On Some Polynomials of The Chemical Nanotubes

By

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A Post Graduate Thesis submitted to the Department of Mathematics as partial fulfilment of the requirement for the award of Degree of M.S.

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I Nighat Farah **CIIT/FA14-MSMATH-003/LHR** hereby declare that I have produced the work presented in this thesis, during the scheduled period of study. I also declare that I have not taken any material from any source except referred to wherever due that amount of plagiarism is within acceptable range. If a violation of HEC rules on research has occurred in this thesis, I shall be liable to punishable action under the plagiarism rules of the HEC.

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It is certified that Nighat Farah **CIIT/FA14-MSMATH-003/LHR** has carried out all the work related to this thesis under my supervision at the Department of Mathematics, COMSATS Institute of Information Technology, Lahore and the work fulfills the requirement for award of MS degree.

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To my beloved parents, my husband and my teachers

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Quran has revealed for the fact in SURAH YASIN, ”It is not permitted to the sun to catch the moon, nor can the night outstrip the day, each swims in their orbits”. Allah the great creator who created me and this universe. He also give me thinking power and willpower to do something in literature. Due to HIS kindness I have completed this thesis and make a little part in the vast sea of knowledge. It is THE Almighty Allah who blessed me with talented teachers, potential and succeed me. My special praise for ”HOLY PROPHET MUHAMMAD (PBUH)” the backbone of knowledge WHO guided HIS ”Umma” to seek knowledge from cradle to grave and WHO is forever touch of the guidance and knowledge for humanity as a whole. If pearls are words and flowers shows feelings it would be much easier to express our heartful gratitude and indebtedness to the people who helped me to complete this manuscript in such a short duration. Words are short space is limited and appreciation for their health is more than we can express in such a short duration. Words are short space is limited and appreciation for their health is more than we can express in such confines. Still I would like to pay thanks and appreciation to my profound supervisor Dr. SARFRAZ AHMAD under whose inspiring guidance I reach to take the completion of this work. I would like also thanks to MAM UZMA for her cooperation and guidance. My heart bowing thanks to my beloved daughter ADAN BILAL for her prayers and love. Sincere thanks to my sisters SHAMA and SHUMAILA for their support and obedience. Special thanks to my brothers M. SAEED, SAMEED and ALI HAIDER whose love, care and help make us able to complete this manuscript. May Allah give all above mentioned personalities a long happy life. (Amin)

Lahore, Pakistan Nighat Farah

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Abstract

In the thesis we have calculated toplogical indices of some Carbon and Boron nanotubes. We have formulated for Omega and Counting polynomials of these nanotubes very firstly in literature. The counting polynomials are valuable in forecasting of different structures. It also helps to describe its topological indices by virtue of quasi-orthogonal cuts of the edge strips in the polycyclic graphs. In this thesis we have given a complete description of the Omega and the Sadhana polynomial of the nanotube $TUC_4[p,q]$ and provide its mathematical proof. We also give explicit formulae for the PI and the theta polynomial of $TUC_4[p,q]$ nanotubes. We have also given a brief note on different types of the Zagreb indices of the nanotubes $\mathrm{TUC}_4[p,q]$ and $\mathrm{TUC}_5C_6C_8[p,q]$. In QSAR/QSPR study, the topological indices are being utilized for envisioning the biological and physical properties of compunds. These indices are very important in mathematical chemistry as well. These topological indices have many applications of statistical tools in chemical reactivity, physical properties and biological activities. In this thesis we have exactly computed the Zagreb indices, GA index, the randic index and the ABC index of the $\mathrm{TU}C_5C_8$ nanotubes. In mathematical chemistry, a topological index is computed using structure of the molecular graph and is a numerical parameter which describe its topology. Using combinatorial techniques we also provide explicit formulae of the different types of the Zagreb indices, GA index, the Randic index and ABC index of *the zigzag boron triangular* nanotubes $\mathrm{BNT}[p,q]$ and armchair boron triangular nanotubes.

Chapter 1

Introduction

We have divided the first chapter into two halves. In the first half, we have discussed some carbon nano structures in nanotechnology with basic notations. These structures include TUC_4, formed from C_4, $TUC_5C_6C_8$, formed from C_5, C_6, C_8 and TUC_5C_8 formed from C_5, C_8. There are also we defined some definitions like topological index, distance between two points, orthogonal cuts, Omega polynomial, Sadhana polynomial, Pi polynomial, Theta polynomial and sadhana index for any connected graph G. These polynomials are already defined for TUC_4C_8 nanotubes and nanotorus[30], $F_{12(2n+1)}$ Fullerenes[29], anthracene, phenanthrene, polyhex toroidal structures [18], Cuneane[16], tubular nanostructures [17], polyomino chains of 8-cycle, TiO_2, triangular benezenoid graphs[28], a planar bipartite cage and its corresponding nets. These polynomials are being computed for more carbon nanotubes nanotori structures. In the second half, we discuss boron nanotubes. The nanotechnology involves different structures of nanotubes including boron nanotubes. Recent discovery of boron nanotubes provocation the production of carbon due to their triangular structure. In this section, we have introduced some topological indices. These indices include Zagreb indices, Hyper Zagreb index, Atom-bond index, Geometric arithmetic index, the Augmented index, the Randic index. In literature, The hyper zagreb indices of $TUSC_4C_8$ nanotubes[23], hexagonal nanotubes [24], some Connectivity and zagreb indices of polyhex nanotubes[21], Zagreb polynomials and indices of $VAC_5C_7(S)$ nanotube [25], Zagreb indices and zagreb polynomial of $HAC_5C_6C_7$ nanotubes[25], some topological indices of $TUC_4C_6C_8$ nanotubes[43], In the second chapter we have given a brief description on the counting polynomials of TUC_4. The counting polynomials are those polynomials are being supporter of any quality division in correspondance of another characteristics. In mathematical chemistry the counting polynomials are related to the name of Hosoya: independent edge sets are counted by $Z(G,x)$ and distances counted by $H(G,x)$ polynomials. Their radicals and coordinates are used for the imitation of topological properties of hydrocarbons. The four counting polynomials, defined by Diudea[6−9], namely the Omega, the Sadhana, the PI and the theta polynomials are given as,

$$\Omega(G,x) = \Sigma_c m(G,c)x^c,$$

$$Sd(G,x) = \sum_c m(G,x)x^{E(G)-c},$$

$$\Pi(G,x) = \Sigma_c m(G,c)x^{|E(G)|-c},$$

$$\Theta(G,x) = \Sigma_c m(G,c)cx^c,$$

respectively. In the third chapter we have discussed and calculated exact formulae for the topological indices i.e zagreb indices, Hyper zagreb index of carbon nanostructures TUC_4 and $TUC_5C_6C_8$. In the fourth chapter degree based topologoical indices have been calculated for TUC_5C_8. These indices are the same as find out in previous chapters. Fifth chapter of this thesis included another important type of nanotubes i.e zigzag boron nanotube $BNT[p,q]$. Its structure formed from boron is more complicated than carbon. But boron nanotubes are most useful in nanotechnology than carbon nanotubes. We have discussed and formulate some topological indices of zigzag boron nanotubes. In general, these indices are first and second zagreb index, Hyper zagreb index, zagreb polynomials, ABC index, Geometric arithmetic index, the Randic index. In the sixth chapter we have discussed degree based indices for another type of boron nanotubes naming armchair boron nanotubes. We also calculated exact formulae of these indices.

Chapter 2

Basic Definitions And Notations

2.1 Omega And Counting Polynomials

One of the extraordinary procurement in the field of nanotechnology is the carbon nanotubes(CNT) amalgam. It was discovered by Iijima[12] in 1991. Single walled carbon nanotubes (SWCNTs) attracted much recognition in the World were introduced two years later. The nanotechnology is a study of the nanostructures between 1 to 100 nanometers in size. With the help of the nanotechnology nanotubes have a lot of applications in the field of pharmaceutics and communications. Carbon nanotubes are made from graphene. The diameter of (SWNT) and (MWNT) are 0.8 to 2nm and 5nm to 20nm respectively, form a rope like structure, although the diameter of multi walled nanotubes may be more than 100 nm with length 100 nm to 0.5m [54]. Due to the potential and physical properties carbon nanotubes have immense interest in community. Carbon nanotubes may be metallic or semiconductor according to their orientation of lattice i.e these are chiral and armchair. The nanotubes, named after the thick sheets of graphene, are consisting of such sheets rotate at explicit and distinct angles. Also the combination of the rolling angles effect on shapes of nanotubes. The radius of nanotubes decides whether these are metals and semiconductors. In actual nanotubes form a small part of sports goods. Carbon nanotubes production is increased more than thousands tons yearly from 2013. These nanotubes are used in energy storage devices, automotive parts, filters, thin film electronics, coatings, and electromagnetic shields[51]. However, it is not easy to harmonize CNTs with undeniable surface features as needed for the specific accomplishments. Some interested work on the CNTs in chemistry has recently been studied in literature [1]-[53]. Let us consider any connected graph be represented by

$$G = (V, E),$$

where V denotes vertices of the graph and E presents the edges of a graph. We use G to represent any graph in this thesis. This branch of theoretical chemistry is being used to explore latest important ideas in Chemistry. The first topological index defined in mathematical chemistry is Hosoya index. Other than this older indices are Randic index, Wiener index, Balban's J index. Hosea and Wiener index are known as Global indices. The ETA (The Extended Topological atom) indices have been applied in the development of QSAR/QSPR/QSTR models. These topological indices have many applications of statistical tools in chemical reactivity, physical properties and biological activities e.g therapy and side effects of drugs, toxicity prediction, environmental pollutants, regulatory decisions[10]-[11],[46] and lead optimization.

Definition 2.1.1. *There is an important branch of chemistry which is used for studying the structures of different nanotubes, with the help of graph theory it has great preferences in nanotechnology is called mathematical chemistry.*

For consultation we refer the reader to [1]-[12], [14].

Definition 2.1.2. *Let us consider any connected graph be represented by*

$$G = (V, E).$$

A graph G can be described by a connection table, a sequence of numbers, a matrix, a polynomial or by a derived unique number often called a topological index.

Definition 2.1.3. *Suppose G be a connected graph with vertex set and the edge set represent as $V(G)$, $E(G)$ respectively. It is to be noted that there should not be loops and multiple edges. Then the smallest path connecting any two vertices say x and y of G, is called distance between x and y and it is denoted by $d(x, y)$.*

Definition 2.1.4. *Let $e_1 = a_1b_1$ and $e_2 = a_2b_2$ be the two distinct edges of G then e_1 is said to be codistant to e_2, written as e_1 co e_2, with satisfaction of the following properties:*

$$d(a_1a_2) = d(b_1b_2) = k$$

$$d(a_1b_2) = d(b_1a_2) = k + 1.$$

If the reflexive and symmetric properties are satisfied for $C(e)$ but transitivity is not necessary. If the set

$$C(e) = \{e_i \in E(G) | e_i \text{ co } e\}$$

satisfies transitivity then $C(e)$ is said to be orthogonal cut "oc" of G. The graph G is called oc-graph if and only if the $E(G)$ is the union of disjoint orthogonal cuts, i.e $C(e_1) \cup C(e_2) \cup C(e_3) \cup \ldots \cup C(e_n)$ and $C(e_i) \cap C(e_j) = \phi$.

Definition 2.1.5. *Let $m(G, c)$ be the number of orthogonal cuts in the graph G. Then the omega polynomial is defined as*

$$\Omega(G, x) = \Sigma_c m(G, c) x^c.$$

The counting polynomials are the supporter for the strength of an attribute division and radicles the circumstances of the corresponding partition. In mathematical chemistry the counting polynomials are related to the name of Hosoya: independent edge sets are counted by $Z(G, x)$ and distances counted by $H(G, x)$ polynomials. These polynomials have application for studying the nature of hydrocarbons. The four counting polynomials, defined by Diudea[6–9], namely the Omega, the Sadhana, the PI and the theta polynomials are given as,

$$\Omega(G, x) = \Sigma_c m(G, c) x^c,$$

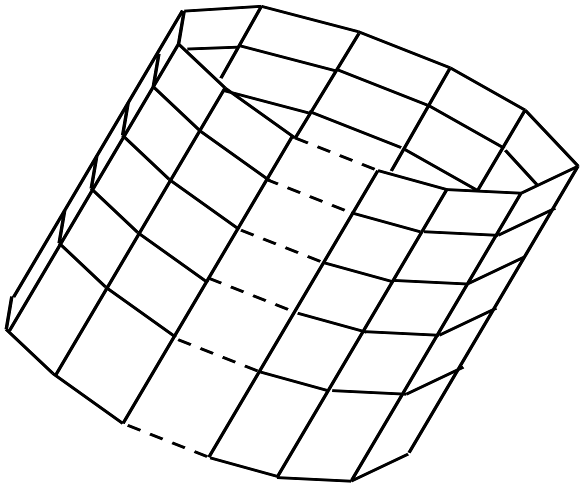

Figure 2.1: $\mathrm{TUC}_4[p, 5]$

$$Sd(G, x) = \sum_c m(G, x)x^{E(G)-c},$$

$$\Pi(G, x) = \Sigma_c m(G, c)cx^{|E(G)|-c},$$

$$\Theta(G, x) = \Sigma_c m(G, c)cx^c,$$

respectively. In this thesis we have calculated these four counting polynomials for the nanotubes covered by C_4 mathematically. These nanotubes are denoted by $\mathrm{TUC}_4[p, q]$. Figure 9.1.1 depicts $\mathrm{TUC}_4[p, 5]$. Let q and p be the number of levels in $\mathrm{TUC}_4[p, q]$ and the number of squares at one level, respectively. In this thesis topological indices of some more carbon structures have discussed. These structures included TUC_5C_8 and $TUC_5C_6C_8$ formed from C_5C_8 and $C_5C_6C_8$ nets respectively.

2.2 Boron Nanotubes And Topological Indices

In this section we have discussed another valuable nanostructure, called boron nanotubes and after that defined some topological indices. The nanotechnology is the

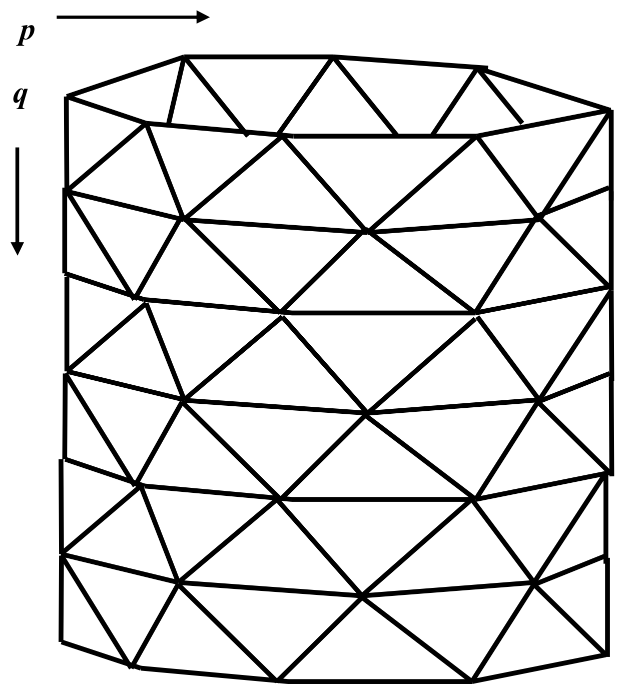

Figure 2.2: Zigzag Boron Triangular Nanotubes $BNT[p, q]$

study of nanostructures which helps to create many new materials and devices having applications in space, pharmaceutics and communication. The nanotechnology involves different structures of nanotubes including boron nanotubes. Boron nanotubes were created very recently in 2004 but it challenges the carbon nanotubes. A boron triangular sheet is same as that of a hexagonal sheet with addition of extra atom in the center as shown in figure 8.2. Most of the scientists think that carbon nanotubes are not better than boron nanotubes [7], [48]. The boron sheets are formed from self doping i.e when we have added an atom at the center of hexagonal structure like benzene. The number of electrons may change. This triangular sheet can be flat or buckled. The shape of the boron sheet depends on the ratio between hexagons and triangles. The single walled boron nanotubes are less stable than double boron nanotubes. These boron sheets are used in semiconductors and for transmission. There are different types of boron nanotubes depending angles and chirality e.g zigzag, armchair and chiral boron nanotubes. The *zagreb indices*, adherent to one of the most studied index, were introduced by I. Gutman and N. Trinajstic.

Definition 2.2.1. *The first and second zagreb indices of the graph G are defined as:*

$$\begin{aligned} \mathrm{M}_1(G) &= \sum_{e=uv\in E(G)} (d_u + d_v) \\ \mathrm{M}_2(G) &= \sum_{e=uv\in E(G)} (d_u * d_v), \end{aligned}$$

where d_u and d_v denote the degrees for the respective vertices.

Similarly the *zagreb polynomials* for the graph G in variable x are given as:

$$\begin{aligned} \mathrm{Zg}_1(G,x) &= \sum_{e=uv\in E(G)} x^{(d_u+d_v)} \\ \mathrm{Zg}_2(G,x) &= \sum_{e=uv\in E(G)} x^{(d_u*d_v)}. \end{aligned}$$

In 2013 another important index based on distance, named *hyper-zagreb index* created by Sayadi, A. M., Shirdel, G. H., and Rezapour, H. citeF2.

Definition 2.2.2. *Hyper-Zagreb index of any graph G is defined as*

$$\mathrm{HM}(G) = \sum_{e=uv\in E(G)} (d_u + d_v)^2.$$

In [31], [53], the *Augmented Zagreb* index was introduced.

Definition 2.2.3. *The Augmented Zagreb index of the graph G is defined as*

$$\mathrm{AZI}(G) = \sum_{uv\in E(G)} (\frac{d_u d_v}{d_u + d_v - 2})^3.$$

The Randic index was introduced in 1975 by Milan Randic [34], [41], [47], [52] who proved the reflection of this index in splitting of molecular structures.

Definition 2.2.4. *The Randic Index is defined as follows:*

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Definition 2.2.5. *Another important topological index namely, the Geometric-Arithmetic index [50] defined by Vukicevic and Furtula as follows:*

$$\mathrm{GA}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

Atom-bond connectivity index ABC was invented by Furtula et al.[20]. This index applied for study of alkanes and cycloalkanes.

Definition 2.2.6. *The atom-bond connectivity index is defined as:*

$$\mathrm{ABC}(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

For studying the properties of these indices can be studied in [3], [21]-[27], [42]-[44] in detail for the historical background and computational techniques. Throughout in this thesis we use standard notations for the Hyper-Zagreb index HM, the Augmented Zagreb index AZI, Randic index $\chi(G)$, Geometric-Arithmetic index GA and Atom-Bond Connectivity index ABC.

Chapter 3

The Omega And Sadhana Polynomial Of $TUC_4[p,q]$

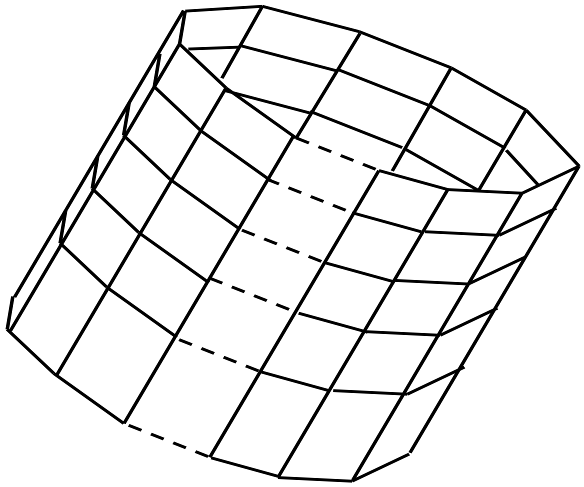

Figure 3.1: 3-dimensional lattice of $\mathrm{TUC}_4[p, 5]$

3.1 The Omega Polynomials Of $\mathrm{TUC}_4[p, q]$ Nanotubes

In this section the closed form of the Omega and the Sadhana polynomials for $\mathrm{TUC}_4[p, q]$ nanotubes as shown in figure 2.1, are being calculated. For that we start with the following lemma about the orthogonal cuts of $\mathrm{TUC}_4[p, q]$ nanotubes.

Lemma 3.1.1. *Let p be an even number and q be non negative integer; then $C(e_{0r}) = C(a_{0(r-1)}a_{0r})$ and $C(e_{u0}) = C(a_{(u-1)0}a_{u0})$ are the orthogonal cuts of $\mathrm{TUC}_4[p, q]$ nanotubes predicted in figure 2.2 and are given as follows:*

$$C(e_{0r}) = C(a_{0(r-1)}a_{0r}) = \{a_{k(r-1)}a_{kr}, a_{k(r+\frac{p}{2}-1)}a_{k(r+\frac{p}{2})} : 1 \leq k \leq q\},$$

and

$$C(e_{u0}) = C(a_{(u-1)0}a_{u0}) = \{a_{(u-1)h}a_{uh} : 1 \leq h \leq p\},$$

where

$1 \leq r \leq p/2$, $1 \leq u \leq q$ *and* $a_{jp} = a_{j0}$.

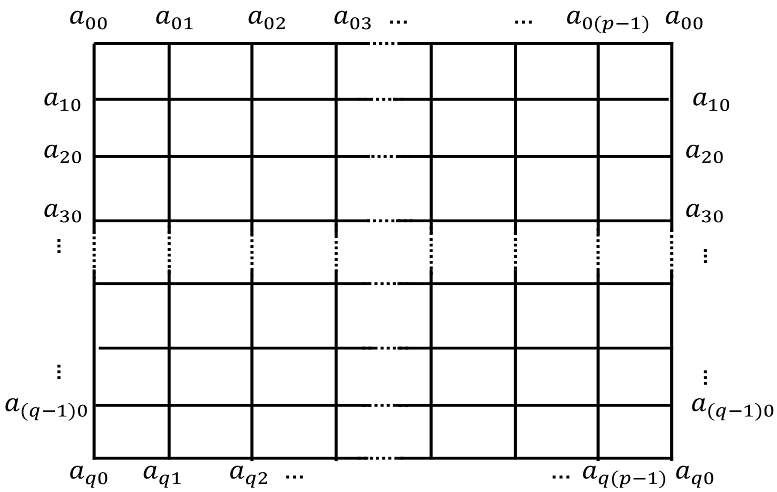

Figure 3.2: 2-dimensional representation of $\mathrm{TUC}_4[p,q]$

Proof. For $1 \leq r \leq p/2$, let $e_{0r} = a_{0(r-1)}a_{0r}$ and

$$C(e_{0r}) = C(a_{0(r-1)}a_{0r}) = \{e : \quad e \ co \ e_{0r}\}.$$

Let $e \in C(e_{0r})$. First we claim that it is of the form $e = a_{i(j-1)}a_{ij}$(i.e., the horizontal edge). In the case if e is a vertical edge i.e., $e = a_{(i-1)j}a_{ij}$ and $d(a_{0(r-1)}, a_{(i-1)j}) = u$ and $d(a_{0r}, a_{(i-1)j}) = v$. Then either the edge $a_{0(r-1)}a_{0r}$ is the part of the shortest path between $a_{0(r-1)}$ and $a_{(i-1)j}$ or not. If it is, then $r = u-1$, $d(a_{0(r-1)}, a_{ij}) = u+1$ and $d(a_{0r}, a_{ij}) = u$ which shows that e_{0r} is not codistant with e. Now if $a_{0(r-1)}a_{0r}$ is not part of the shortest path between $a_{0(r-1)}$ and $a_{(i-1)j}$ but it is in the shortest path between a_{0r} and $a_{(i-1)j}$, then again it is easy to see that e_{0r} is not codistant with e in this case. Now assume $a_{0(r-1)}a_{0r}$ is not the part of both paths i.e., between $a_{0(r-1)}$ and $a_{(i-1)j}$ and between a_{0r} and $a_{(i-1)j}$. It is easy to see that $d(a_{0(r-1)}, a_{ij}) = u+1$ and $d(a_{0r}, a_{ij}) = v+1$. Now $u = v$ or $u < v$ or $u > v$. In all cases, e_{or} is not codistant with e. Hence e must be a horizontal edge i.e., $e = a_{i(j-1)}a_{ij}$. By using the similar arguments, we can show that e is of the form $a_{k(r-1)}a_{kr}$ or $a_{k(r+\frac{p}{2}-1)}a_{k(r+\frac{p}{2})}$, where

$1 \leq k \leq q$. Similarly we can show that

$$C(e_{u0}) = C(a_{(u-1)0}a_{u0}) = \{a_{(u-1)h}a_{uh} : 1 \leq h \leq p\},$$

$1 \leq u \leq q$. Now note that $E(\mathrm{TUC}_4[p,q]) = \cup_{r=1}^{p/2} C(e_{0r}) \cup_{u=1}^{q} C(e_{u0})$ and reflexive and symmetric properties are satisfied for $C(e_{0r})$ and $C(e_{u0})$. To prove transitivity property in $C(e_{0r})$, let e_1, e_2 co $a_{0(r-1)}a_{0r}$ i.e., $e_1, e_2 \in C(e_{0r})$, then there arise three cases:

Case 1: Let

$$e_1 = a_{s(r-1)}a_{sr},$$

and

$$e_2 = a_{t(\frac{p}{2}+r-1)}a_{t(\frac{p}{2}+r)},$$

such that $s \leq t$ and $0 \leq s, t, \leq q$. It is easy to see that

$$\begin{aligned} d(a_{s(r-1)}, a_{t(\frac{p}{2}+r-1)}) &= d(a_{t(r-1)}, a_{t(\frac{p}{2}+r-1)}) + d(a_{t(\frac{p}{2}+r-1)}, a_{s(\frac{p}{2}+r-1)}) \\ &= \frac{p}{2} + r - 1 - (r-1) + t - s = \frac{p}{2} + t - s. \end{aligned}$$

Similarly,

$$d(a_{sr}, a_{t(\frac{p}{2}+r)}) = \frac{p}{2} + t - s,$$

and

$$d(a_{sr}, a_{t(\frac{p}{2}+r-1)}) = d(a_{s(r-1)}, a_{t(\frac{p}{2}+r-1)}) - 1 = \frac{p}{2} + t - s - 1.$$

Now the shortest path from $a_{s(r-1)}$ to $a_{t(\frac{p}{2}+r)}$ is $a_{s(r-1)}$, $a_{s(r-2)}$, $a_{s(r-3)}$,$\cdots$, a_{s0}, $a_{s(\frac{p}{2}+(\frac{p}{2}-1))}$, $\cdots$, $a_{s(\frac{p}{2}+r)}$,$a_{(s+1)(\frac{p}{2}+r)}$, $\cdots$, $a_{t(\frac{p}{2}+r)}$. Hence

$$d(a_{s(r-1)}, a_{t(\frac{p}{2}+r)}) = r - 1 + \frac{p}{2} - r + t - s = \frac{p}{2} + t - s - 1.$$

Since $e_1 = a_{s(r-1)}a_{sr} = a_{sr}a_{s(r-1)}$, so e_1 co e_2.

Case 2: Let

$$e_1 = a_{s(r-1)}a_{sr},$$

and

$$e_2 = a_{t(r-1)}a_{tr},$$

such that $s \leq t$ and $0 \leq s, t, \leq q$. The shortest path from $a_{s(r-1)}$ to $a_{t(r-1)}$ is computed as $a_{s(r-1)}$, $a_{(s+1)(r-1)}$,$\cdots$,$a_{t(r-1)}$ which gives

$$d(a_{s(r-1)}, a_{t(r-1)}) = t - s,$$

and

$$d(a_{sr}, a_{tr}) = t - s.$$

Similarly

$$d(a_{s(r-1)}, a_{tr}) = t - s + 1,$$

and

$$d(a_{sr}, a_{t(r-1)}) = t - s + 1.$$

This implies that e_1 co e_2.

Case 3: Let

$$e_1 = a_{s(\frac{p}{2}+r-1)}a_{s(\frac{p}{2}+r)},$$

and

$$e_2 = a_{t(\frac{p}{2}+r-1)}a_{t(\frac{p}{2}+r)}.$$

By using the same arguments as in Case 2, we can show that e_1 co e_2. This implies that $C(e_{0r})$ for $1 \leq r \leq \frac{p}{2}$ are orthogonal cuts "oc" of $\mathrm{TUC}_4[p, q]$ nanotubes.

Similarly it can be proved that $C(e_{u0})$ for $1 \leq u \leq q$ are also orthogonal cuts of $\mathrm{TUC}_4[p,q]nanotubes$.

$\square$

Lemma 3.1.2. *Let p be an odd number and q be non negative integer; then $C(e_{0r}) = C(a_{0(r-1)}a_{0r})$ and $C(e_{u0}) = C(a_{(u-1)0}a_{u0})$ are the orthogonal cuts $\mathrm{TUC}_4[p,q]$ nanotubes and are given as follows:*

$$C(e_{0r}) = \{a_{j(r-1)}a_{jr} | \quad 0 \leq j \leq q\},$$

$$C(e_{u0}) = \{a_{(u-1)i}a_{ui} | \quad 0 \leq i \leq p-1\},$$

where $1 \leq r \leq p$ and $1 \leq u \leq q$.

Proof. The proof is similar to that of Lemma 3.1.1 $\square$

Here are the main results.

Theorem 3.1.3. *The Omega polynomial of $\mathrm{TUC}_4[p,q]$ nanotubes is given by*

$$\Omega(\mathrm{TUC}_4[p,q],x) = \begin{cases} \frac{p}{2}x^{(2q+2)} + qx^p, & \textit{if } p \textit{ is even,} \\ px^{q+1} + qx^p, & \textit{otherwise.} \end{cases}$$

Proof. Suppose p is even. By Lemma 3.1.1, the oc strips are $C(e_{0r})$ and $C(e_{u0})$. Since every oc is qoc, the length of $p/2$ qoc strips is $2q+2$ and the length of q strips is p. Then the omega polynomial of $G = \mathrm{TUC}_4[p,q]nanotubes$ is as follows

$$\Omega(G,x) = \frac{p}{2}x^{2q+2} + qx^p.$$

The proof for odd p is similar. $\square$ $\square$

3.2 Sadhana And Counting Polynomials Of $\mathrm{TUC}_4[p,q]$

In this section Sadhana polynomials, Theta polynomials, PI polynomials and The Cluj-Ilmenau index are to be calculated for $\mathrm{TUC}_4[p,q]$.

Theorem 3.2.1. *The Sadhana polynomials of* $\mathrm{TUC}_4[p,q]$ *nanotubes are computed as*

$$Sd(\mathrm{TUC}_4[p,q],x) = \begin{cases} \frac{p}{2}x^{2pq+p-2q-2} + qx^{2pq}, & \text{if } p \text{ is even,} \\ px^{2pq+p-q-1} + qx^{2pq}, & \text{otherwise.} \end{cases}$$

Theorem 3.2.2. *The theta and PI polynomials of* $\mathrm{TUC}_4[p,q]$ *nanotubes are computed as*

$$\Theta(\mathrm{TUC}_4[p,q],x) = \begin{cases} p(q+1)x^{2q+2} + pqx^{p}, & \text{if } p \text{ is even,} \\ p(q+1)x^{q+1} + pqx^{p}, & \text{otherwise.} \end{cases}$$

$$\Pi(\mathrm{TUC}_4[p,q],x) = \begin{cases} p(q+1)x^{2pq+p-2q-2} + pqx^{2pq}, & \text{if } p \text{ is even,} \\ p(q+1)x^{2pq+q-q-1} + pqx^{2pq}, & \text{if } p \text{ is odd.} \end{cases}$$

The Cluj-Ilmenau index [19], $CI = CI(G)$, is calculated from the Omega polynomial as

$$CI(G) = [\Omega'(G,x)]^2 - [\Omega'(G,x) + \Omega''(G,x)]_{x=1}.$$

We conclude with the following important result.

Corollary 3.2.3. *The PI index and Cluj index for* $\mathrm{TUC}_4[p,q]$ *nanotubes coincide.*

Proof. Suppose p is even. The Omega polynomial and its first and second derivatives are given as

$$\Omega(\mathrm{TUC}_4[p,q],x) = \frac{p}{2}x^{2q+2} + qx^{p}.$$

$$\Omega'(\mathrm{TUC}_4[p,q],x) = \frac{p}{2}(2q+2)x^{2q+1} + qpx^{p-1}.$$

$$\Omega''(\mathrm{TUC}_4[p,q],x) = \frac{p}{2}(2q+2)(2q+1)x^{2q} + qp(p-1)x^{p-2}.$$

$$CI(\mathrm{TUC}_4[p,q],x) = 4p^2q^2 + 3p^2q - 2pq^2 - 4pq + p^2 - 2p. \tag{3.2.1}$$

Now the theta polynomial and its first derivative are computed as

$$\Theta(\mathrm{TUC}_4[p,q],x) = p(q+1)x^{2q+2} + pqx^p$$

$$\Theta'(\mathrm{TUC}_4[p,q],x) = p(q+1)(2q+2)x^{2q+1} + p^2qx^{p-1}$$

$$PI(\mathrm{TUC}_4[p,q]) = 4p^2q^2 + 3p^2q - 2pq^2 - 4pq + p^2 - 2p. \tag{3.2.2}$$

From equations (9.1.6) and (9.1.7), $CL(\mathrm{TUC}_4[p,q]) = PI(\mathrm{TUC}_4[p,q])$. Similarly the Omega and the theta polynomials and their derivatives for odd p are computed as .

$$\Omega(G,x) = px^{q+1} + qx^p$$

$$\Omega'(\mathrm{TUC}_4[p,q],x) = p(q+1)x^q + qpx^{p-1}$$

$$\Omega''(\mathrm{TUC}_4[p,q],x) = pq(q+1)x^{q-1} + qp(p-1)x^{p-2}$$

$$\Theta(G,x) = p(q+1)x^{q+1} + pqx^p$$

$$\Theta'(\mathrm{TUC}_4[p,q],x) = p(q+1)^2x^q + p^2qx^{p-1}.$$

The Cluj-index and PI index for odd p is calculated as

$$CI(\mathrm{TUC}_4[p,q],x) = 4p^2q^2 + 3p^2q - pq^2 - 2pq + p^2 - p = PI(\mathrm{TUC}_4[p,q],x).$$

Thus the Cluj-index and PI index for all values of p and q are equal. □ □

3.3 Conclusion

In this chapter the Omega and Sadhana polynomials are being studied which are very important tools in the description of topological properties of nanotubes and have a significant role in the QSAR/QSPR study. We used mathematical tools to compute these polynomials for the nanotube $\mathrm{TUC}_4[p, q]$. We also give explicit formulae for the PI and the theta polynomial of $\mathrm{TUC}_4[p, q]$ nanotubes and prove that the Cluj index and PI index coincide in this case.

Chapter 4

The Hyper Zagrb Index Of $TUC_4[p,q]$ And $TUC_5 C_6 C_8[p,q]$

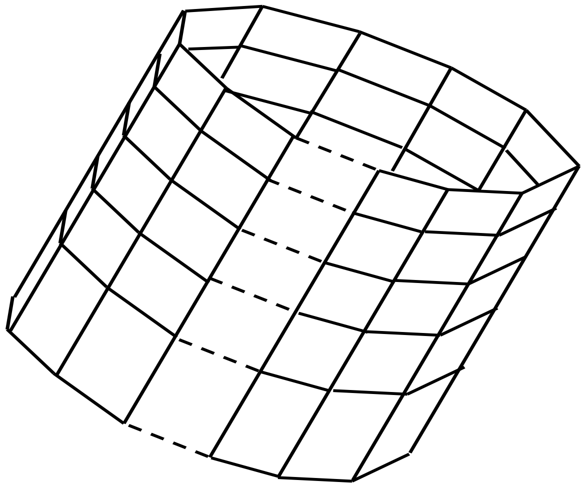

Figure 4.1: 3-dimensional lattice of $\mathrm{TUC}_4[p, 5]$

4.1 The Hyper-Zagreb Index Of $\mathrm{TUC}_4[p, q]$

In this section the closed form of the formulae for the two Zagreb indices, Zagreb polynomials and the Hyper-Zagreb index of carbon nanotubes $\mathrm{TUC}_4[p, q]$ predicted in figure 3.1, and figure 3.2 are computed. Also the Augmented Zagreb index is also computed. Here is the first result.

Theorem 4.1.1. *Let $G = \{V, E\}$ be the $\mathrm{TUC}_4[p, q]$ nanotube as shown in Figure 3.1. Here p denotes the number of horizontal squares and q denotes the tube levels. Then both of the Zagreb indices of G are*

$$\begin{aligned} \mathrm{M}_1(G) &= 2p(8q + 1) \\ \mathrm{M}_2(G) &= 2p(16q - 3), \end{aligned}$$

respectively.

Proof. Let $G = TUC_4[p, q]$ with $G = \{V, E\}$. There are two types of vertices in G namely of degree 3 and 4 which is clear from the Figure 9.1. Thus we have $V = V_3 \oplus V_4$,

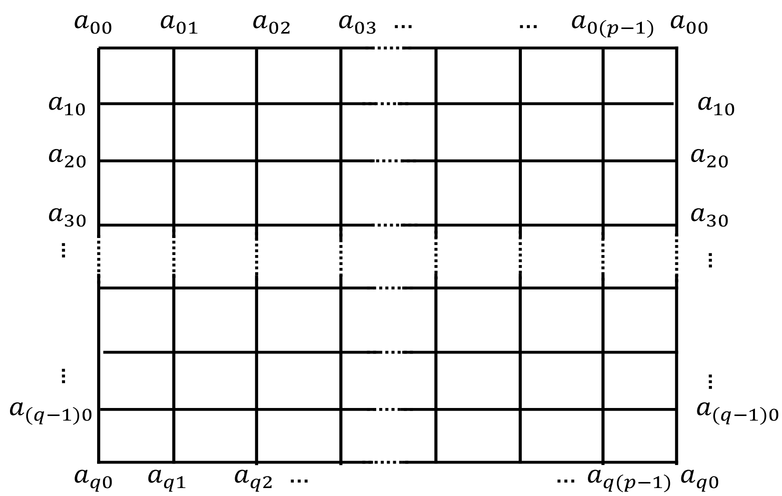

Figure 4.2: 2-dimensional representation of $\mathrm{TUC}_4[p, q]$

where

$$\begin{aligned} V_3 &= \{v \in V(G) | d_v = 3\} \\ V_4 &= \{v \in V(G) | d_v = 4\} \end{aligned}$$

with $|V_3| = 2p$ and $|V_4| = p(q-1)$. Clearly from the structure of G, there are three partitions of edges in G i.e $E = E_{\{3,3\}} \oplus E_{\{3,4\}} \oplus E_{\{4,4\}}$. Here

$$\begin{aligned} E_{\{3,3\}} &= \{e = uv \in E(G) | d_u = d_v = 3\}, \\ E_{\{3,4\}} &= \{e = uv \in E(G) | d_u = 3, d_v = 4\}, \\ E_{\{4,4\}} &= \{e = uv \in E(G) | d_u = d_v = 4\}. \end{aligned}$$

The cardinalities of these sets are given as follows

$$\begin{aligned} |E_{\{3,3\}}| &= 2p, \\ |E_{\{3,4\}}| &= 2p, \\ |E_{\{4,4\}}| &= 2pq - 3p. \end{aligned}$$

Thus the first Zagreb index is given by

$$\begin{aligned}
\mathrm{M}_1(G) &= \sum_{uv\in E_{\{3,3\}}}(d_u+d_v)+\sum_{uv\in E_{\{3,4\}}}(d_u+d_v)+\sum_{uv\in E_{\{4,4\}}}(d_u+d_v)\\
&= 6(2p)+7(2p)+8(2pq-3p)=2p(8q+1).
\end{aligned}$$

Similarly, the second Zagreb index of $TUC_4[p,q]$ is given by

$$\begin{aligned}
\mathrm{M}_2(G) &= \sum_{uv\in E(TUC_4[p,q])}(d_u*d_v)\\
&= \sum_{uv\in E_{\{3,3\}}}(d_u*d_v)+\sum_{uv\in E_{\{3,4\}}}(d_u*d_v)+\sum_{uv\in E_{\{4,4\}}}(d_u*d_v)\\
&= 9(2p)+12(2p)+16(2pq-3p)=2p(16q-3),
\end{aligned}$$

which completes the proof. □

Now using the statement of above theorem we have the following obvious corollary.

Corollary 4.1.2. *Let G be the nanotube* $\mathrm{TUC}_4[p,q]$. *The Zagreb polynomials for G are given as follows*

$$\begin{aligned}
\mathrm{Zg}_1(G,x) &= 2px^6+2px^7+(2pq-3p)x^8\\
\mathrm{Zg}_2(G,x) &= 2px^9+2px^{12}+(2pq-3p)x^{16},
\end{aligned}$$

respectively.

Theorem 4.1.3. *Let G be the nanotube* $\mathrm{TUC}_4[p,q]$. *Then the HM index of G is computed as follows*

$$\mathrm{HM}(G)=2p(64q-11).$$

Proof. To compute the Hyper-Zagreb index for the nanotube $\mathrm{TUC}_4[p,q]$, we proceed, using the proof of Theorem 3.1.1, as follows

$$\begin{aligned} \mathrm{HM}(G) &= \sum_{uv \in E(G)} (d_u + d_v)^2, \\ &= 6^2 * 2p + 7^2 * 2p + 8^2 * (2pq - 3p), \\ &= 2p(64q - 11). \end{aligned}$$

which completes the proof. □

We finish this section by giving the following corollary.

Corollary 4.1.4. *Let G be the nanotubes $TUC_4[p, q]$. The Augmented Zagreb index of G is given by*

$$\mathrm{AZI}(G) = p(37.916q - 6.44475).$$

Proof. The proof proceed as follows.

$$\begin{aligned} AZI(G) &= \sum_{uv \in E(TUC_4[p,q])} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \\ &= 11.390625(2p) + 13.824(2p) + 18.958(2pq - 3p). \end{aligned}$$

On simplification we are done. □

4.2 Hyper-Zagreb Index Of $\mathrm{TUC}_5 C_6 C_8[p, q]$

The goal of this section is to compute the Zagreb indices, the Zagreb polynomials, the Hyper-Zagreb index and the Augmented Zagreb index of molecular structure $\mathrm{TUC}_5 C_6 C_8[p, q]$ nanotube. Here is the first result.

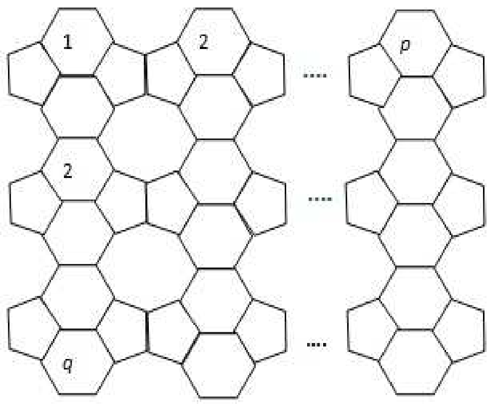

Figure 4.3: 2-dimensional view of $\mathrm{TUC}_5C_6C_8[p,q]$

Theorem 4.2.1. *Let* $\mathrm{TUC}_5C_6C_8[p,q]$ *be the nanotube as predicted in Figure 3.3. The first and second Zagreb indices of* G *are given be*

$$\begin{aligned} \mathrm{M}_1(G) &= 8p(9q+2), \\ \mathrm{M}_2(G) &= 2p(54q+7), \end{aligned}$$

respectively. Hence the Zagreb polynomials of $G = TUC_5C_6C_8[p,q]$ *are given by*

$$\begin{aligned} \mathrm{Zg}_1(G,x) &= 2px^4 + 4px^5 + (12pq-2p)x^6, \\ \mathrm{Zg}_2(G,x) &= 2px^4 + 4px^6 + (12pq-2p)x^9, \end{aligned}$$

respectively.

Proof. Let $G = \{V, E\}$ be a graph such that $G = \mathrm{TUC}_5C_6C_8[p,q]$ nanotubes. Since G consists of several $C_5C_6C_8$ net, the number of $C_5C_6C_8$ nets in the first row are denoted by p. Similarly the number of repetitions of $C_5C_6C_8$ in first column is denoted by q. Since there are two types of vertices in G namely of degree 2 and of degree 3. Thus we can write $V = V_2 \oplus V_3$, where

$$\begin{aligned} V_2 &= \{v \in V(G) | d_v = 2\}, \\ V_3 &= \{v \in V(G) | d_v = 3\}. \end{aligned}$$

Now by the structure of G we have

$$\begin{aligned} |V_2| &= 4p, \\ |V_3| &= 8pq. \end{aligned}$$

Thus the total number of bonds/edges of $G = \mathrm{TUC}_5C_6C_8[p,q]$ are given as

$$E(G) = \frac{1}{2}[2(4p) + 3(8pq)] = 4p + 12pq.$$

Again it is clear from the structure of G there are three types of edges of G i.e $E = E_{\{2,2\}} \oplus E_{\{2,3\}} \oplus E_{\{}3,3\}$, where

$$\begin{aligned} E_{\{2,2\}} &= \{e = uv \in E(TUC_5C_6C_8[p,q]) | d_u = d_v = 2\}, \\ E_{\{2,3\}} &= \{e = uv \in E(TUC_5C_6C_8[p,q]) | d_u = 2, d_v = 3\}, \\ E_{\{3,3\}} &= \{e = uv \in E(TUC_5C_6C_8[p,q]) | d_u = d_v = 3\}. \end{aligned}$$

Now the cardinalities of these sets are as follows

$$\begin{aligned} |E_{\{2,2\}}| &= 2p, \\ |E_{\{2,3\}}| &= 4p, \\ |E_{\{3,3\}}| &= 12pq - 2p. \end{aligned}$$

The $M_1(G)$ index of G is computed as follows:

$$\begin{aligned}
\mathrm{M}_1(G) &= \sum_{uv\in E_{\{2,2\}}}(d_u+d_v)+\sum_{uv\in E_{\{2,3\}}}(d_u+d_v)+\sum_{uv\in E_{\{3,3\}}}(d_u+d_v),\\
&= 4(2p)+5(4p)+6(12pq-2p),\\
&= 16p+72pq,\\
&= 8p(9q+2).
\end{aligned}$$

Now the first Zagreb polynomial of the graph G is calculated as follows

$$\begin{aligned}
\mathrm{Zg}_1(G,x) &= \sum_{uv\in E(G)} x^{(d_u+d_v)}\\
&= 2px^4+4px^5+(12pq-2p)x^6
\end{aligned}$$

Again the second Zagreb index of $TUC_5C_6C_8[p,q]$ is to be find out as

$$\begin{aligned}
\mathrm{M}_2(TUC_5C_6C_8[p,q]) &= \sum_{uv\in E_{\{2,2\}}}(d_u*d_v)+\sum_{uv\in E_{\{2,3\}}}(d_u*d_v)+\sum_{uv\in E_{\{3,3\}}}(d_u*d_v),\\
&= 4(2p)+6(4p)+9(12pq-2p),\\
&= 14p+108pq,\\
&= 2p(54q+7).
\end{aligned}$$

The second Zagreb polynomial of any G is given by

$$\begin{aligned}
\mathrm{Zg}_2(G,x) &= \sum_{e=uv\in E(G)} x^{(d_u*d_v)},\\
&= 2px^4+4px^6+(12pq-2p)x^9.
\end{aligned}$$

It completes the proof. $\square$

Theorem 4.2.2. *Let $G=\{V,E\}$ be the nanotube $TUC_5C_6C_8[p,q]$. Then the HM index of G is computed as follows*

$$\mathrm{HM}(G)=4p(108q+15).$$

Proof. To compute the Hyper-Zagreb index for G we will use the proof of theorem 4.2.1. Since

$$\mathrm{HM}(G) = \sum_{uv \in E} (d_u + d_v)^2$$

Thus

$$\begin{aligned} \mathrm{HM}(G) &= \sum_{uv \in E_{\{2,2\}}} (d_u + d_v)^2 + \sum_{uv \in E_{\{2,3\}}} (d_u + d_v)^2 + \sum_{uv \in E_{\{3,3\}}} (d_u + d_v)^2, \\ &= 4^2 * 2p + 5^2 * 4p + 6^2 * (12pq - 2p), \\ &= 4p(108q + 15), \end{aligned}$$

which completes the proof. □

Corollary 4.2.3. *Let $G = \{V, E\}$ be the nanotubes $TUC_5C_6C_8[p, q]$. The Augmented Zagreb index of G is*

$$\mathrm{AZI}(G) = p(25.21875 + 136.6875q)$$

Proof. We proceed as follows:

$$\begin{aligned} \mathrm{AZI}(G) &= \sum_{uv \in E} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \\ &= 48p + 11.390625(12pq - 2p), \end{aligned}$$

on simplification we are done. □

Chapter 5

The Hyper Zagrb Index Of *$TUC_5C_8[p,q]$*

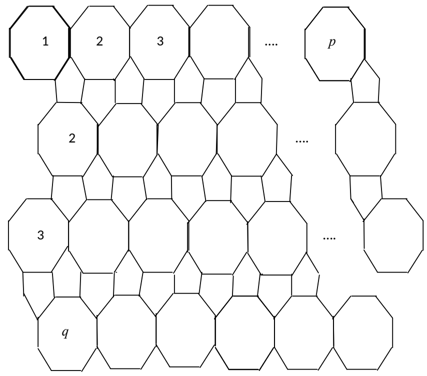

Figure 5.1: 2-dimensional view of C_5C_8

5.1 The Hyper-Zagreb Index Of $\mathrm{TU}C_5C_8$ Nanotubes

In this section, the exact formulae for the first and second Zagreb indices, related Zagreb polynomials and the Hyper-Zagreb index of the family of $\mathrm{TU}C_5C_8$ nanotubes are computed. Also the Augmented Zagreb index of the same family is also computed. The first result caries the following shape.

theorem 5.1.1. *Let $G = \{V, E\}$ be the $\mathrm{TU}C_5C_8$ as shown in Figure 9.1.1. Here p denotes the number of C_5C_8 nets horizontally and q denotes the tube levels. Then the first Zagreb index $\mathrm{M}_1(G)$ and second $\mathrm{M}_2(G)$ Zagreb index of G are*

$$\begin{aligned} \mathrm{M}_1(G) &= 4p(9q+4) \\ \mathrm{M}_2(G) &= 2p(27q+7). \end{aligned}$$

Proof. Consider the graph of $\mathrm{TU}C_5C_8$ with $G = \{V, E\}$. There are two types of vertices in G namely of degree 2 and 3 which is clear from the figure 9.1.1. Thus we have $V = V_2 \oplus V_3$, where

$$\begin{aligned} V_4 &= \{v \in V(\mathrm{TU}C_5C_8) | d_v = 2\} \\ V_6 &= \{v \in V(\mathrm{TU}C_5C_8) | d_v = 3\} \end{aligned}$$

with $|V_2| = 4p$ and $|V_3| = 4pq$. Clearly from the structure of G, there are three partitions of edges in G i.e $E = E_{\{2,2\}} \oplus E_{\{2,3\}} \oplus E_{\{3,3\}}$. Here

$$\begin{aligned} E_{\{2,2\}} &= \{e = uv \in E(G) | d_u = d_v = 2\}, \\ E_{\{2,3\}} &= \{e = uv \in E(G) | d_u = 2, d_v = 3\}, \\ E_{\{3,3\}} &= \{e = uv \in E(G) | d_u = d_v = 3\}. \end{aligned}$$

The cardinalities of these sets are given as follows

$$\begin{aligned} |E_{\{2,2\}}| &= 2p, \\ |E_{\{2,3\}}| &= 4p, \\ |E_{\{3,3\}}| &= 6pq - 2p. \end{aligned}$$

Thus the first Zagreb index is given by

$$\begin{aligned} \mathrm{M}_1(\mathrm{TU}C_5C_8) &= \sum_{uv \in EG} (d_u + d_v) \\ &= 4(2p) + 5(4p) + 6(6pq - 2p) \\ &= 4p(9q + 4). \end{aligned}$$

Similarly, the second Zagreb index of $\mathrm{TU}C_5C_8$ is given by

$$\begin{aligned} \mathrm{M}_2(\mathrm{TU}C_5C_8) &= \sum_{uv \in E(G)} (d_u * d_v) \\ &= 4(2p) + 6(4p) + 9(6pq - 2p), \\ &= 2p(27q + 7). \end{aligned}$$

which completes the proof. $\square$

Now using the statement of above theorem:

Corollary 5.1.2. *Let G be the $\mathrm{TU}C_5C_8$. Then the first $\mathrm{Zg}_1(\mathrm{TU}C_5C_8, x)$ and second $\mathrm{Zg}_2(\mathrm{TU}C_5C_8, x)$ Zagreb polynomials for $\mathrm{TU}C_5C_8$ are given as follows:*

$$\begin{aligned}\mathrm{Zg}_1(\mathrm{TU}C_5C_8, x) &= 2px^4 + 4px^5 + (6pq - 2p)x^6, \\ \mathrm{Zg}_2(\mathrm{TU}C_5C_8, x) &= 2px^4 + 4px^6 + (6pq - 2p)x^9.\end{aligned}$$

theorem 5.1.3. *Let $\mathrm{TU}C_5C_8$ be the nanotubes. Then the HM index of $\mathrm{TU}C_5C_8$ is computed as follows*

$$\mathrm{HM}(\mathrm{TU}C_5C_8) = 12p(18q + 5).$$

Proof. To compute the Hyper-Zagreb index for the $\mathrm{TU}C_5C_8$ nanotubes, we proceed, using the proof of theorem 7.1.1, as follows

$$\begin{aligned}\mathrm{HM}(\mathrm{TU}C_5C_8) &= \sum_{uv \in E(G)} (d_u + d_v)^2, \\ &= 4^2 * 2p + 5^2 * 4p + 6^2 * (6pq - 2p), \\ &= 12p(18q + 5).\end{aligned}$$

which completes the proof. □

We finish this section by giving the following corollary.

Corollary 5.1.4. *Let G be the family of nanotubes $\mathrm{TU}C_5C_8$. The Augmented Zagreb index of G is given by*

$$\mathrm{AZI}(G) = 48p + 22.78125p(3q - 1).$$

Proof. The proof proceed as follows.

$$\begin{aligned}AZI(\mathrm{TU}C_5C_8) &= \sum_{uv \in E(\mathrm{TU}C_5C_8)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \\ &= 8(2p) + 8(4p) + 11.390625(3q - 1)p.\end{aligned}$$

On simplification we are done. □

5.2 Other Results

Here we will compute exact formulae of Geometric-Arithmetic index, Atom-Bond Connectivity index and Randic index for $\mathrm{TU}C_5C_8$.

theorem 5.2.1. *Let G be the graph of $\mathrm{TU}C_5C_8$. Then the Geometric-Arithmetic index of $\mathrm{TU}C_5C_8$ is given by*

$$GA(\mathrm{TU}C_5C_8) = \frac{(8\sqrt{6})p}{5} + 6pq.$$

Proof. Let G be the graph of $\mathrm{TU}C_5C_8$ nanotubes. Then $GA(G)$ is computed as follows

$$\begin{aligned}
GA(\mathrm{TU}C_5C_8) &= \sum_{uv\in E(\mathrm{TU}C_5C_8)} \frac{2\sqrt{d_ud_v}}{d_u+d_v} \\
&= \sum_{uv\in E_{\{2,2\}}} \frac{2\sqrt{d_ud_v}}{d_u+d_v} + \sum_{uv\in E_{\{2,3\}}} \frac{2\sqrt{d_ud_v}}{d_u+d_v} + \sum_{uv\in E_{\{3,3\}}} \frac{2\sqrt{d_ud_v}}{d_u+d_v}, \\
&= \frac{2p(2\sqrt{2*2})}{2+2} + \frac{4p(2\sqrt{2*3})}{2+3} + (6pq-2p)\frac{2\sqrt{3*3}}{3+3} \\
&= 2p + \frac{8p\sqrt{6}}{5} + 6pq - 2p \\
&= \frac{p(8\sqrt{6})}{5} + 6pq.
\end{aligned}$$

which completes the proof. □

theorem 5.2.2. *Let G be a graph of $\mathrm{TU}C_5C_8$ nanotubes. Then the Atom-Bond Connectivity index of G is given by*

$$ABC(\mathrm{TU}C_5C_8) = \frac{P(9\sqrt{2}-4)}{3} + 4pq.$$

Proof. The proof proceed as follows:

$$\begin{aligned}
ABC(\mathrm{TU}C_5C_8) &= \sum_{e=uv\in E(\mathrm{TU}C_5C_8)} \sqrt{\frac{d_u+d_v-2}{d_ud_v}} \\
&= \sum_{uv\in E_{\{2,2\}}} \sqrt{\frac{d_u+d_v-2}{d_ud_v}} + \sum_{uv\in E_{\{2,3\}}} \sqrt{\frac{d_u+d_v-2}{d_ud_v}} + \\
&\quad \sum_{uv\in E_{\{3,3\}}} \sqrt{\frac{d_u+d_v-2}{d_ud_v}}, \\
&= p\sqrt{2} + \frac{4p\sqrt{2}}{2} + \frac{2(6pq-2p)}{3} \\
&= \frac{P(9\sqrt{2}-4)}{3} + 4pq.
\end{aligned}$$

which completes the proof of the theorem. □

theorem 5.2.3. *Suppose G be* $\mathrm{TU}C_5C_8$ *nanotubes. Then the Randic index of G is given as:*

$$\chi(\mathrm{TU}C_5C_8) = \frac{p(2\sqrt{6}+1)}{3} + 2pq.$$

Proof. Let G be a graph predicts $\mathrm{TU}C_5C_8$. We calculate $\chi(\mathrm{TU}C_5C_8)$ index as follows:

$$\begin{aligned}
\chi(\mathrm{TU}C_5C_8) &= \sum_{uv\in E(\mathrm{TU}C_5C_8)} \frac{1}{\sqrt{d_ud_v}} \\
&= \sum_{uv\in E_{\{2,2\}}} \frac{1}{\sqrt{d_ud_v}} + \sum_{uv\in E_{\{2,3\}}} \frac{1}{\sqrt{d_ud_v}} + \sum_{uv\in E_{\{3,3\}}} \frac{1}{\sqrt{d_ud_v}}, \\
&= \frac{2p}{\sqrt{4}} + \frac{4p}{\sqrt{6}} + \frac{6pq-2p}{\sqrt{9}} \\
&= p + \frac{2p\sqrt{6}}{3} + 2pq - \frac{2p}{3} \\
&= \frac{p(2\sqrt{6}+1)}{3} + 2pq.
\end{aligned}$$

Hence completes the proof of the theorem. □

Chapter 6

The Hyper Zagrb Index Of Zigzag Boron Nanotubes *BNT[p,q]*

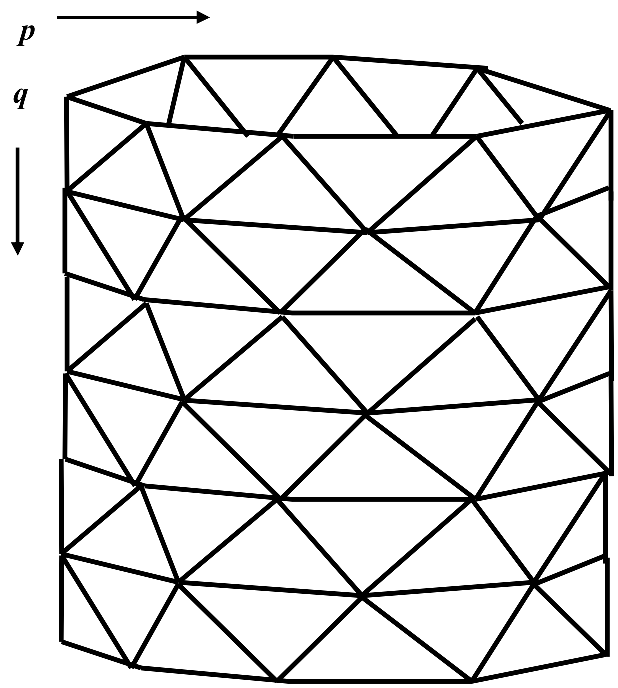

Figure 6.1: 3-dimensional lattice of zigzag boron triangular nanotubes

6.1 The Hyper-Zagreb Index Of Boron Triangular Nanotubes BNT$[p, q]$

In this section we calculated formulae for the first and second Zagreb indices, related Zagreb polynomials and the Hyper-Zagreb index of the family of zigzag boron triangular nanotubes BNT$[p, q]$ as shown in figure 5.1, are computed. Also the Augmented Zagreb index is computed. Here is the first result.

Theorem 6.1.1. *Let $G = \{V, E\}$ be the boron triangular nanotubes* BNT$[p, q]$. *Here p denotes the number of horizontal triangles and q denotes the tube levels. Then*

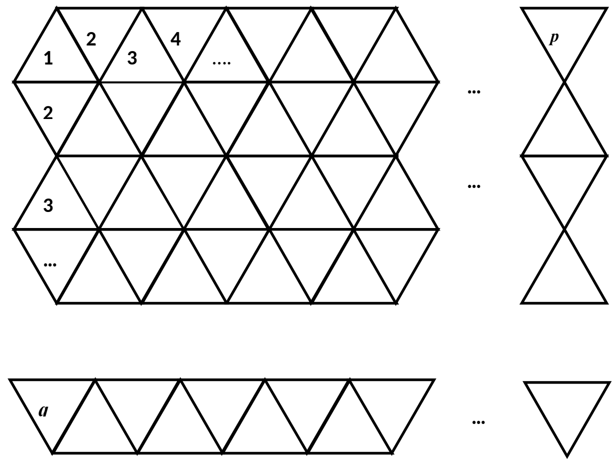

Figure 6.2: 2-dimensional lattice of zigzag boron triangular nanotubes

$\mathrm{M}_1(G)$ *and* $\mathrm{M}_2(G)$ *indices of* G *are*

$$\mathrm{M}_1(G) = 2p(9q+5)$$
$$\mathrm{M}_2(G) = 2p(27q+5).$$

Proof. Consider the graph of BNT$[p,q]$ with $G = \{V, E\}$. There are two types of vertices in G namely, of degree 4 and 6 which is clear from the figure 5.2. Thus we have $V = V_4 \oplus V_6$, where

$$V_4 = \{v \in V(G) | d_v = 4\}$$
$$V_6 = \{v \in V(G) | d_v = 6\}$$

with $|V_4| = p$ and $|V_6| = (q-1)\frac{p}{2}$. Clearly from the structure of G, there are three partitions of edges in G i.e $E = E_{\{4,4\}} \oplus E_{\{4,6\}} \oplus E_{\{6,6\}}$. Here

$$E_{\{4,4\}} = \{e = uv \in E(G) | d_u = d_v = 4\},$$
$$E_{\{4,6\}} = \{e = uv \in E(G) | d_u = 4, d_v = 6\},$$
$$E_{\{6,6\}} = \{e = uv \in E(G) | d_u = d_v = 6\}.$$

The cardinalities of these sets are given as follows

$$\begin{aligned}
|E_{\{4,4\}}| &= p, \\
|E_{\{4,6\}}| &= 2p, \\
|E_{\{6,6\}}| &= (q-1)\frac{3p}{2}.
\end{aligned}$$

Thus the first Zagreb index is given by

$$\begin{aligned}
\mathrm{M}_1(G) &= \sum_{uv\in E_{\{4,4\}}} (d_u + d_v) + \sum_{uv\in E_{\{4,6\}}} (d_u + d_v) + \sum_{uv\in E_{\{6,6\}}} (d_u + d_v) \\
&= 8(p) + 10(2p) + 12(q-1)\frac{3p}{2} \\
&= 2p(9q+5).
\end{aligned}$$

Similarly, the second Zagreb index of boron triangular nanotubes is given by

$$\begin{aligned}
\mathrm{M}_2(G) &= \sum_{uv\in E(G)} (d_u * d_v) \\
&= 16(p) + 24(2p) + 36(q-1)\frac{3p}{2}, \\
&= 2p(27q+5).
\end{aligned}$$

This completes the proof. □

Now using the statement of above theorem :

Corollary 6.1.2. *Let G be the* $\mathrm{BNT}[p,q]$. *Then the first* $\mathrm{Zg}_1(G,x)$ *and second* $\mathrm{Zg}_2(G,x)$ *Zagreb polynomials for G are given as follows:*

$$\begin{aligned}
\mathrm{Zg}_1(G,x) &= px^8 + 2px^{10} + (q-1)\frac{3p}{2}x^{12}, \\
\mathrm{Zg}_2(G,x) &= px^{16} + 2px^{24} + (q-1)\frac{3p}{2}x^{36}.
\end{aligned}$$

Theorem 6.1.3. *Let G be the boron triangular nanotube* $\mathrm{BNT}[p,q]$*. Then $HM(G)$ G is given by*

$$\mathrm{HM}(G) = 24p(9q+2).$$

Proof. To compute the Hyper-Zagreb index for the boron triangular nanotube $\mathrm{BNT}[p,q]$, we proceed, using the proof of theorem 7.1.1, as follows

$$\begin{aligned}\mathrm{HM}(G) &= \sum_{uv\in E(G)} (d_u+d_v)^2,\\ &= 8^2 * p + 10^2 * 2p + 12^2 * (q-1)\frac{3p}{2},\\ &= 24p(9q+2).\end{aligned}$$

which completes the proof. ☐

We finish this section by giving the following corollary.

Corollary 6.1.4. *Let G be the nanotubes* $\mathrm{BNT}[p,q]$*. The Augmented Zagreb index of G is given by*

$$\mathrm{AZI}(G) = p(69.984q + 2.98607).$$

Proof. The proof proceed as follows.

$$\begin{aligned}\mathrm{AZI}(G) &= \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u+d_v-2}\right)^3\\ &= 18.97007(p) + 27(2p) + 69.984(q-1)p.\end{aligned}$$

On simplification we are done. ☐

6.2 Other Results

In this section, we will compute exact formulae of the Geometric-Arithmetic index, the Atom-Bond Connectivity index and Randic index for the boron triangular nanotubes

BNT$[p, q]$.

Theorem 6.2.1. *Let G be the graph of the boron triangular nanotubes* BNT$[p, q]$. *Then the Geometric-Arithmetic index of G is given by*

$$\mathrm{GA}(G) = \frac{(8\sqrt{6} - 5)p}{10} + \frac{3pq}{2}.$$

Proof. Let G be the graph of boron triangular nanotubes. Then GA(G) is computed as follows

$$\begin{aligned}
\mathrm{GA}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} & \\
&= \sum_{uv \in E_{\{4,4\}}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv \in E_{\{4,6\}}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv \in E_{\{6,6\}}} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \\
&= \frac{2p\sqrt{4 * 4}}{4 + 4} + \frac{2p(2\sqrt{4 * 6})}{4 + 6} + (q - 1)\frac{3p}{2}\frac{2\sqrt{6 * 6}}{6 + 6} \\
&= p + \frac{4p\sqrt{6}}{5} + \frac{3pq - 3p}{2} \\
&= \frac{(8\sqrt{6} - 5)p}{10} + \frac{3pq}{2}.
\end{aligned}$$

This completes the proof. ☐

Theorem 6.2.2. *Let G be a graph of the boron triangular nanotubes* BNT$[p, q]$. *Then the Atom-Bond Connectivity index of G is given by*

$$\mathrm{ABC}(G) = \frac{P(3\sqrt{6} - 3\sqrt{10} + 8\sqrt{3})}{12} + \frac{pq\sqrt{10}}{4}.$$

Proof. Using the proof of theorem 7.1.1, we get

$$
\begin{aligned}
\mathrm{ABC}(G) = & \sum_{e=uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\
&= \sum_{uv\in E_{\{4,4\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E_{\{4,6\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \\
&\quad \sum_{uv\in E_{\{6,6\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}, \\
&= \frac{p\sqrt{6}}{4} + \frac{2p\sqrt{3}}{3} + \frac{p(q-1)\sqrt{10}}{4} \\
&= \frac{P(3\sqrt{6}-3\sqrt{10}+8\sqrt{3})}{12} + \frac{pq\sqrt{10}}{4},
\end{aligned}
$$

and we are done. □

Theorem 6.2.3. *Suppose G be boron triangular nanotubes* BNT$[p, q]$. *Then the Randic index of G is given as:*

$$\chi(G) = \frac{p(2\sqrt{6}+3q)}{12}.$$

Proof. Let G be a graph predicts boron triangular nanotubes. We calculate Randic index as follows:

$$
\begin{aligned}
\chi(G) = & \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&= \sum_{uv\in E_{\{4,4\}}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv\in E_{\{4,6\}}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv\in E_{\{6,6\}}} \frac{1}{\sqrt{d_u d_v}}, \\
&= \frac{p}{\sqrt{16}} + \frac{2p}{\sqrt{24}} + \frac{3p(q-1)}{2\sqrt{36}} \\
&= \frac{p}{4} + \frac{p\sqrt{6}}{6} + \frac{pq-p}{4} \\
&= \frac{p(2\sqrt{6}+3q)}{12}.
\end{aligned}
$$

This completes the proof. □

Chapter 7

The Hyper Zagrb Index Of Armchair Boron Nanotubes *BNT[p,q]*

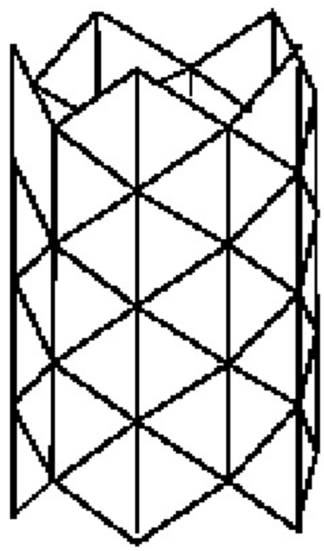

Figure 7.1: 3-dimensional armchair nanotube

7.1 The Hyper-Zagreb Index Of Armchair Boron Triangular Nanotubes $BNT[p, q]$

In this section the formulae for the first and second Zagreb indices, related Zagreb polynomials and the Hyper-Zagreb index of the family of armchair boron triangular nanotubes $BNT[p, q]$, predicted in figure 1, are computed. Also the Augmented Zagreb index is computed. Here is the first result.

Theorem 7.1.1. *Let $G = \{V, E\}$ be the $BNT[p, q]$ as shown in figure 2. Here p denotes the number of horizontal triangular nets and q denotes the tube levels. Then the Zagreb index of G are*

$$\begin{aligned} \mathrm{M}_1(G) &= 4p(18q + 17) \\ \mathrm{M}_2(G) &= 12p(18q + 11), \end{aligned}$$

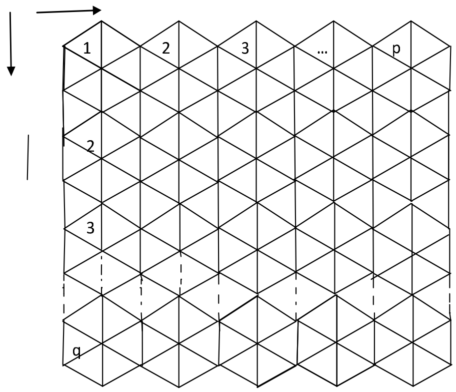

Figure 7.2: 2-dimensional armchair nanotube

respectively.

Proof. Consider the graph of $BNT[p, q]$ with $G = \{V, E\}$. There are three types of vertices in G namely of degree 3, 5 and 6 which is clear from the Figure 9.1. Thus we have $V = V_3 \oplus V_5 \oplus V_6$, where

$$\begin{aligned} V_3 &= \{v \in V(G) | d_v = 3\} \\ V_5 &= \{v \in V(G) | d_v = 5\} \\ V_5 &= \{v \in V(G) | d_v = 6\} \end{aligned}$$

with $|V_3| = 2p$, $|V_5| = 2p$ and $|V_6| = 2pq$. And total number of edges of the given tube can be calculated as

$$|E(G)| = \frac{1}{2}[3(2p) + 5(2p) + 6(2pq)].$$

Clearly from the structure of G, there are six partitions of edges in G i.e $E = E_{\{3,3\}} \oplus$

$E_{\{3,5\}} \oplus E_{\{3,6\}} E_{\{5,5\}} \oplus E_{\{5,6\}} \oplus E_{\{6,6\}}$. Here

$$\begin{aligned}
E_{\{3,3\}} &= \{e = uv \in E(G) | d_u = d_v = 3\}, \\
E_{\{3,5\}} &= \{e = uv \in E(G) | d_u = 3, d_v = 5\}, \\
E_{\{3,6\}} &= \{e = uv \in E(G) | d_u = 3, d_v = 6\}, \\
E_{\{5,5\}} &= \{e = uv \in E(G) | d_u = d_v = 5\}, \\
E_{\{5,6\}} &= \{e = uv \in E(G) | d_u = 5, d_v = 6\}, \\
E_{\{6,6\}} &= \{e = uv \in E(G) | d_u = 6, d_v = 6\}.
\end{aligned}$$

The cardinalities of these sets are given as follows

$$\begin{aligned}
|E_{\{3,3\}}| &= 0, \\
|E_{\{3,5\}}| &= 4p, \\
|E_{\{3,6\}}| &= 2p, \\
|E_{\{5,5\}}| &= 0, \\
|E_{\{5,6\}}| &= 6p, \\
|E_{\{6,6\}}| &= 6pq - 4p.
\end{aligned}$$

Thus the first Zagreb index is given by

$$\begin{aligned}
\mathrm{M}_1(G) &= \sum_{uv \in E_{\{3,5\}}} (d_u + d_v) + \sum_{uv \in E_{\{3,6\}}} (d_u + d_v) + \sum_{uv \in E_{\{5,6\}}} (d_u + d_v) + \sum_{uv \in E_{\{6,6\}}} (d_u + d_v) \\
&= 8(4p) + 9(2p) + 11(6p) + 12(6pq - 4p) \\
&= 4p(18q + 17).
\end{aligned}$$

Similarly, the second Zagreb index of armchair boron triangular nanotubes is given by

$$\begin{aligned}
\mathrm{M}_2(G) &= \sum_{uv\in E(G)} (d_u * d_v) \\
&= 15(4p) + 18(2p) + 30(6p) + 36(6pq - 4p), \\
&= 12p(18q + 11).
\end{aligned}$$

which completes the proof. □

Now using the statement of above theorem.

Corollary 7.1.2. *Let G be the $BNT[p,q]$. Then the first and second Zagreb polynomials for G are given as follows*

$$\begin{aligned}
\mathrm{Zg}_1(G,x) &= 4px^8 + 2px^9 + 6px^{11} + (6pq - 4p)x^{12}, \\
\mathrm{Zg}_2(G,x) &= 4px^{15} + 2px^{18} + 6px^{30} + (6pq - 4p)x^{36},
\end{aligned}$$

respectively.

Theorem 7.1.3. *Let G be the boron triangular nanotube. Then the HM index of G is computed as follows*

$$\mathrm{HM}(G) = 8p(108q + 71).$$

Proof. To compute the Hyper-Zagreb index for the boron triangular nanotube, we proceed, using the proof of Theorem 7.1.1, as follows

$$\begin{aligned}
\mathrm{HM}(G) &= \sum_{uv\in E(G)} (d_u + d_v)^2, \\
&= 8^2 * 4p + 9^2 2p + 11^2 * 6p + 12^2 * (6pq - 4p), \\
&= 8p(108q + 71).
\end{aligned}$$

which completes the proof. □

We finish this section by giving the following corollary.

Corollary 7.1.4. *Let G be the nanotubes $BNT[p,q]$. The Augmented Zagreb index of G is given by*

$$\mathrm{AZI}(G) = p(279.936q + 132.0963).$$

Proof. The proof proceed as follows.

$$\begin{aligned} AZI(G) &= \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \\ &= 15.625(4p) + 17.0023(2p) + 37.0359(6p) + 46.656(6pq - 4p). \end{aligned}$$

On simplification we are done. □

7.2 Other Results And Discussion

In this we will calculate exact formulae of Geometric-Arithmetic index, Atom-Bond connectivity index and Randic index for $BNT[p,q]$.

Theorem 7.2.1. *Consider G be the graph of $BNT[p,q]$. Then the Geometric-Arithmetic index of G is given by*

$$GA(G) = \frac{88\sqrt{15} + 220\sqrt{2} + 180\sqrt{30} - 660}{165} + 6pq.$$

Proof. Let G be the graph of armchair boron triangular nanotubes. Then $GA(G)$ is computed as follows

$$
\begin{aligned}
GA(G) &= \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\
&= \sum_{uv\in E_{\{3,5\}}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{uv\in E_{\{3,6\}}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \\
&\quad \sum_{uv\in E_{\{5,6\}}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{uv\in E_{\{6,6\}}} \frac{2\sqrt{d_u d_v}}{d_u+d_v}, \\
&= \frac{4p\sqrt{3*5}}{3+5} + \frac{2p(2\sqrt{3*6})}{3+6} + 6p\frac{2\sqrt{5*6}}{5+6} + \frac{2(6pq-4p)\sqrt{6*6}}{6+6} \\
&= 8p\frac{\sqrt{15}}{15} + \frac{4p\sqrt{2}}{3} + \frac{12p\sqrt{30}}{11} + (6pq-4p) \\
&= \frac{88\sqrt{15}+220\sqrt{2}+180\sqrt{30}-660}{165} + 6pq.
\end{aligned}
$$

which completes the proof. □

Theorem 7.2.2. *Let G be a graph of boron triangular nanotubes. Then the Atom-Bond connectivity index of G is given by*

$$ABC(G) = \frac{P(3\sqrt{6}-3\sqrt{10}+8\sqrt{3})}{12} + \frac{pq\sqrt{10}}{4}.$$

Proof. The proof proceed as follows:

$$
\begin{aligned}
ABC(G) &= \sum_{e=uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\
&= \sum_{uv\in E_{\{3,5\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E_{\{3,6\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\
&\quad + \sum_{uv\in E_{\{5,6\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E_{\{6,6\}}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}.
\end{aligned}
$$

which completes the proof of the theorem. □

Theorem 7.2.3. *Suppose G be the family of armchair boron triangular nanotubes. Then the Randic index of G is given as:*

$$\chi(G) = \frac{p(12\sqrt{15} + 5\sqrt{18} + 9\sqrt{30} - 30)}{45} + pq.$$

Proof. Let G be a graph predicts boron triangular nanotubes. We calculate Randic index as follows:

$$
\begin{aligned}
\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} & \\
&= \sum_{uv \in E_{\{3,5\}}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{\{3,6\}}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{\{5,6\}}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{\{6,6\}}} \frac{1}{\sqrt{d_u d_v}}, \\
&= \frac{4p}{\sqrt{15}} + \frac{2p}{\sqrt{18}} + \frac{6p}{\sqrt{30}} + \frac{6pq - 4p}{\sqrt{36}} \\
&= \frac{4p\sqrt{15}}{15} + \frac{p\sqrt{18}}{9} + \frac{p\sqrt{30}}{5\sqrt{}} + \frac{6pq - 4p}{6} \\
&= \frac{p(12\sqrt{15} + 5\sqrt{18} + 9\sqrt{30} - 30)}{45} + pq.
\end{aligned}
$$

Hence completes the proof of the theorem. □

Chapter 8

The Omega And Sadhana Polynomial Of Zigzag Boron Nanotubes ***BNT[p,q]***

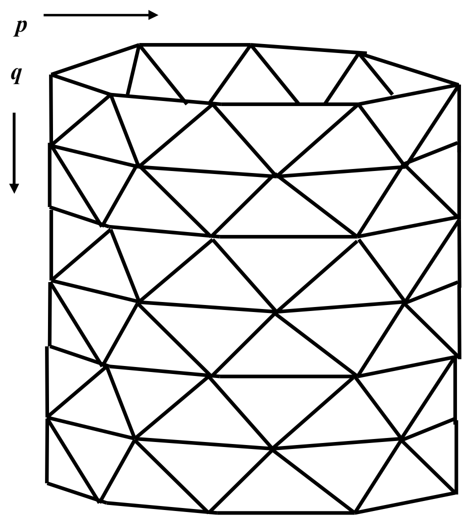

Figure 8.1: 3-dimensional lattice of zigzag boron triangular nanotubes

8.1 The Omega And Sadhana Polynomial Of Zigzag Boron Triangular Nanotubes $BNT[p,q]$

In this chapter exact formulae of the Omega and the Sadhana polynomials of BNT$[p,q]$ are being calculated. And also given explicit formulae for counting polynomials of BNT$[p,q]$ as shown in figure 1..

Theorem 8.1.1. *Let G be the family of zigzag boron nanotubes $BNT[p,q]$. The Omega polynomials of* BNT$[p,q]$*, are given by*

$$\Omega(\mathrm{BNT}[p,q],x) = \begin{cases} px^{(q+1)} + 2px^{q}, & \text{if } p \text{ is even and } q \text{ is odd,} \\ \frac{p}{2}x^{q+2} + \frac{5p}{2}x^{q}, & \text{if } p \text{ is even and } q \text{ is even.} \end{cases}$$

Proof. Suppose p is even, q is odd. It is clear from the figure 2 that there are four types of orthogonal cuts. We denote these edges by e_1, e_2, e_3 and e_4 are given in the following table.

Then by using the table 1, the proof of the theorem 2.1 i.e. the omega polynomial

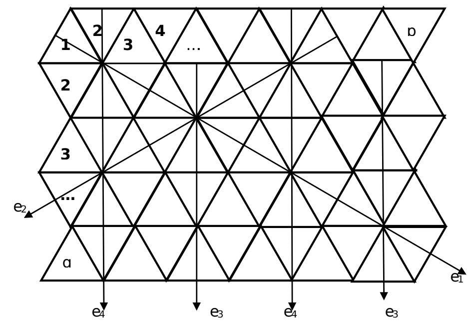

Figure 8.2: 2-dimensional lattice of zigzag boron triangular nanotubes for odd q

Edges	No. of qoc strips	No. of cut off edges
e_1	p	q
e_2	p	q
e_3	$\frac{p}{2}$	q+1
e_4	$\frac{p}{2}$	q+1

Table 8.1: The number of equidistant edges for odd q

of $G = \mathrm{BNT}[p, q]$ is as follows

$$\begin{aligned}\Omega(G, x) &= \frac{p}{2}x^{q+1} + \frac{p}{2}x^{q+1} + 2px^q, \\ &= px^{(q+1)} + 2px^q.\end{aligned}$$

Which completes the proof. Now when both p and q are even. There are also four types of oc strips i.e f_1, f_2, f_3 and f_4 as shown in figure 3. These edges are defined as in table 2

Then by the table 2, the Omega polynomial of $G = \mathrm{BNT}[p, q]$ for even p, q is

Edges	No. of qoc strips	No. of cut off edges
f_1	p	q
f_2	p	q
f_3	$\frac{p}{2}$	q+2
f_4	$\frac{p}{2}$	q

Table 8.2: The number of equidistant edges for even q

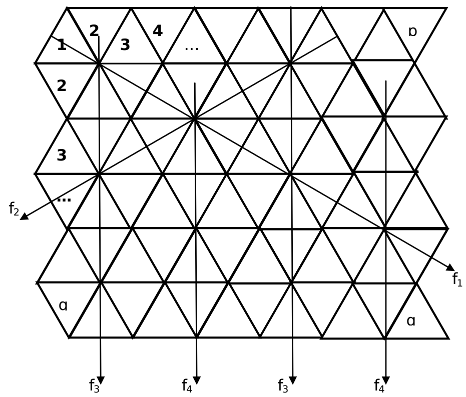

Figure 8.3: 2-dimensional lattice of zigzag boron triangular nanotubes

given by

$$\begin{aligned}\Omega(G,x) &= \frac{p}{2}x^{q+2}+\frac{p}{2}x^{q}+2px^{q},\\ &= \frac{p}{2}x^{q+2}+\frac{5p}{2}x^{q}.\end{aligned}$$

Which completes the proof of the Theorem. $\square$

Now we wish to find out Sadhana polynomial and Sadhana index for the discussed Omega polynomials. The total number of edges for the given family of Zigzag boron nanotubes are

$$\Omega'(\mathrm{BNT}[p,q],x)_{x=1} = |E(\mathrm{BNT}[p,q])|.$$

$$\Omega(\mathrm{BNT}[p,q],x) = px^{q+1}+2px^{q}.$$

$$\Omega'(\mathrm{BNT}[p,q],x) = p(q+1)x^{q}+2pqx^{q-1}.$$

Theorem 8.1.2. *The Sadhana polynomials of* $\mathrm{BNT}[p,q]$ *are computed as*

$$Sd(\mathrm{BNT}[p,q],x) = \begin{cases} px^{3pq+p-q-1}+2px^{3pq+p-q}, & \textit{if } p \textit{ is even, } q \textit{ is odd,}\\ \frac{p}{2}x^{3pq+p-q-2}+\frac{5p}{2}x^{3pq+p-q}, & \textit{if } p \textit{ is even, } q \textit{ is even.}\end{cases}$$

Also Sahana index is computed as

$$| Sd'(BNT[p,q],x) |_{x=1} = \begin{cases} 9p^2q+3p^2-3pq-p, & \textit{if } p \textit{ is even, } q \textit{ is even or odd .} \end{cases}$$

Theorem 8.1.3. *Theta and PI polynomials of* BNT$[p,q]$ *are computed as*

$$\Theta(\mathrm{BNT}[p,q],x) = \begin{cases} p(q+1)x^{q+1}+2pqx^q, & \textit{if } p \textit{ is even, } q \textit{ is odd} \\ \frac{p}{2}(q+2)x^{q+2}+\frac{5pq}{2}x^q, & \textit{if } p \textit{ is even, } q \textit{ is even.} \end{cases}$$

$$\Pi(\mathrm{BNT}[p,q],x) = \begin{cases} p(q+1)x^{3pq+p-q-1}+2pqx^{3pq+p-q}, & \textit{if } p \textit{ is even, } q \textit{ is odd} \\ \frac{p}{2}(q+2)x^{3pq+p-q-2}+\frac{5pq}{2}x^{3pq+p-q}, & \textit{if } p \textit{ is even, } q \textit{ is even.} \end{cases}$$

The Cluj-Ilmenau index [19], $CI = CI(G)$, is calculated from the Omega polynomial as

$$CI(G) = [\Omega'(G,x)]^2 - [\Omega'(G,x)+\Omega''(G,x)]_{x=1}.$$

We are computing the following important result.

Corollary 8.1.4. *The PI index and Cluj index for* BNT$[p,q]$ *coincide.*

Proof. By definitions the Cluj index and PI index Suppose p is even, q is odd. The Omega polynomial and its first and second derivatives are given as

$$\Omega(\mathrm{BNT}[p,q],x) = px^{q+1}+2px^q.$$

$$\Omega'(\mathrm{BNT}[p,q],x) = p(q+1)x^q+2pqx^{q-1}.$$

$$\Omega''(\mathrm{BNT}[p,q],x) = pq(q+1)x^{q-1}+2pq(q-1)x^{q-2}.$$

$$CI(\mathrm{BNT}[p,q],x) = 9p^2q^2+p^2+6p^2q-3pq^2-2pq-p. \tag{8.1.1}$$

Now the Theta polynomial and its first derivative is computed as

$$\Theta(\mathrm{BNT}[p,q],x) = p(q+1)x^{q+1}+2pqx^q$$

$$\Theta'(\text{BNT}[p,q],x) = p(q+1)(q+1)x^{q} + 2pq^2x^{q-1}$$

Thus PI index is calculated as:

$$PI(\text{BNT}[p,q]) = 9p^2q^2 + p^2 + 6p^2q - 3pq^2 - 2pq - p. \tag{8.1.2}$$

From equations (9.1.6) and (9.1.7), $CL(\text{BNT}[p,q]) = PI(\text{BNT}[p,q])$. Similarly the Omega and the Theta polynomials and their derivatives for even p, q are calculated as

$$\Omega(\text{BNT}[p,q],x) = \frac{p}{2}x^{q+2} + \frac{5p}{2}x^{q}$$
$$\Omega'(\text{BNT}[p,q],x) = \frac{p}{2}(q+2)x^{q+1} + \frac{5pq}{2}x^{q-1}$$
$$\Omega''(\text{BNT}[p,q],x) = \frac{p}{2}(q+2)(q+1)x^{q} + \frac{5pq}{2}(q-1)x^{q-2}$$
$$\Theta(G,x) = \frac{p}{2}(q+2)x^{q+2} + \frac{5p}{2}qx^{q}$$
$$\Theta'(\text{BNT}[p,q],x) = \frac{p}{2}(q+2)(q+2)x^{q+1} + \frac{5p}{2}q^2x^{q-1}.$$

Then the Cluj-index and PI index for even q is calculated as

$$CI(\text{BNT}[p,q],x) = 9p^2q^2 + p^2 + 6p^2q - 3pq^2 - 2pq - 2p = PI(\text{BNT}[p,q],x).$$

Thus The Cluj-index and PI index for even p and all values of q are equal. □

Theorem 8.1.5. *Consider G be a graph representing the family of zigzag boron nanotubes. Suppose p be an odd number and q be a positive integer. Then the Omega polynomial of G is as follows*

$$\Omega(\text{BNT}[p,q],x) = px^{q+1} + 2px^{q}.$$

Proof. Consider G be a graph of family of $BNT[p,q]$. There are three types of oc strips i.e h_1, h_2, h_3. These edges are shown in figure 4 and computed in table 3.

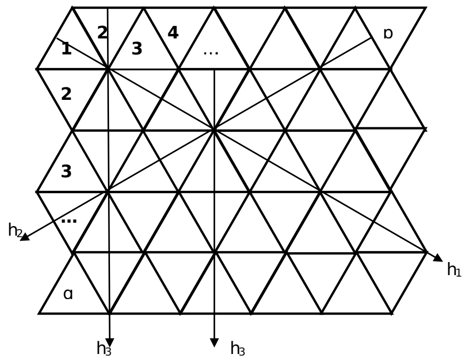

Figure 8.4: 2-dimensional lattice of zigzag boron triangular nanotubes

Edges	No. of qoc strips	No. of cut off edges
h_1	p	q
h_2	p	q
h_3	p	q+1

Table 8.3: The number of equidistant edges for odd p

Then with the help of table 3, Omega polynomial is computed as

$$\Omega(\mathrm{BNT}[p,q],x) = px^{q+1} + 2px^{q}.$$

Hence the theorem. $\square$

The Omega polynomial for odd p becomes the same formula as that of Omega polynomial of $BNT[p,q]$ when p is even with odd q. So that the results for Sadhana polynomial, Theta and PI polynomials are also same which are discussed above for even p.

Chapter 9

The Omega And Sadhana Polynomial Of Armchair Boron Nanotubes ***BNT[p,q]***

In this chapter exact formulae of the Omega and the Sadhana polynomials of BNT$[p,q]$ are being calculated. And also given explicit formulae for counting polynomials of BNT$[p,q]$.

9.1 The Omega And Sadhana Polynomial Of Armchair Boron Triangular Nanotubes $BNT[p,q]$

In this section exact formulae of the Omega and the Sadhana polynomials of BNT$[p,q]$ are being calculated .

Theorem 9.1.1. *Suppose G be a graph presenting the armchair boron nanotubes* BNT$[p,q]$ *where p and q be the number of parallelograms horizontally and vertically respectively, in the given tube as shown in figure 1. The Omega polynomials of* BNT$[p,q]$ *when q is odd, are being calculated as*

$$\Omega(\mathrm{BNT}[p,q],x) = 6px^{q-2} + 2qx^{p} \tag{9.1.1}$$

Proof. Let us consider a graph of armchair BNT$[p,q]$ when q is odd and p be a non-negative integer. One can easily see from the figure 2 that there are eight types of orthogonal cuts. We denote these edges by e_i, where $1 \leq i \leq 8$ are given in the following table.

Then by using the table 1, the proof of the theorem is quite easy. Thus the omega polynomial of $G = \mathrm{BNT}[p,q]$ is as follows

$$\begin{aligned}\Omega(G,x) &= 2px^{q-2} + qx^{p} + 2px^{q-2} + qx^{p} + 2px^{q-2}, \\ &= 6px^{(q-2)} + 2qx^{p}.\end{aligned}$$

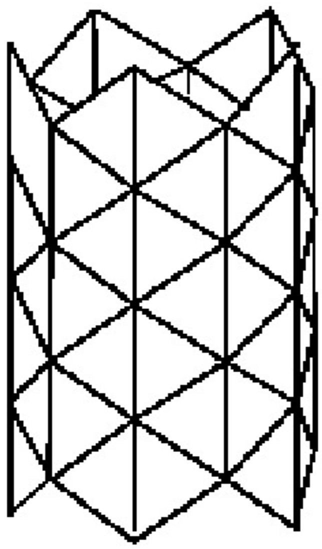

Figure 9.1: 3-dimensional armchair nanotube

Edges	No. of qoc strips	No. of cut off edges
e_1	p	q-2
e_2	p	q-2
e_3	q	p
e_4	p	q-2
e_5	p	q-2
e_6	q	p
e_7	p	q-2
e_8	p	q-2

Table 9.1: The number of equidistant edges for odd q

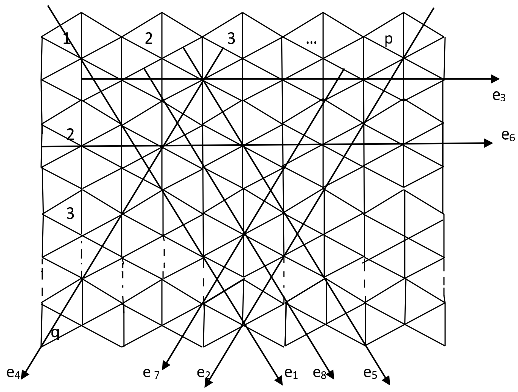

Figure 9.2: 2-dimensional armchair nanotube for odd q

Hence the result. Which completes the proof of the Theorem. □

Now we wish to find out Sadhana polynomial and Sadhana index for the discussed Omega polynomials. The total number of edges for the given family of armchair boron nanotubes are

$$\Omega'(\mathrm{BNT}[p,q],x)_{x=1} = |E(\mathrm{BNT}[p,q])|.$$

The derivative of Omega polynomial gives the total number of edges. i.e

$$\begin{aligned}\Omega^{'}(\mathrm{BNT}[p,q],x) &= 6p(q-2)x^{q-3} + 2pqx^{p-1}, \\ &= 8pq - 12p.\end{aligned}$$

Theorem 9.1.2. *The Sadhana polynomials of armchair boron nanotubes* BNT$[p,q]$ *are computed as*

$$Sd(\mathrm{BNT}[p,q],x) = 6px^{8pq-12p-q+2} + 2qx^{8pq-13p}. \tag{9.1.2}$$

And Sahana index is computed as follows

$$\begin{aligned}Sd^{'}(\mathrm{BNT}[p,q],x) &= 6p(8pq-12p-q+2)x^{8pq-12p-q+1} + 2q(8pq-13p)x^{8pq-14p}, \\ &= 48p^2q + 16pq^2 - 32pq - 60p.\end{aligned}$$

Theorem 9.1.3. *Theta and PI polynomials of* $\mathrm{BNT}[p,q]$ *are computed as*

$$\Theta(\mathrm{BNT}[p,q],x) = (6pq-12p)x^{q-2} + 2pqx^{p}.$$

And

$$\Pi(\mathrm{BNT}[p,q],x) = (6pq-12p)x^{8pq-12p-q+2} + 2pqx^{8pq-13p}.$$

The Cluj-Ilmenau index [19], $CI = CI(G)$, is calculated from the Omega polynomial as

$$CI(G) = [\Omega'(G,x)]^2 - [\Omega'(G,x) + \Omega''(G,x)]_{x=1}.$$

Here we are computing the following important result.

Corollary 9.1.4. *The PI index and Cluj index for* $\mathrm{BNT}[p,q]$ *coincide.*

Proof. Since

$$CI(G) = [\Omega'(G,x)]^2 - [\Omega'(G,x) + \Omega''(G,x)]_{x=1},$$

And the PI index $PI(G)$ is defined as follows

$$PI(G) = \mid \Pi'(G,x) \mid_{x=1} = e^2 - \sum_{c} m(G,x)c^2 = [(\Omega'(G,x))^2 - \Theta'(G,x)]_{x=1}.$$

Consider p is non-negative, q is odd. The Omega polynomial, its first and second derivatives are given as

$$\Omega(\mathrm{BNT}[p,q],x) = 6px^{q-2} + 2qx^{p}.$$

$$\Omega(\mathrm{BNT}^{'}[p,q],x) = 6p(q-2)x^{q-3} + 2pqx^{p-1}.$$

$$\Omega(\mathrm{BNT}^{''}[p,q],x) = (6pq-12p)(q-3)x^{q-4} + 2p(p-1)qx^{p-2}.$$

$$CI(\mathrm{BNT}[p,q],x) = 64p^2q^2 + 144p^2 - 194p^2q - 6pq^2 + 24pq - 24p. \tag{9.1.3}$$

Now the Theta polynomial and its first derivative at

$$x = 1$$

is computed as

$$\Theta(\mathrm{BNT}[p,q],x) = (6pq - 12p)x^{q-2} + 2pqx^{p}$$

and

$$\Theta^{'}(\mathrm{BNT}[p,q],x) = 6pq^{2} + 24p - 24pq + 2p^{2}q$$

respectively. Thus PI index is calculated as:

$$PI(\mathrm{BNT}[p,q]) = 64p^{2}q^{2} + 144p^{2} - 194p^{2}q - 6pq^{2} + 24pq - 24p. \tag{9.1.4}$$

From equations (9.1.6) and (9.1.7), $CL(\mathrm{BNT}[p,q]) = PI(\mathrm{BNT}[p,q])$. □

Theorem 9.1.5. *Suppose G be a graph representing the family of armchair boron nanotubes. Consider q be an even number and p be a positive integer. Then the Omega polynomial of G is as follows*

$$\Omega(\mathrm{BNT}[p,q],x) = 2px^{q-1} + 4px^{q-2} + 2qx^{p}.$$

Proof. Let us consider G be a graph of family of $BNT[p,q]$. There are eight types of oc strips i.e h_i such that $1 \leq i \leq 8$. These edges are shown in figure 2 and computed in table below.

Then with the help of table 2, Omega polynomial of $G = \mathrm{BNT}[p,q]$ is computed as

$$\begin{aligned}\Omega(G,x) &= 2px^{q-1} + qx^{p} + 2px^{q-2} + qx^{p} + 2px^{q-2}, \\ &= 2px^{q-1} + 4px^{(q-2)} + 2qx^{p}.\end{aligned}$$

Which completes the proof of the Theorem. □

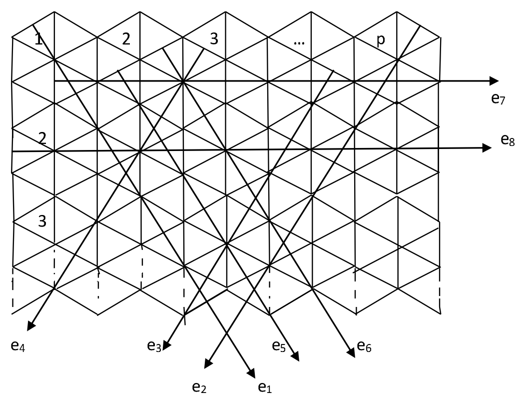

Figure 9.3: 2-dimensional armchair nanotube for even q

Edges	No. of qoc strips	No. of cut off edges
h_1	p	q-1
h_2	p	q-1
h_3	p	q-2
h_4	p	q-2
h_5	p	q-2
h_6	p	q-2
h_7	q	p
h_8	q	p

bm/

Table 9.2: The number of equidistant edges for even q

Now we want to compute Sadhana polynomial and Sadhana index for the discussed Omega polynomials. The total number of edges for the given family of armchair boron nanotubes are

$$\Omega'(\mathrm{BNT}[p,q],x)_{x=1} = |E(\mathrm{BNT}[p,q])|.$$

The derivative of Omega polynomial gives the total number of edges. i.e

$$\begin{aligned}\Omega^{'}(\mathrm{BNT}[p,q],x) &= 2p(q-1)x^{q-2} + 4p(q-2)x^{q-3} + 2pqx^{p-1}, \\ &= 8pq - 10p.\end{aligned}$$

Theorem 9.1.6. *The Sadhana polynomials of armchair boron nanotubes* $\mathrm{BNT}[p,q]$ *are computed as*

$$Sd(\mathrm{BNT}[p,q],x) = 4px^{8pq-10p-q+2} + 2px^{8pq-10p-q+1} + 2qx^{8pq-11p}. \tag{9.1.5}$$

And Sahana index is computed as follows:

$$Sd(G) = 48p^2q + 16pq^2 - 32pq - 60p.$$

Theorem 9.1.7. *Theta and PI polynomials of* $\mathrm{BNT}[p,q]$ *are computed as*

$$\Theta(\mathrm{BNT}[p,q],x) = (4pq-8p)x^{q-2} + (2pq-2p)x^{q-1} + 2pqx^{p}.$$

And

$$\Pi(\mathrm{BNT}[p,q],x) = (4pq-8p)x^{8pq-12p-q+2} + (2pq-2p)x^{8pq-12p-q+1} + 2pqx^{8pq-11p}.$$

The Cluj-Ilmenau index [19], $CI = CI(G)$, is calculated from the Omega polynomial as

$$CI(G) = [\Omega'(G,x)]^2 - [\Omega'(G,x) + \Omega''(G,x)]_{x=1}.$$

Here we are computing the following important result.

Corollary 9.1.8. *The PI index and Cluj index for* $\mathrm{BNT}[p,q]$ *coincide.*

Proof. Consider p is non-negative, q is odd. The Omega polynomial, its first and second derivatives are given as

$$\Omega(\mathrm{BNT}[p,q],x) = 4px^{q-2} + 2px^{q-1} + 2qx^{p}.$$

$$\Omega(\mathrm{BNT}^{'}[p,q],x) = 4p(q-2)x^{q-3} + 2p(q-1)x^{q-2} + 2pqx^{p-1}.$$

$$\Omega(\mathrm{BNT}^{''}[p,q],x) = (4pq-8p)(q-3)x^{q-4} + (2pq-2p)(q-2)x^{q-3} + 2p(p-1)qx^{p-2}.$$

$$CI(\mathrm{BNT}[p,q],x) = 64p^2q^2 + 100p^2 - 162p^2q - 6pq^2 + 20pq - 18p. \tag{9.1.6}$$

Now the Theta polynomial and its first derivative at

$$x = 1$$

is computed as

$$\Theta(\mathrm{BNT}[p,q],x) = (4pq-8p)x^{q-2} + (2pq-2p)x^{q-1} + 2pqx^{p}.$$

$$\Theta^{'}(\mathrm{BNT}[p,q],x) = 2pq^2 + 2p - 4pq + 4pq^2.$$

Thus PI index is calculated as:

$$PI(\mathrm{BNT}[p,q]) = 64p^2q^2 + 100p^2 - 162p^2q - 6pq^2 + 20pq - 18p. \tag{9.1.7}$$

From equations (9.1.6) and (9.1.7), $CL(\mathrm{BNT}[p,q]) = PI(\mathrm{BNT}[p,q])$. □

Chapter 10

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