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EXTENSION OF M-POLYNOMIAL AND DEGREE BASED TOPOLOGICAL INDICES FOR NANOTUBE

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Abstract. The *M-polynomial* of a graph $G(V(G), E(G))$ is defined as $M(G; u, v) = \sum_{i \leq j} m_{ij} u^i v^j$, where m_{ij} denotes the number of edges $xy \in E(G)$ such that $\{d_x, d_y\} = \{i, j\}$, where d_x, d_y denote degree of the vertex x and y in the graph $G(V(G), E(G))$. In this paper, we show how to compute the degree-based indices such as Forgotten index, Reduced Second Zagreb index, Sigma index, Hyper-Zagreb index and Albertson index using the *M-polynomial*. In addition, we present as an application how to quickly and effectively compute the degree-based topological indices using *M-polynomial* for two carbon nanotube structures, namely $HC_5C_7[p, q]$ and $VC_5C_7[p, q]$.

Keywords: M-Polynomial, Carbon Nanotubes, Degree-based topological index, Graph Polynomials
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1. Introduction

In the study of graphs, an invariant of a graph depends only on the topological structure of graphs and does not depend on its representation, such as the drawing/labelling of graphs. A graph invariant represents a topological index when a numerical value expresses the structure of the graph. For decades, topological indices have found application in the field of chemical graph theory. Here, the structure of a molecule/chemical network is analyzed quantitatively for its structure-activity/structure-property relationships *(QSAR/QSPR)*.

In this paper, we focus on degree-based topological indices, which is a collection of indices computed using the degree-sequence of a graph. Among many degree-based indices, we focus on the Zagreb indices and its variations, given by Gutman and Trinajstić in [17]. They were the first to introduce the degree based indices, called the first Zagreb index $M_1(G)$, which was defined by

$$M_1(G) = \sum_{x \in V(G)} {d_x}^2 = \sum_{xy \in E(G)} (d_x + d_y),$$

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where d_x denotes the degree of vertex $x \in V(G)$. For more study of Zagreb index, we refer to [12, 13, 31]. The second Zagreb index $M_2(G)$ is given by

$$M_2(G) = \sum_{xy \in E(G)} d_x d_y.$$

Following this work by Gutman and Trinajstić, there was a plethora of literature published on Zagreb indices. Further, many modified forms and variants also introduced. For a recent survey of more degree-based indices, we refer to [14, 15].

One of the modified Zagreb index ${}^mM_2(G)$ introduced by J. Hao [18], in 2009, is defined by

$${}^mM_2(G) = \sum_{xy \in E(G)} \frac{1}{d_x d_y}.$$

For chemical graphs, another index proven useful in the study of heat formation of heptanes and octanes is Augmented Zagreb index [9], which is defined as

$$AZI(G) = \sum_{xy \in E(G)} \left(\frac{d_x d_y}{d_x + d_y - 2} \right)^3.$$

In similar lines of Zagreb indices another interesting and well studied in the field of drug design is the Randić index [25] defined by

$$R(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d_x d_y}}.$$

A generalized version of Randić index [24] is defined by

$$R_\alpha(G) = \sum_{xy \in E(G)} (d_x d_y)^\alpha,$$

where $\alpha \in \mathbb{R}$, and for $\alpha = -\frac{1}{2}$, we obtain the Randić index.

Another variation of the Randić index was first introduced by Siemion Fajtlowicz [6] known as Harmonic index is defined as

$$H(G) = \sum_{xy \in E(G)} \frac{2}{d_x + d_y}.$$

Favaron *et al.* [8] has given the relationship between Harmonic index and eigenvalue of the graph.

The Inverse sum index introduced by Vukičević and Gašperov [29] in 2010 and shown to be a significant predictor of the total surface area of octane isomer.The Inverse sum index $ISI(G)$ is defined as

$$ISI(G) = \sum_{xy \in E(G)} \frac{1}{\frac{1}{d_x} + \frac{1}{d_y}} = \sum_{xy \in E(G)} \frac{d_x d_y}{d_x + d_y}.$$

Symmetric division degree index [27, 28] $SDD(G)$ is defined as

$$SDD(G) = \sum_{xy \in E(G)} \left(\frac{min(d_x, d_y)}{max(d_x, d_y)} + \frac{max(d_x, d_y)}{min(d_x, d_y)} \right).$$

Traditionally, the computation of topological indices involved only their definitions. Such computations are known to be time-consuming. In order to reduce the computation time of topological indices, several techniques were introduced by many researchers. Among them, the polynomial representation of indices has received wide attention in the literature. For instance, Hosoya polynomial also known as Wiener polynomial [11,21], we used to compute various indices such as Wiener index [30], Hosoya index [20] and Hyper Wiener index [22] etc. For example, the derivative of Hosoya polynomial when evaluated at 1, gives the Weiner index. Hyper Weiner index and Tratch-Zefirov index can be obtained similarly [3].

In 2015, Deutsch and Klavžar introduced a polynomial known as *M-polynomial* [4]. It is a general polynomial because, with the help of this polynomial, one can determine at-least nine degree-based topological indices. For more study of *M-polynomial*, we refer to [5].

In this paper, we find representations of five degree-based topological indices using *M-polynomial*, such as Forgotten index, Reduced Second Zagreb index, Sigma index, Hyper Zagreb index and Albertson index. Further, we also determine the value of these indices with the help of *M-polynomial* for carbon nanotube structures $HC_5C_7[p,q]$, and $VC_5C_7[p.q]$.

2. Preliminaries

In this section, we will mention some of the definitions and related results required for this article. Mainly, the five indices that we focus on this paper is listed below.

F-index or Forgotten index [10] of a graph $G(V(G),E(G))$ is defined as

$$F(G) = \sum_{x\in V(G)} {d_x}^3 = \sum_{xy\in E(G)} ({d_x}^2 + {d_y}^2). \tag{1}$$

Reduced Second Zagreb index [14] of a graph $G(V(G),E(G))$ is defined as

$$RM_2(G) = \sum_{xy\in E(G)} (d_x - 1)(d_y - 1). \tag{2}$$

Sigma index [16] of a graph $G(V(G),E(G))$ is defined as

$$\sigma(G) = \sum_{xy\in E(G)} (d_x - d_y)^2. \tag{3}$$

Hyper Zagreb index [26] of a graph $G(V(G),E(G))$ is defined as

$$Hyp(G) = \sum_{xy\in E(G)} (d_x + d_y)^2. \tag{4}$$

Albertson index [1] of graph $G(V(G),E(G))$ is defined as

$$Alb(G) = \sum_{xy\in E(G)} |d_x - d_y|. \tag{5}$$

Definition 2.1. *[4] Let $G(V(G),E(G))$ be a graph, then M-polynomial of G is given by*

$$M(G;u,v) = \sum_{i\le j} m_{ij} u^i v^j,$$

where m_{ij} denotes the number of edges xy of G such that $\{d_x,d_y\} = \{i,j\}$, where d_x,d_y denotes the degree of the vertex x and y in the graph G.

Definition 2.2. *[4] A degree based topological index for a graph G is defined as*

$$I(G) = \sum_{e=xy\in E(G)} f(d_x,d_y), \tag{6}$$

where $f(u,v)$ is a function which is suitable for some degree based topological indices.

For instance, the first Zagreb index $M_1(G)$ is defined with equation (6) by putting $f(u,v) = u + v$. Counting edges which have same end-degrees, then we can rewrite equation (6) as

$$I(G) = \sum_{i \le j} m_{ij} f(i,j). \tag{7}$$

We require some of the operators as defined in [4]. The operators are listed below :

$$D_u f(u,v) = u\frac{\partial f(u,v)}{\partial u},\ D_v f(u,v) = v\frac{\partial f(u,v)}{\partial v}. \tag{8}$$

$$S_u f(u,v) = \int_0^u \frac{f(t,v)}{t}dt,\ S_v f(u,v) = \int_0^v \frac{f(u,t)}{t}dt. \tag{9}$$

$$J(f(u,v)) = f(u,u),\ Q_\alpha(f(u,v)) = u^\alpha f(u,v). \tag{10}$$

Now we recall the theorems from which are required for our proofs :

Theorem 2.1. *[4] Let $G(V(G), E(G))$ be a graph and let $I(G) = \sum_{xy \in E(G)} f(d_x, d_y)$, where $f(u,v)$ is a polynomial in u and v, then $I(G) = f(D_u, D_v)(M(G;u,v))|_{u=v=1}$.* □

Theorem 2.2. *[4] Let $G(V(G), E(G))$ be a graph and let $I(G) = \sum_{xy \in E(G)} f(d_x, d_y)$, where $f(u,v) = \sum_{i,j \in \mathbb{Z}} \alpha_{i,j} u^i v^j$, $\alpha_{i,j} \in \mathbb{R}$ for each i,j. Then $I(G)$ can be obtain from M-polynomial using operators D_u, D_v, S_u and S_v.* □

Theorem 2.3. *[4] Let $G(V(G), E(G))$ be a graph and $I(G) = \sum_{xy \in E(G)} f(d_x, d_y)$, where $f(u,v) = \dfrac{u^r v^s}{(u+v+\alpha)^k}$, for all $r,s \ge 0$, $k \ge 1$ and $\alpha \in \mathbb{Z}$. Then $I(G) = S_u^k Q_\alpha J D_u^r D_v^s (M(G;u,v))|_{u=v=1}$.* □

With the help of the above three theorems, the authors in [4], have proved that certain topological indices can be computed directly from *M-polynomial*. We summarize these results in Table 1.

TABLE 1. Degree based topological indices derived from *M-polynomial*:

Degree based topological index	$f(u,v)$	Derivation from $M(G;u,v)$
$M_1(G)$	$u+v$	$(D_u + D_v)(M(G;u,v))\|_{u=v=1}$
$M_2(G)$	uv	$(D_u D_v)(M(G;u,v))\|_{u=v=1}$
${}^mM_2(G)$	$\frac{1}{uv}$	$(S_u S_v)(M(G;u,v))\|_{u=v=1}$
For $\alpha \in \mathbb{N}$, $R_\alpha(G)$	$(uv)^\alpha$	$(D_u^\alpha D_v^\alpha)(M(G;u,v))\|u=v=1$
For $\alpha \in \mathbb{N}$, $RR_\alpha(G)$	$\frac{1}{(uv)^\alpha}$	$(S_u^\alpha S_v^\alpha)(M(G;u,v))\|_{u=v=1}$
$SDD(G)$	$\frac{u^2+v^2}{uv}$	$(D_u S_v + D_v S_u)(M(G;u,v))\|u=v=1$
$H(G)$	$\frac{2}{u+v}$	$2S_u J(M(G;u,v))\|_{u=v=1}$
$ISI(G)$	$\frac{uv}{u+v}$	$S_u J D_u D_v(M(G;u,v))\|_{u=v=1}$
$AZI(G)$	$\frac{(uv)^3}{(u+v-2)^3}$	$S_u^3 Q_{-2} J D_u^3 D_v^3(M(G;u,v))\|_{u=v=1}$

3. Main results

In this section, we present our main results of computing various degree based indices using the *M-polynomial*. As the first step, applying the operator $D_u,\ D_v$ on *M-polynomial*, we get:

$$D_u M(G;u,v) = u\frac{\partial M(u,v)}{\partial u} = u\left\{\sum_{i\le j} i m_{ij} u^{i-1} v^j\right\} = \sum_{i\le j} i m_{ij} u^i v^j. \tag{11}$$

$$D_u^2 M(G;u,v) = u\frac{\partial}{\partial u}\left\{u\frac{\partial}{\partial u}M(G;u,v)\right\} = \sum_{i\le j} i^2 m_{ij} u^i v^j. \tag{12}$$

Similarly,

$$D_v M(G;u,v) = \sum_{i\le j} j m_{ij} u^i v^j, \tag{13}$$

and

$$D_v^2 M(G;u,v) = \sum_{i\le j} j^2 m_{ij} u^i v^j. \tag{14}$$

$$D_u D_v M(G;u,v) = u\frac{\partial}{\partial u}\left\{v\frac{\partial}{\partial v}M(G;u,v)\right\} = \sum_{i\le j} ij m_{ij} u^i v^j. \tag{15}$$

Next we derive the five topological indices given by equations (1) to (5) from the *M-polynomial*

Theorem 3.1. *Let $M(G;u,v)$ be an M-polynomial for a graph $G(V(G),E(G))$, then the Forgotten index is given by*

$$F(G) = (D_u^2 + D_v^2)M(G;u,v)|_{u=v=1}.$$

Proof. Forgotten index of a graph $G(V(G),E(G))$ is defined as

$$F(G) = \sum_{x\in V(G)} {d_x}^3 = \sum_{xy\in E(G)} ({d_x}^2 + {d_y}^2).$$

Now using equations (6) and (7), we can rewrite the above equation as

$$F(G) = \sum_{xy\in E(G)} ({d_x}^2 + {d_y}^2) = \sum_{i\le j} m_{ij}(i^2 + j^2). \tag{16}$$

Using equations (12) and (14) in (16), we get $F(G) = (D_u^2 + D_v^2)M(G;u,v)|_{u=v=1}$.

Theorem 3.2. *Let $M(G;u,v)$ be an M-polynomial for a graph $G(V(G),E(G))$, then the Reduced Second Zagreb index is given by*

$$RM_2(G) = (D_u - 1)(D_v - 1)M(G;u,v)|_{u=v=1}.$$

Proof. Since,

$$\begin{aligned}(D_u - 1)(D_v - 1)M(G;u,v) &= (D_uD_v - D_u - D_v + 1)M(G;u,v)\\ &= D_uD_vM(G;u,v) - D_uM(G;u,v) - D_vM(G;u,v) + M(G;u,v).\end{aligned} \tag{17}$$

Using equations (11), (13) and (15) in equation (17), then

$$(D_u - 1)(D_v - 1)M(G;u,v) = \sum_{i\le j}(i-1)(j-1)m_{ij}u^iv^j. \tag{18}$$

Rewriting Reduced Second Zagreb index with the help of equations (6) and (7), we get

$$RM_2(G) = \sum_{xy \in E(G)} (d_x - 1)(d_y - 1) = \sum_{i \leq j} m_{ij}(i-1)(j-1). \tag{19}$$

Hence $RM_2(G) = (D_u - 1)(D_v - 1)M(G; u, v)|_{u=v=1}$.

Theorem 3.3. *Let $M(G; u, v)$ be a polynomial for a graph $G(V(G), E(G))$, then Sigma index is given by*

$$\sigma(G) = (D_u - D_v)^2 M(G; u, v)|_{u=v=1}.$$

Proof. Since,

$$\begin{aligned}(D_u - D_v)^2 M(G; u, v) &= (D_u^2 + D_v^2 - 2D_u D_v)M(G; u, v) \\ &= D_u^2 M(G; u, v) + D_v^2 M(G; u, v) - 2D_u D_v M(G; u, v). \end{aligned}\tag{20}$$

Now using equations (12), (14) and (15) in equation (20), then

$$(D_u - D_v)^2 M(G; u, v) = \sum_{i \leq j} (i - j)^2 m_{ij} u^i v^j. \tag{21}$$

Sigma index can be rewritten using equations (6) and (7), as

$$\sigma(G) = \sum_{xy \in E(G)} (d_x - d_y)^2 = \sum_{i \leq j} m_{ij}(i - j)^2. \tag{22}$$

Comparing equations (21) and (22), we get $\sigma(G) = (D_u - D_v)^2 M(G; u, v)|_{u=v=1}$.

Theorem 3.4. *Let $M(G; u, v)$ be an M-polynomial for a graph $G(V(G), E(G))$, then Hyper-Zagreb index is given by*

$$Hyp(G) = (D_u + D_v)^2 M(G; u, v)|_{u=v=1}.$$

Proof. Since,

$$\begin{aligned}(D_u + D_v)^2 M(G; u, v) &= (D_u^2 + D_v^2 + 2D_u D_v)M(G; u, v) \\ &= D_u^2 M(G; u, v) + D_v^2 M(G; u, v) + 2D_u D_v M(G; u, v). \end{aligned}\tag{23}$$

Now using equations (12), (14) and (15) in equation (23), then

$$(D_u + D_v)^2 M(G; u, v) = \sum_{i \leq j} (i + j)^2 m_{ij} u^i v^j. \tag{24}$$

With the help of equations (6) and (7), Hyper Zagreb index can be rewritten as,

$$Hyp(G) = \sum_{xy \in E(G)} (d_x + d_y)^2 = \sum_{i \leq j} m_{ij}(i + j)^2. \tag{25}$$

Now from equations (24) and (25), we get $Hyp(G) = (D_u + D_v)^2 M(G; u, v)|_{u=v=1}$.

Theorem 3.5. *Let $M(G; u, v)$ be an M-polynomial for a given graph $G(V(G), E(G))$, then Albertson index is given by*

$$Alb(G) = (D_v - D_u)M(G; u, v)|_{u=v=1}.$$

Proof. Since,

$$(D_v - D_u)M(G; u, v) = D_v M(G; u, v) - D_u M(G; u, v). \tag{26}$$

Now using equations (11) and (13) in the equation (26), we have

$$(D_v - D_u)M(G; u, v) = \sum_{i \leq j} (j - i) m_{ij} u^i v^j. \tag{27}$$

By using equations (6) and (7), we can rewrite Albertson index as :

$$Alb(G) = \sum_{xy \in E(G)} |d_x - d_y| = \sum_{i \leq j} m_{ij}(j - i). \tag{28}$$

Now from equations (27) and (28), we get $Alb(G) = (D_v - D_u)M(G; u, v)|_{u=v=1}$.

In this section, we have computed the polynomial of five degree based indices other than those mentioned in Table 1 and we have consolidated these results in Table 2.

TABLE 2

Degree based topological index	$f(u, v)$	derivation from $M(G; u, v)$
$F(G)$	$u^2 + v^2$	$(D_u^2 + D_v^2)(M(G; u, v))\|_{u=v=1}$
$RM_2(G)$	$(u - 1)(v - 1)$	$(D_u - 1)(D_v - 1)(M(G; u, v))\|_{u=v=1}$
$\sigma(G)$	$(u - v)^2$	$(D_u - D_v)^2(M(G; u, v))\|_{u=v=1}$
$Hyp(G)$	$(u + v)^2$	$(D_u + D_v)^2(M(G; u, v))\|_{u=v=1}$
$Alb(G)$	$\|u - v\|$	$(D_v - D_u)(M(G; u, v))\|_{u=v=1}$

4. Carbon Nanotubes

In this section, we apply the theoretical results proposed in section 3 to a collection of chemical graphs, namely carbon nanotubes. Carbon nanotubes are a particular type of fullerenes. It constitutes the carbon allotropes formed with a cylindrical structure. Carbon nanotubes are known to have outstanding properties such as high Young's modulus, high tensile strength, high electronics flow, to name a few. At room temperature, the thermal conductivity of nanotubes is higher than that of natural diamond and the basal plane of graphite. Superconductivity has been observed but only at low temperatures [23]. Owing to such properties, carbon nanotubes are well-suited for virtually any application requiring high strength, durability, electrical conductivity, thermal conductivity and lightweight properties compared to conventional materials. For a detailed study on the properties of nanotubes, we refer to [2].

The structural and physical properties of carbon nanotubes have attracted a wide range of application in the field of nanotechnology, electronics, material science, architecture, to name a few. We focus on two nanotubes namely HC_5C_7 and VC_5C_7, the structure of these carbon nanotubes consist of alternating pentagons (C_5) and heptagons (C_7). A three-dimensional representation of these carbon nanotubes is given in Figure 1. The two-dimensional lattice structure of these carbon nanotubes are given in Figure 4, and Figure 7 respectively. For a detailed study of the structural properties of these nanotubes using topological indices, we refer to [7, 19].

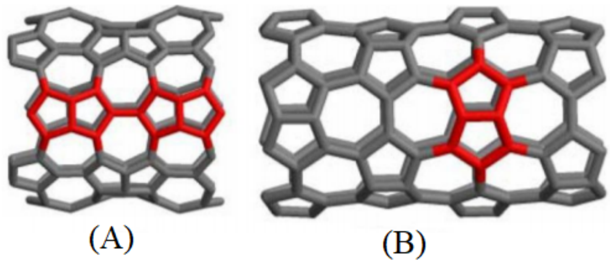

FIGURE 1. 3-D geometry of nanotubes $HC_5C_7(A)$ and $VC_5C_7(B)$.

4.1. $HC_5C_7[p,q]$, $p,q \geq 1$ **Nanotube.** In this section, we compute the degree based indices for graph carbon nanotubes $HC_5C_7[p,q]$ from the *M-polynomial.* As stated before, this nanotube is C_5C_7 net whose two-dimensional lattice structure consists of alternatively arranged pentagons C_5 and heptagons C_7 with a trivalent decoration as shown in Figure 2. In $HC_5C_7[p,q]$, p denotes the number of heptagons C_7 in the first row of its $2-D$ lattice representation and q denotes the number of periods in the whole lattice. Here, a period consists of the four rows, as shown in Figure 3, which represents the i^{th} period. The lattice structure consists of $16p$ vertices in each period along with a set of $2p$ vertices joined as pendants at the last row. Thus, the total number of vertices in this lattice is $|V(HC_5C_7[p,q])| = 16pq + 2p$. Similarly, counting the number of edges, we find that there are $24p$ edges in each period with an additional $2p$ edges which were added (as extra) to connect the pendant vertices to get a $2-D$ lattice, that is, $|E(HC_5C_7[p,q])| = 24pq - 2p$.

Theorem 4.1. *Let G be the graph of the nanotube $HC_5C_7[p,q]$, for $p,q \geq 1$ then its M-polynomial is given by*

$$M(G;u,v) = 8pu^2v^3 + (24pq - 10p)u^3v^3.$$

Proof. To compute the *M-polynomial*, we partition the edges of this nanotube based on the degree of the end vertices. We find that the edges can be partitioned in to exactly two sets given by:

$$\begin{aligned} E_1(G) &= \{xy \in E(G) | d_x = 2 \text{ and } d_y = 3\}, \\ E_2(G) &= \{xy \in E(G) | d_x = d_y = 3\}. \end{aligned}$$

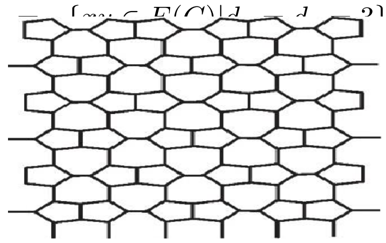

FIGURE 2. 2-D structure of $HC_5C_7[3,3]$ nanotube.

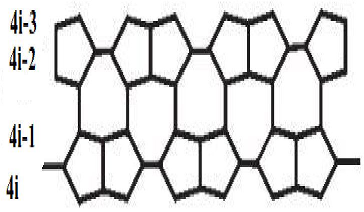

FIGURE 3. i^{th} period of HC_5C_7 nanotube.

FIGURE 4. Structure of $HC_5C_7[3,3]$ nanotube

Number of edges in $E_1(G)$ and $E_2(G)$ are $8p$ and $24pq - 10p$ respectively. Now we compute the *M-polynomial* for given graph $G = HC_5C_7[p,q]$. Since, $\{d_x, d_y\} = \{i,j\}$ and $(i,j) \in \{(2,3),(3,3)\}$ then from Definition 2.1, we have

$$\begin{aligned} M(G;u,v) &= m_{23}u^2v^3 + m_{33}u^3v^3 = |E_1(G)|u^2v^3 + |E_2(G)|u^3v^3 \\ &= 8pu^2v^3 + (24pq - 10p)u^3v^3. \end{aligned}$$

Now using the expression for the *M-polynomial* of $HC_5C_7[p,q]$, and the polynomial representations of the 5 degree based indices (given in Table 2) we compute the exact value of the indices for $HC_5C_7[p,q]$ nanotube as follows:

Theorem 4.2. *The computed value of the degree based indices for the graph $HC_5C_7[p,q]$, $p,q \geq 1$, is given by*

$RM_2(G) = 96pq - 24p, \quad Hyp(G) = 864pq - 160p, \quad F(G) = 432pq - 76p, \quad \sigma(G) = 8p$ *and* $Alb(G) = 8p$.

Proof. From Theorem 4.1, *M-polynomial* for the graph $G = HC_5C_7[p,q]$ is

$$M(G;u,v) = 8pu^2v^3 + (24pq - 10p)u^3v^3,$$

then

$$\begin{aligned} D_uM(G;u,v) &= 16pu^2v^3 + 3(24pq - 10p)u^3v^3, && (29)\\ D_vM(G;u,v) &= 24pu^2v^3 + 3(24pq - 10p)u^3v^3, && (30)\\ D_vD_uM(G;u,v) &= 48pu^2v^3 + 9(24pq - 10p)u^3v^3, && (31)\\ D_u^2M(G;u,v) &= 32pu^2v^3 + 9(24pq - 10p)u^3v^3, && (32)\\ D_v^2M(G;u,v) &= 72pu^2v^3 + 9(24pq - 10p)u^3v^3. && (33) \end{aligned}$$

Applying these operators values given by (29) to (33) in the expressions given in Table 2, we get the required results of the theorem.

4.2. $VC_5C_7[p,q]$, $p,q \geq 1$ **Nanotubes.** In this section, we compute the degree based indices for graph carbon nanotubes $VC_5C_7[p,q]$ from *M-polynomial.* As stated before, this nanotube is a C_5C_7 net whose two-dimensional lattice structure consists of alternatively arranged pentagons C_5 and heptagons C_7 with a trivalent decoration as shown in Figure 5. In $VC_5C_7[p,q]$, p denotes the number of pentagons C_5 in the first row of its $2-D$ lattice representation and q denotes the number of periods in the whole lattice. Here, a period consists of the four rows, as shown in Figure 6, which represents the i^{th} period. In this lattice structure again, there are $16p$ vertices in each period along with a set of $3p$ vertices joined as degree two vertices at the last row. Thus, the total number of vertices in this lattice is $|V(VC_5C_7[p,q])| = 16pq + 3p$. Similarly, counting the number of edges, we find that there are $24p$ edges in each period and there are extra $3p$ edges added to connect the degree two vertices to get a $2-D$ lattice, that is, $|E(VC_5C_7[p,q])| = 24pq - 3p$.

Theorem 4.3. *Let G be the graph of the nanotube $VC_5C_7[p,q]$, for $p,q \geq 1$, then its M-polynomial is given by*

$$M(G;u,v) = pu^2v^2 + 10pu^2v^3 + (24pq - 14p)u^3v^3.$$

Proof. To compute the *M-polynomial*, we partition the edges of this nanotube based on the degree of the end vertices. We find that the edges can be partitioned in to exactly three sets given by:

$$\begin{aligned} E_1(G) &= \{xy \in E(G) | d_x = d_y = 2\},\\ E_2(G) &= \{xy \in E(G) | d_x = 2 \text{ and } d_y = 3\},\\ E_3(G) &= \{xy \in E(G) | d_x = d_y = 3\}. \end{aligned}$$

The number of edges in $E_1(G)$, $E_2(G)$ and $E_3(G)$ are p, $10p$, and $24pq - 14p$. Now we compute the *M-polynomial* for given graph $G = VC_5C_7[p,q]$. Since, $\{d_x, d_y\} = \{i,j\}$, and $(i,j) \in \{(2,2),(2,3),(3,3)\}$ then from Definition 2.1, we have

$$\begin{aligned} M(G;u,v) &= m_{22}u^2v^2 + m_{23}u^2v^3 + m_{33}u^3v^3\\ &= |E_1(G)|u^2v^2 + |E_2(G)|u^2v^3 + |E_3(G)|u^3v^3\\ &= pu^2v^2 + 10pu^2v^3 + (24pq - 14p)u^3v^3. \end{aligned}$$

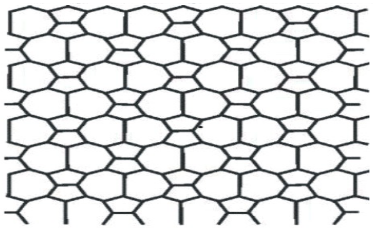

FIGURE 5. $2-D$ graph of $VC_5C_7[3,4]$ nanotube.

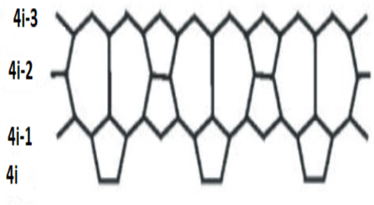

FIGURE 6. Graph of i^{th} period of lattice $VC_5C_7[3,4]$

FIGURE 7. Structure of $VC_5C_7[3,4]$

Now using the expression for the *M-polynomial* of $VC_5C_7[p.q]$, and the polynomial representations of the 5 degree based indices (given in Table Table 2) we compute the exact value of the indices for $VC_5C_7[p.q]$ nanotube as follows:

Theorem 4.4. *The computed value of the degree based indices for the graph of* $VC_5C_7[p,q]$, $p,q \geq 1$ *are given by*

$$\begin{aligned} RM_2(G) &= 96pq - 35p. \\ Hyp(G) &= 864pq - 238p. \\ F(G) &= 432pq - 114p. \\ \sigma(G) &= 10p. \\ Alb(G) &= 10p. \end{aligned}$$

Proof. From Theorem 4.3, *M-polynomial* for the $G = VC_5C_7[p,q]$ is

$$M(G;u,v) = pu^2v^2 + 10pu^2v^3 + (24pq - 14p)u^3v^3,$$

then

$$\begin{aligned} D_uM(G;u,v) &= 2pu^2v^2 + 20pu^2v^3 + 3(24pq - 14p)u^3v^3, && (34) \\ D_vM(G;u,v) &= 2pu^2v^2 + 30pu^2v^3 + 3(24pq - 14p)u^3v^3, && (35) \\ D_uD_vM(G;u,v) &= 4pu^2v^2 + 60pu^2v^3 + 9(24pq - 14p)u^3v^3, && (36) \\ D_u^2M(G;u,v) &= 4pu^2v^2 + 40pu^2v^3 + 9(24pq - 14p)u^3v^3. && (37) \\ D_v^2M(G;u,v) &= 4pu^2v^2 + 90pu^2v^3 + 9(24pq - 14p)u^3v^3. && (38) \end{aligned}$$

Substitute these values given by (34) to (38) in Table 2 we get the required results of the theorem.

5. CONCLUSION

In this paper, we have shown a way to calculate the Reduced Second Zagreb index, Hyper Zagreb index, Forgotten index, Sigma index and Albertson index using *M-polynomial*.

Further, we have shown that computation of these topological indices for carbon nanotubes $HC_5C_7[p,q]$ and $VC_5C_7[p,q]$ becomes very simple and easy when using the M-polynomial.

We observe that the Sigma index and Albertson index behave identically to any nanotube, and it is independent of the number of periods in the lattice structure of a nanotube. Further, the Sigma index of HC_5C_7 depends only on heptagons while Sigma index of VC_5C_7 depends only on pentagons in a period.

In both nanotube structures, the formula obtained for Zagreb indices and the Forgotten index depend on both the total number of pentagons/heptagons in the lattice as well as in each of the period. Another interesting observation is that even though these indices mathematically look dependent, that is, has a similar formulaic pattern, but they differ significantly and hence are incomparable.

Finally, we see that by the application of *M-polynomial* we can reduce drastically the computational effort required to compute most of the degree-based topological indices.

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