\eta(x,y))|_{x=y=1} = \frac{1}{2}(21n^2 - 39n + 19).$$

General Randić index

$$R_\alpha(SHDN3[n]) = D_x^\alpha D_y^\alpha(\eta(x,y))|_{x=y=1} = \\ = 72\cdot 8^\alpha(n-1)^2 + 42\cdot 14^\alpha + 60\cdot 20^\alpha(n-2) + 18\cdot 36^\alpha(3n^2-9n+7).$$

Inverse Randić index

$$RR_\alpha(SHDN3[n]) = S_x^\alpha S_y^\alpha(\eta(x,y))|_{x=y=1} = \frac{72}{8^\alpha}(n-1)^2 + \frac{42}{14^\alpha} + \frac{60}{20^\alpha}(n-2) + \frac{18}{36^\alpha}(3n^2-9n+7).$$

Symmetric division (deg) index

$$SDD(SHDN3[n]) = (S_yD_x + S_xD_y)(\eta(x,y))|_{x=y=1} = 672n^2 - 1524n + 863.$$

Harmonic index

$$H(SHDN3[n]) = 2S_xJ(\eta(x,y))|_{x=1} = \frac{147}{5}n^2 - \frac{271}{5}n + \frac{389}{15}.$$

Inverse sum (indeg) index

$$ISI(SHDN3[n]) = S_xJD_xD_y(\eta(x,y))|_{x=1} = \frac{966}{5}n^2 - \frac{1918}{5}n + \frac{2822}{15}.$$

Augmented Zagreb index

$$AZ(SHDN3[n]) = S_x^3Q_{-2}JD_x^3D_y^3(\eta(x,y))|_{x=1} = 48(21n^2 - 41n + 20). \qquad \square$$

4. Experimental outcomes associated with the M-polynomial

In Table 3, we have listed the M-polynomial and related degree-based topological indices of the $SHDN3[n]$ network for different values of n. Using the Maple-13 software we have created 3-D plots of the M-polynomial of the subdivided Hex-derived network of third type of dimension 3 ($SHDN3[3]$) in the different domain ranges from $-2 \leq x, y \leq 2$ in Fig. 2, *a*, $-1 \leq x, y \leq 1$ in Fig. 2, *b* and $-0.5 \leq x, y \leq 0.5$ in Fig. 2, *c*.

Furthermore, we have drawn the related degree-based topological indices of the $SHDN3[n]$ network for several n ($3 \leq n \leq 7$). Figure 3 shows the characteristics of the first Zagreb, general Randić ($\alpha = 1/2$), second Zagreb, symmetric division (deg), inverse sum (indeg), and augmented Zagreb indices of the $SHDN3[n]$ network. The characteristics of the modified second Zagreb, harmonic, and inverse Randić ($\alpha = 1/2$) indices of the $SHDN3[n]$ network are graphically represented in Fig. 4. By inspecting them, we can conclude that the values of each of the topological indices have been increasing with the increment of dimension n of the structure.

T a b l e 3. Evaluation of M-polynomial and the corresponding degree-based topological indices of the $SHDN3[n]$ network at distinct values of n

Topological Index	Dimension				
	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
	M-polynomial				
	$288x^2y^4 + 42x^2y^7 + 60x^2y^{10} + 126x^2y^{18}$	$648x^2y^4 + 42x^2y^7 + 120x^2y^{10} + 342x^2y^{18}$	$1152x^2y^4 + 42x^2y^7 + 180x^2y^{10} + 666x^2y^{18}$	$1800x^2y^4 + 42x^2y^7 + 240x^2y^{10} + 1098x^2y^{18}$	$2592x^2y^4 + 42x^2y^7 + 300x^2y^{10} + 1638x^2y^{18}$
First Zagreb index	5346	12 546	22 770	36 018	52 290
Second Zagreb index	8628	20 484	37 380	59 316	86 292
Modified second Zagreb index	45.50	99.50	174.50	270.50	387.50
General Randić index ($\alpha = 1/2$)	1996.0648	4578.6267	8216.4821	12 909.6311	18 658.0735
Inverse Randić index ($\alpha = 1/2$)	147.4648	324.1604	569.7677	884.2867	1267.7174
Symmetric division (deg) index	2339	5519	10 043	15 911	23 123
Harmonic index	127.9333	279.5333	489.9333	759.1333	1087.1333
Inverse sum (indeg) index	776.1333	1744.9333	3100.1333	4841.7333	6969.7333
Augmented Zagreb index	4128	9216	16 320	25 440	36 576

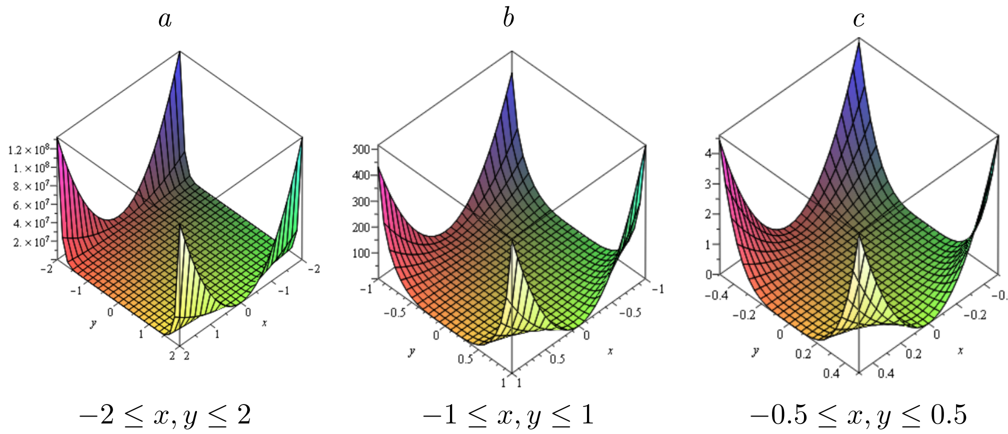

Fig. 2. The graph of the M-polynomial of $SHDN3[3]$ network in various x and y regions

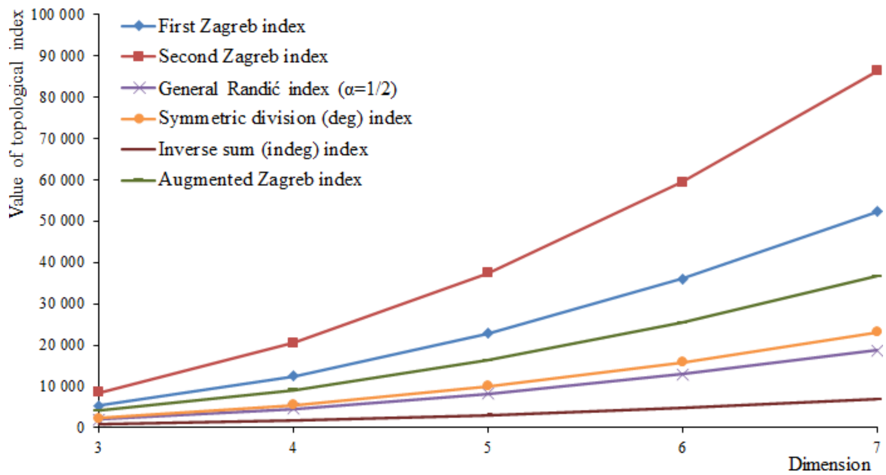

Fig. 3. Pictorial representation of first Zagreb, general Randić ($\alpha = 1/2$), second Zagreb, symmetric division (deg), inverse sum (indeg), and augmented Zagreb indices of $SHDN3[n]$ network for different values of n ($3 \le n \le 7$)

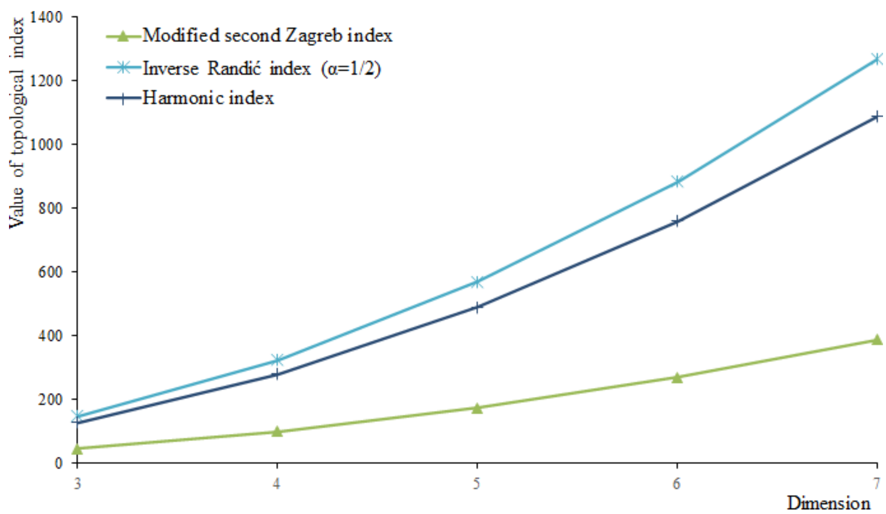

Fig. 4. Pictorial representation of modified second Zagreb, harmonic, and inverse Randić ($\alpha = 1/2$) indices of $SHDN3[n]$ network for different values of n ($3 \le n \le 7$)

Conclusions

In the present study, we have considered the subdivided Hex-derived network of third type of dimension n ($SHDN3[n]$) which we have derived from the structure of $HDN3[n]$ network by the graph subdivision. Observe that the structure of $SHDN3[n]$ network is more compact than the $HDN3[n]$ network. We have calculated the degree-based topological indices of the $SHDN3[n]$ network by the direct method and M-polynomial method. In the direct method, we have computed the degree-based topological indices using their direct mathematical formulas. In the M-polynomial based method, we have obtained the exact expression of M-polynomial for the $SHDN3[n]$ network and then derived the respective degree-based topological indices. One can observe that the latter method is very quick, compact, easy and more appropriate to compute the degree-based topological indices of the network. Additionally, we have graphically represented the behavior of the M-polynomial in different regions and the degree-based topological indices of the $SHDN3[n]$ network for different dimensions. The obtained outcomes can set a base for advanced research into subdivided Hex-derived networks, their characteristics and appliances.

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ВЫЧИСЛИТЕЛЬНЫЕ ТЕХНОЛОГИИ

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О М-полиномиальных и связанных с ними топологических дескрипторах подразделенной сотовой сети третьего типа

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Аннотация

Топологические индексы имеют то числовое значение, которое обычно описывает многочисленные свойства молекулярных графов, такие как физические, химические, биологические и т. д. Сегодня очень распространено вычисление различных топологических индексов на основе степеней с помощью М-полинома. Шестнадцатеричные сети широко используются в области фармацевтики, телекоммуникационных сетей и электроники. В настоящем исследовании построена подразделенная сотовая сеть третьего типа размерности n и получен соответствующий М-полином. Вычислены основанные на степени топологические индексы вышеуказанной сети с использованием их прямых формул и, альтернативно, точного выражения М-полинома. Кроме того, очерчен М-полином и связанные с ним топологические индексы для различных значений n. Достигнутые результаты могут стать основой для дальнейшего изучения подразделенных сотовых сетей, их свойств и устройства.

Ключевые слова: М-полином, подразделенная сотовая сеть третьего типа, степенные топологические индексы, полином-граф.

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