Chapter 6

M-Polynomial And VDB Indices

6.1 Introduction

In this chapter, 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 carbon nanotube structures, namely $HC_5C_7[p,q]$, $SC_5C_7[p,q]$ and $VC_5C_7[p.q]$.

The chapter is organized as follows. Section 6.2, we recall some definitions and results. In Section 6.3, we compute degree based indices using the M-polynomial and in the last section 6.4, we apply the M-polynomial to compute the VDB indices for three classes of carbon nanotubes.

6.2 Definitions and Required Results

In this section, we recall some of the definitions stated in Chapter 1 and state related results required for this chapter. Mainly, the five indices that we focus in this chapter is listed below.

For a simple connected graph $G(V(G), E(G))$, the indices are defined as

1. F-index or Forgotten index [77]

$$F(G) = \sum_{u \in V(G)} d(u)^3 = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2). \tag{6.1}$$

2. Reduced Second Zagreb index [40]

$$RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1). \tag{6.2}$$

3. Sigma index [79]

$$\sigma(G) = \sum_{uv \in E(G)} (d(u) - d(v))^2. \tag{6.3}$$

4. Hyper Zagreb index [64]

$$Hyp(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2. \tag{6.4}$$

5. Albertson index [78]

$$Alb(G) = \sum_{uv \in E(G)} |d(u) - d(v)|. \tag{6.5}$$

Definition 6.1. [111] Let $G(V(G), E(G))$ be a graph, then *M-polynomial* of G is given by

$$M(G; x, y) = \sum_{i \leq j} m_{ij} x^i y^j,$$

where m_{ij} denotes the number of edges uv of G whose end vertices have degrees i and j, that is, $\{d(u), d(v)\} = \{i, j\}$.

Definition 6.2. [111] A degree based topological index for a graph G is defined as

$$I(G) = \sum_{e=uv \in E(G)} f(d(u), d(v)), \tag{6.6}$$

where $f(x, y)$ is a function suitably representing some degree based topological indices.

For instance, the first Zagreb index $M_1(G)$ is defined with Equation (6.6) by putting $f(x, y) = x+y$. By counting the edges which have same end-degrees, we can rewrite Equation (6.6) as

$$I(G) = \sum_{i \leq j} m_{ij} f(i, j). \tag{6.7}$$

We require some of the operators as defined in [111]. The operators are listed below :

$$D_x f(x, y) = x \frac{\partial f(x, y)}{\partial x}, \qquad D_y f(x, y) = y \frac{\partial f(x, y)}{\partial y}. \tag{6.8}$$

$$S_x f(x, y) = \int_0^x \frac{f(t, y)}{t} dt, \qquad S_y f(x, y) = \int_0^y \frac{f(x, t)}{t} dt. \tag{6.9}$$

$$J(f(x, y)) = f(x, x), \qquad Q_\alpha(f(x, y)) = x^\alpha f(x, y). \tag{6.10}$$

Note that these operators are well-defined, especially in our case where we consider f(x,y) as a polynomial function.

Next we consolidate the results from [111] as a theorem which is required for our proofs.

Theorem 6.3. *([111],Theorems 2.1, 2.2 and 2.3) Let $G(V(G), E(G))$ be a graph.*

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

2. *If* $I(G) = \sum_{uv\in E(G)} f(d(u), d(v))$, *where* $f(x,y) = \sum_{i,j\in\mathbb{Z}} \alpha_{i,j}x^iy^j$, $\alpha_{i,j} \in \mathbb{R}$ *for each* i, j. *Then* $I(G)$ *can be obtained from M-polynomial using the operators* D_x, D_y, S_x *and* S_y.

3. *If* $I(G) = \sum_{uv\in E(G)} f(d(u), d(v))$, *where* $f(x,y) = \frac{x^ry^s}{(x+y+\alpha)^k}$, *for all* $r, s \geq 0$, $k \geq 1$ *and* $\alpha \in \mathbb{Z}$. *Then* $I(G) = S_x^kQ_\alpha JD_x^rD_y^s(M(G;x,y))|_{x=y=1}$.

With the help of the above theorem, the authors in [111], have proved that certain topological indices can be computed directly from *M-polynomial*. We summarize these results in Table 6.1.

TABLE 6.1: Degree based topological indices derived from *M-polynomial*:

Degree based topological index	$f(x,y)$	Derivation from $M(G;x,y)$
$ZM_1(G)$	$x+y$	$(D_x+D_y)(M(G;x,y))\|_{x=y=1}$
$ZM_2(G)$	xy	$(D_xD_y)(M(G;x,y))\|_{x=y=1}$
$^mM_2(G)$	$\frac{1}{xy}$	$(S_xS_y)(M(G;x,y))\|_{x=y=1}$
For $\alpha\in\mathbb{N}$, $R_\alpha(G)$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\|x=y=1$
For $\alpha\in\mathbb{N}$, $RR_\alpha(G)$	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\|_{x=y=1}$
$SDD(G)$	$\frac{x^2+y^2}{xy}$	$(D_xS_y+D_yS_x)(M(G;x,y))\|x=y=1$
$H(G)$	$\frac{2}{x+y}$	$2S_xJ(M(G;x,y))\|_{x=y=1}$
$ISI(G)$	$\frac{xy}{x+y}$	$S_xJD_xD_y(M(G;x,y))\|_{x=y=1}$
$AZI(G)$	$\frac{(xy)^3}{(x+y-2)^3}$	$S_x^3Q_{-2}JD_x^3D_y^3(M(G;x,y))\|_{x=y=1}$

6.3 Main Results

In this section, we present our main results on computing various degree based indices using the *M-polynomial*. As the first step, when applying the operator D_x, D_y on *M-polynomial*, we get:

$$D_xM(G;x,y) = x\frac{\partial M(x,y)}{\partial x} = x\left\{\sum_{i\leq j} im_{ij}x^{i-1}y^j\right\} = \sum_{i\leq j} im_{ij}x^iy^j. \tag{6.11}$$

$$D_x^2M(G;x,y) = x\frac{\partial}{\partial x}\left\{x\frac{\partial}{\partial x}M(G;x,y)\right\} = \sum_{i\leq j} i^2m_{ij}x^iy^j. \tag{6.12}$$

Similarly,

$$D_y M(G;x,y) = \sum_{i\leq j} j m_{ij} x^i y^j, \tag{6.13}$$

and

$$D_y^2 M(G;x,y) = \sum_{i\leq j} j^2 m_{ij} x^i y^j. \tag{6.14}$$

$$D_x D_y M(G;x,y) = x\frac{\partial}{\partial x}\left\{ y\frac{\partial}{\partial y} M(G;x,y)\right\} = \sum_{i\leq j} ij m_{ij} x^i y^j. \tag{6.15}$$

Next we derive the five topological indices given by Equations (6.1) to (6.5) from the *M-polynomial*

Theorem 6.4. *Let $M(G;x,y)$ be an M-polynomial for a graph $G(V(G),E(G))$, then the Forgotten index is given by*

$$F(G) = (D_x^2 + D_y^2)M(G;x,y)|_{x=y=1}.$$

Proof. Now using Equations (6.6) and (6.7) in the Equation 6.1 of the Forgotten index, we get

$$F(G) = \sum_{uv\in E(G)} (d(u)^2 + d(v)^2) = \sum_{i\leq j} m_{ij}(i^2+j^2). \tag{6.16}$$

Now by using the Equations (6.12) and (6.14) in (6.16), we immediately obtain that $F(G) = (D_x^2 + D_y^2)M(G;x,y)|_{x=y=1}$. □

Theorem 6.5. *Let $M(G;x,y)$ be an M-polynomial for a graph $G(V(G),E(G))$, then the Reduced Second Zagreb index is given by*

$$RM_2(G) = (D_x - 1)(D_y - 1)M(G;x,y)|_{x=y=1}.$$

Proof. Note that

$$\begin{aligned}(D_x-1)(D_y-1)M(G;x,y) &= (D_xD_y - D_x - D_y + 1)M(G;x,y)\\ &= D_xD_yM(G;x,y) - D_xM(G;x,y) - D_yM(G;x,y) + M(G;x,y).\end{aligned} \tag{6.17}$$

By using Equations (6.11), (6.13) and (6.15) in Equation (6.17) and upon simplification, we then get

$$(D_x - 1)(D_y - 1)M(G; x, y) = \sum_{i \leq j} (i-1)(j-1)m_{ij}x^i y^j. \tag{6.18}$$

Rewriting Reduced Second Zagreb index with the help of Equations (6.6) and (6.7), we get

$$RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1) = \sum_{i \leq j} m_{ij}(i-1)(j-1). \tag{6.19}$$

Hence $RM_2(G) = (D_x - 1)(D_y - 1)M(G; x, y)|_{x=y=1}$. □

Theorem 6.6. *Let $M(G; x, y)$ be a polynomial for a graph $G(V(G), E(G))$, then Sigma index is given by*

$$\sigma(G) = (D_x - D_y)^2 M(G; x, y)|_{x=y=1}.$$

Proof. Since,

$$\begin{aligned}(D_x - D_y)^2 M(G; x, y) =& (D_x^2 + D_y^2 - 2D_x D_y)M(G; x, y) \\ =& D_x^2 M(G; x, y) + D_y^2 M(G; x, y) - 2D_x D_y M(G; x, y).\end{aligned} \tag{6.20}$$

Now using Equations (6.12), (6.14) and (6.15) in Equation (6.20), then

$$(D_x - D_y)^2 M(G; x, y) = \sum_{i \leq j} (i-j)^2 m_{ij} x^i y^j. \tag{6.21}$$

Sigma index can be rewritten using Equations (6.6) and (6.7), as

$$\sigma(G) = \sum_{uv \in E(G)} (d(u) - d(v))^2 = \sum_{i \leq j} m_{ij}(i-j)^2. \tag{6.22}$$

Comparing Equations (6.21) and (6.22), we get $\sigma(G) = (D_x - D_y)^2 M(G; x, y)|_{x=y=1}$. □

Theorem 6.7. *Let $M(G; x, y)$ be an M-polynomial for a graph $G(V(G), E(G))$, then Hyper-Zagreb index is given by*

$$Hyp(G) = (D_x + D_y)^2 M(G; x, y)|_{x=y=1}.$$

Proof. Note that

$$\begin{aligned}(D_x + D_y)^2 M(G;x,y) =& (D_x^2 + D_y^2 + 2D_xD_y)M(G;x,y)\\ =& D_x^2M(G;x,y) + D_y^2M(G;x,y) + 2D_xD_yM(G;x,y).\end{aligned} \tag{6.23}$$

Now using Equations (6.12), (6.14) and (6.15) in Equation (6.23), then

$$(D_x + D_y)^2 M(G;x,y) = \sum_{i\leq j}(i+j)^2 m_{ij}x^iy^j. \tag{6.24}$$

With the help of Equations (6.6) and (6.7), Hyper Zagreb index can be rewritten as,

$$Hyp(G) = \sum_{uv\in E(G)} (d(u)+d(v))^2 = \sum_{i\leq j} m_{ij}(i+j)^2. \tag{6.25}$$

Now from Equations (6.24) and (6.25), we get $Hyp(G) = (D_x + D_y)^2 M(G;x,y)|_{x=y=1}$. □

Theorem 6.8. *Let $M(G;x,y)$ be an M-polynomial for a given graph $G(V(G),E(G))$, then Albertson index is given by*

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

Proof. : Since,

$$(D_y - D_x)M(G;x,y) = D_yM(G;x,y) - D_xM(G;x,y). \tag{6.26}$$

Now using Equations (6.11) and (6.13) in the Equation (6.26), we have

$$(D_y - D_x)M(G;x,y) = \sum_{i\leq j}(j-i)m_{ij}x^iy^j. \tag{6.27}$$

By using Equations (6.6) and (6.7), we can rewrite Albertson index as :

$$Alb(G) = \sum_{uv\in E(G)} |d(u)-d(v)| = \sum_{i\leq j} m_{ij}(j-i). \tag{6.28}$$

Now from Equations (6.27) and (6.28), we get $Alb(G) = (D_y - D_x)M(G;x,y)|_{x=y=1}$. □

In this section, we have computed the polynomial of five degree based indices other than those mentioned in Table 6.1 and have consolidated these results in Table 6.2.

Table 6.2: M-Polynomial for more degree based topological indices

Degree based topological index	$f(x,y)$	derivation from $M(G;x,y)$
$F(G)$	x^2+y^2	$(D_x^2+D_y^2)(M(G;x,y))\|_{x=y=1}$
$RM_2(G)$	$(x-1)(y-1)$	$(D_x-1)(D_y-1)(M(G;x,y))\|_{x=y=1}$
$\sigma(G)$	$(x-y)^2$	$(D_x-D_y)^2(M(G;x,y))\|_{x=y=1}$
$Hyp(G)$	$(x+y)^2$	$(D_x+D_y)^2(M(G;x,y))\|_{x=y=1}$
$Alb(G)$	$\|x-y\|$	$(D_y-D_x)(M(G;x,y))\|_{x=y=1}$

6.4 Application to Nanotubes

In this section, we apply the theoretical results proposed in section 6.3 to a collection of chemical graphs, namely carbon nanotubes. Carbon nanotubes are a particular type of fullerenes. It constitutes the carbon allotropes formed in 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 [127]. 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 [128].

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 three nanotubes namely HC_5C_7, SC_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 6.1. The two-dimensional lattice structure of these carbon nanotubes are given in Figure 6.2, Figure 6.3 and Figure 6.4 respectively. For a detailed study of the structural properties of these nanotubes using topological indices, we refer to [125, 129].

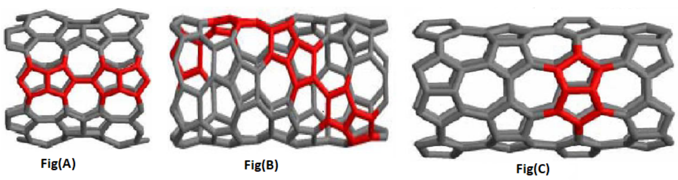


Figure 6.1: 3-D geometry of nanotubes $HC_5C_7(A)$, $SC_5C_7(B)$ and $VC_5C_7(C)$.

6.4.1 HC5C7 Nanotubes

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 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 6.2. 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 6.2, 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, $|E(HC_5C_7[p,q])| = 24pq - 2p$.

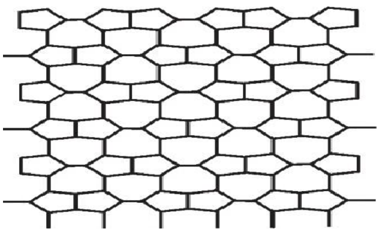
Theorem 6.9. *Let G be the graph of the nanotube $HC_5C_7[p,q]$, for $p,q \geq 1$ then its M-polynomial is given by*

$$M(G;x,y) = 8px^2y^3 + (24pq - 10p)x^3y^3.$$

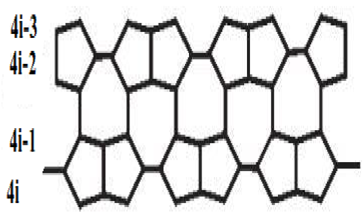
Proof. To compute the *M-polynomial*, we partition the edges of this nanotube based on the degree of the end vertices. We find that the edges can be partitioned in to exactly two sets given by:

$$E_1(G) = \{uv \in E(G)|d(u) = 2 \text{ and } d(v) = 3\}, \ E_2(G) = \{uv \in E(G)|d(u) = d(v) = 3\}.$$

Number of edges in $E_1(G)$ and $E_2(G)$ are $8p$ and $24pq - 10p$ respectively. Now we compute the *M-*



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



i^{th} period of HC_5C_7.

FIGURE 6.2: Structure of $HC_5C_7[3,3]$ nanotube.

polynomial for given graph $G = HC_5C_7[p,q]$. Since, $\{d(u), d(v)\} = \{i, j\}$ and $(i,j) \in \{(2,3),(3,3)\}$

then from Definition 6.1, we have

$$M(G;x,y) = m_{23}x^2y^3 + m_{33}x^3y^3 = |E_1(G)|x^2y^3 + |E_2(G)|x^3y^3$$
$$= 8px^2y^3 + (24pq - 10p)x^3y^3.$$

□

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 6.2) we compute the exact value of the indices for $HC_5C_7[p,q]$ nanotube as follows:

Theorem 6.10. *The computed value of the degree based indices for the graph* $HC_5C_7[p,q]$, $p,q \geq 1$, *is given by*

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

Proof. From Theorem 6.9, *M-polynomial* for the graph $G = HC_5C_7[p,q]$ is

$$M(G;x,y) = 8px^2y^3 + (24pq - 10p)x^3y^3,$$

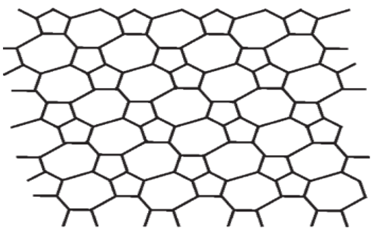
then

$$D_xM(G;x,y) = 16px^2y^3 + 3(24pq - 10p)x^3y^3, \tag{6.29}$$
$$D_yM(G;x,y) = 24px^2y^3 + 3(24pq - 10p)x^3y^3, \tag{6.30}$$
$$D_yD_xM(G;x,y) = 48px^2y^3 + 9(24pq - 10p)x^3y^3, \tag{6.31}$$
$$D_x^2M(G;x,y) = 32px^2y^3 + 9(24pq - 10p)x^3y^3, \tag{6.32}$$
$$D_y^2M(G;x,y) = 72px^2y^3 + 9(24pq - 10p)x^3y^3. \tag{6.33}$$

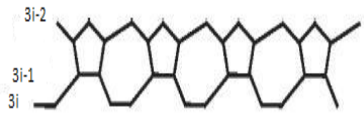
Applying the operators values given by (6.29) to (6.33) in the expressions given in Table 6.2, we get the required results of the theorem. □

6.4.2 SC5C7 Nanotubes

In this section, we compute the degree based indices for the carbon nanotubes $SC_5C_7[p,q]$ from $M-polynomial$. As stated before, this nanotube is a C_5C_7 net whose two-dimensional lattice structure consists of alternately arranged pentagons (C_5) and heptagons (C_7) with a trivalent decoration as shown in Figure 6.3. In $SC_5C_7[p,q]$, 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 three rows, as shown in Figure 6.3, which represents the i^{th}-period. In this lattice structure, there are $8p$ vertices in each period. Thus, the total number of vertices in this lattice is $|V(SC_5C_7)[p,q]| = 8pq$. Similarly, counting the number of edges, we find that there are $12p$ edges in each period and there are additional $2p$ edges which were joined as extra at the ends of the lattice structure, that is $|E(SC_5C_7[p,q])| = 12pq - 2p$.



2-D structure of $SC_5C_7[4,4]$.



i^{th} period of $SC_5C_7[p,q]$.

FIGURE 6.3: Structure of $SC_5C_7[p,q]$ nanotube.

Theorem 6.11. *[117] Let G be the graph of this nanotube, the $M-polynomial$ of $G = SC_5C_7[p,q]$ is given by*

$$M(G;x,y) = px^2y^2 + 6px^2y^3 + (12pq - 9p)x^3y^3.$$

□

Now using the expression for the $M-polynomial$ of $SC_5C_7[p.q]$, and the polynomial representations of the 5 degree based indices (given in Table 6.2) we compute the exact value of the indices for $SC_5C_7[p,q]$ nanotube as follows:

Theorem 6.12. *The computed value of the degree based indices for the graph $G = SC_5C_7[p,q]$, $p,q \geq 1$, are given by*

$$RM_2(G) = 48pq - 23p, \qquad Hyp(G) = 432pq - 158p,$$

$$F(G) = 216pq - 76p, \qquad \sigma(G) = 6p,$$

$$Alb(G) = 6p.$$

Proof. : From Theorem 6.11, $M - polynomial$ for the graph $G = SC_5C_7[p, q]$ is

$$M(G; x, y) = px^2y^2 + 6px^2y^3 + (12pq - 9p)x^3y^3,$$

then

$$D_xM(G; x, y) = 2px^2y^2 + 12px^2y^3 + 3(12pq - 9p)x^3y^3, \quad (6.34)$$

$$D_yM(G; x, y) = 2px^2y^2 + 18px^2y^3 + 3(12pq - 9p)x^3y^3, \quad (6.35)$$

$$D_yD_xM(G; x, y) = 4px^2y^2 + 36px^2y^3 + 9(12pq - 9p)x^3y^3, \quad (6.36)$$

$$D_x^2M(G; x, y) = 4px^2y^2 + 24px^2y^3 + 9(12pq - 9p)x^3y^3, \quad (6.37)$$

$$D_y^2M(G; x, y) = 4px^2y^2 + 54px^2y^3 + 9(12pq - 9p)x^3y^3. \quad (6.38)$$

Substituting these values given by (6.34) to (6.38) in the expressions given in Table 6.2 we get the required results of the theorem. □

6.4.3 VC5C7 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 also 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 6.4. 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 6.4, 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, $|E(VC_5C_7[p, q])| = 24pq - 3p$.

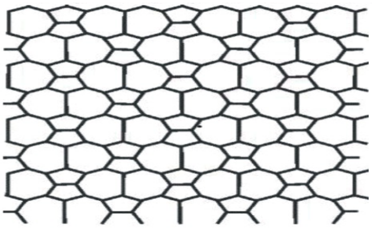
Theorem 6.13. *Let G be the graph of the nanotube $VC_5C_7[p, q]$, for $p, q \geq 1$, then its M-polynomial is given by*

$$M(G; x, y) = px^2y^2 + 10px^2y^3 + (24pq - 14p)x^3y^3.$$

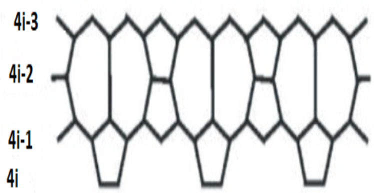
Proof. To compute the *M-polynomial*, we partition the edges of this nanotube based on the degree of the end vertices. We find that the edges can be partitioned in to exactly three sets given by:

$$E_1(G) = \{uv \in E(G)|d(u) = d(v) = 2\},$$
$$E_2(G) = \{uv \in E(G)|d(u) = 2 \ and \ d(v) = 3\},$$
$$E_3(G) = \{uv \in E(G)|d(u) = d(v) = 3\}.$$

The number of edges in $E_1(G)$, $E_2(G)$ and $E_3(G)$ are p, $10p$, and $24pq - 14p$. Now we compute



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



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

FIGURE 6.4: Structure of $VC_5C_7[3, 4]$ nanotube

the *M-polynomial* for given graph $G = VC_5C_7[p, q]$. Since, $\{d(u), d(v)\} = \{i, j\}$, and $(i, j) \in \{(2, 2), (2, 3), (3, 3)\}$ then from Definition 6.1, we have

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

□

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 6.2) we compute the exact value of the indices for $VC_5C_7[p.q]$ nanotube as follows:

Theorem 6.14. *The computed value of the degree based indices for the graph of* $VC_5C_7[p,q]$*,* $p,q \geq 1$ *are given by*

$$RM_2(G) = 96pq - 35p, \qquad Hyp(G) = 864pq - 238p,$$
$$F(G) = 432pq - 114p, \qquad \sigma(G) = 10p,$$
$$Alb(G) = 10p.$$

Proof. From Theorem 6.13, *M-polynomial* for the $G = VC_5C_7[p,q]$ is

$$M(G;x,y) = px^2y^2 + 10px^2y^3 + (24pq - 14p)x^3y^3,$$

then

$$D_xM(G;x,y) = 2px^2y^2 + 20px^2y^3 + 3(24pq - 14p)x^3y^3, \tag{6.39}$$
$$D_yM(G;x,y) = 2px^2y^2 + 30px^2y^3 + 3(24pq - 14p)x^3y^3, \tag{6.40}$$
$$D_xD_yM(G;x,y) = 4px^2y^2 + 60px^2y^3 + 9(24pq - 14p)x^3y^3, \tag{6.41}$$
$$D_x^2M(G;x,y) = 4px^2y^2 + 40px^2y^3 + 9(24pq - 14p)x^3y^3. \tag{6.42}$$
$$D_y^2M(G;x,y) = 4px^2y^2 + 90px^2y^3 + 9(24pq - 14p)x^3y^3. \tag{6.43}$$

Substituting the values given by (6.39) to (6.43) in Table 6.2 we get the required results of the theorem. □

6.5 Summary

In this chapter, 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, SC_5C_7 depends only on heptagons while Sigma index of VC_5C_7 depends only on pentagons in a period.

In each of the nanotube structures, the formula obtained for reduced second Zagreb index 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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