Computing Degree Based Topological Indices of HAC_5C_7 and VC_5C_7 Nanotubes

By

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CIIT/FA14-MSMATH-010/LHR

MS Thesis

In

Mathematics

COMSATS Institute of Information Technology

Lahore Campus-Pakistan

Spring, 2016

COMSATS Institute of Information Technology

Computing Degree Based Topological Indices of HAC_5C_7 and VC_5C_7 Nanotubes

A Thesis Presented To

COMSATS Institute of Information Technology, Islamabad

In partial fulfillment

of the requirement of the degree of

MS (Mathematics)

By

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Spring, 2016

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

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May, 2016

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I Ahsan Raza (CIIT/FA14-MSMATH-010/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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Dedication

To My Mother

And

My Brother Mohsin Raza

Acknowledgements

First of all, I would like to thank, Almighty ALLAH Who is most Gracious, Merciful, Omniscient and Omnipotent, and without the help of Whom nothing is possible.

I would like to thank Dr. Faisal Nadeem, my supervisor, for his many valueable suggestions, constant support and encouragement. His motivation and help combined to make my research experience worthwhile.

My special thanks goes to HOD of mathematics department and all the faculty of CIIT lahore for providing me such a great research environment.

I want to thank all those friends, who remain sincere with me and gave me good suggestions.

Finally, I am thankful to my whole family especially my respectable parents and my brothers, for their prayers and continuing support.

Ahsan raza

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Abstract

Computing Degree Based Topological Indices of HAC_5C_7 and VC_5C_7 Nanotubes

There are certain types of topological indices such as degree based topological indices, distance based topological indices and spectrum based topological indices, which are used by researchers in quantitative structure-property relationship (*QSPR*) and quantitative structure-activity relationship (*QSAR*) to predict physico-chemical properties of chemical compounds. A large number of topological indices are based on vertex-degree of molecular graphs. The purpose of current study is the discussion of the line graphs of $HAC_5C_7[p,q]$ and $VC_5C_7[p,q]$ nanotubes constructed by joinig left right side and as well as constructed by joining upside down, and computing some vertex-degree based topological indices of the line graphs of these nanotubes.

Graph theory is a very powerful tool of applied mathematics. It concerns with different fields of science and has wide applications. In the first chapter we give some basic introduction and some definitions of graph theory.

In the second chapter we give brief description about vertex-degree based topological indices.

In the third chapter of this dissertation, we discussed the line graphs of $HAC_5C_7[p,q]$ nanotube constructed by joinig left right side and as well as constructed by joining upside down. We also computed some well known degree based topological indices of the line graphs of $HAC_5C_7[p,q]$ nanotube.

This dissertation also includes discussion of the line graph of $VC_5C_7[p,q]$ nanotube constructed by joinig left right side and as well as constructed by joining upside down. We also computed some well known degree based topological indices of the line graphs of $VC_5C_7[p,q]$ nanotube given in last chapter.

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Chapter 1

Introduction and Basic Concepts

1.1 Graphs

A **graph** G is an ordered triple $(V(G),\ E(G), \phi_G)$ where $V(G)$ is a non empty set of vertices, $E(G)$ is non empty set of edges disjoint from $V(G)$ and ϕ_G is a function from $E(G)$ to $P(V)$ (power set of V) such that for every $e \in E(G)$, $\phi_G(e)$ is either one element of $P(V)$ or two element of $P(V)$ [1].

ϕ_G is called incidence function and vertices of $\phi_G(e)$ are called end vertices of the edge e. If one element of E is mapped to only one element of $P(V)$ then edges are called simple edges otherwise are called multi edges. Usually we represent vertices with dots and edges with lines (may be curved or straight).

A **simple graph** is a graph without loops and multi edges.

A graph G is **finite** if $V(G)$ and $E(G)$ are finite otherwise G is infinite graph. A simple, finite and undirected graph is shown in Figure 1.1.
$V(G) = \{x_1, x_2, x_3, x_4, x_5\}$ and $E(G) = \{x_1x_2, x_2x_3, , x_3x_4, x_4x_5, x_1x_5, x_2x_5\}$

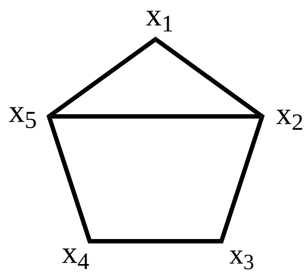

Figure 1.1: Simple graph

Note: Throughout this thesis, we will always consider simple, finite and undirected graphs.

Let G be a graph, then the cardinality of $V(G)$ is called **order** of G and cardinality of $E(G)$ is called **size** of G , denoted by $n(G)$ and $m(G)$ or simply n and m respectively. If $e = xy \in E(G)$, then x, y are adjacent vertices. Symbolically we write it as $x \sim y$. Two distinct edges e and f are said to be adjacent if they have a common end vertex.

The **degree** of a vertex x is the number of vertices that are adjacent to vertex x. It is denoted by $d_x(G)$ or simply d_x. The maximum degree of a vertex of G is called degree of G . The vertex of degree 0 is called isolated vertex and vertex of degree 1 is called end vertex or pendent vertex. An edge is said to be pendent if one of its vertex is pendent.

Theorem 1.1.1. *If a graph G has n vertices and m edges, then*

$$\sum_{x \in V(G)} (d_x) = 2m.$$

The sum of the degrees of all the vertices is equal to double of the edges. This is known as first fundamental theorem of graph theory, given by Euler.

Let x be any vertex of a graph G then $N_G(x) = \{y \in V(G)|xy \in E(G)\}$, i-e set of those vertices of G which are adjacent to x. It is denoted by N_x.

S_x is the sum of degrees of all those vertices which are adjacent to x. Mathematically

$$S_x = \sum_{y \in N_x} d_y.$$

1.2 Subgraphs

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, then H is said to be subgraph of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. In other words if every vertex of H belongs to $V(G)$ and every edge of H belongs to $E(G)$.

Every graph is subgraph of itself. We can obtain a subgraph of a graph G by deleting a vertex or edge of G. If H is a subgraph of G and order of H and G is same then H is said to be **spanning subgraph** of G.

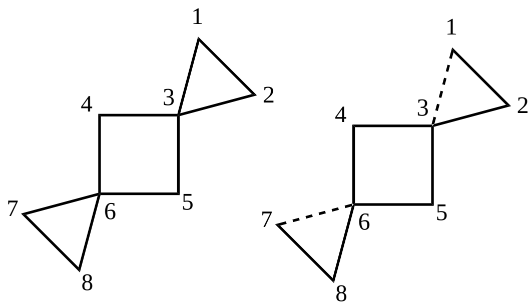

Figure 1.2: A graph and its spanning subgraph

A subgraph H of G is **induced subgraph**, if for every $x, y \in V(H)$ and $xy \in E(G)$, then $xy \in E(H)$.

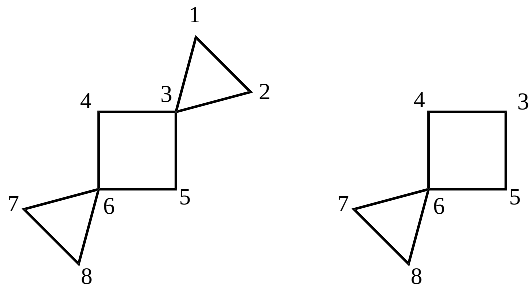

Figure 1.3: A graph and its induced subgraph

1.3 Cycle Graphs

Let $e_i = u_i u_{i+1}$ be edges of G where $i \in [1, t]$, the sequence W of edges such that $W = e_1 e_2 ... e_t$ is called **walk** of length $t-1$, if every two edges are adjacent in W.

A walk W is called a **trail** if all edges of W are distinct.

A walk $W = e_1 e_2 ... e_t (e_i = u_i u_{i+1})$ is called a **path** if all vertices of W are distinct. If starting and ending point of a path is same then it is said to be **closed path** or **cycle**.

A graph G is called **cyclic graph** or **cycle graph** if it contains a cycle. A cycle of n vertices is represented by C_n.

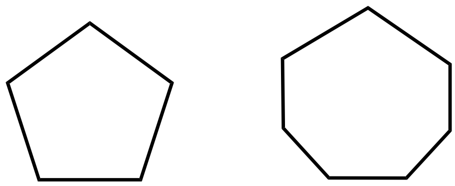

Figure 1.4: C_5 and C_7

1.4 Connected and Disconnected Graphs

If G be a graph, $x, y \in V(G)$ are said to be connected vertices if a path exists between x and y. If every pair of vertices of G is connected then G is said to be **connected graph**.

Any graph which is not connected is called **disconnected graph**. A disconnected graph may contains two or more connected components.

1.5 Some Graph Operations

1.5.1 Union of Graphs

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two graphs, union of G_1 and G_2 is a graph $G_1 \bigcup G_2$, consisting of vertex set $V_1 \bigcup V_2$ and edge set $E_1 \bigcup E_2$.

1.5.2 Join of Graphs

$G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two graphs, join of G_1 and G_2 is a graph $G_1 + G_2$, consisting of vertex set $V_1 \bigcup V_2$ and edge set $E(G_1 + G_2) = \{xy | x \in V(G_1), y \in V(G_2)\}$.

1.5.3 Isomorphic Graphs

A graph $G_1 = (V_1, E_1)$ is said to be isomorphic to $G_2 = (V_2, E_2)$ (denoted by $G_1 \cong G_2$) if there exist a bijection $\beta : V_1 \to V_2$ such that

$$xy \in E_1 \iff \beta(x)\beta(y) \in E_2$$

If G_1 and G_2 are isomorphic, then order, size and degree sequence of G_1 and G_2 are same.

The graphs which are not isomorphic to each other are called non-isomorphic graphs.

1.6 Line Graphs

$G = (V, E)$ be a graph, then $L(G)$ represents the line graph of G , having vertex set $V(L(G)) = E(G)$. The edges of G becomes vertices of $L(G)$. Two vertices in $L(G)$ are adjacent if two edges are adjacent in G .

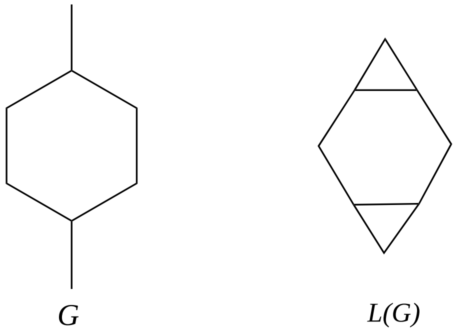

Figure 1.5: A graph G and its line graph L(G)

Graph Theory is widely used in study of networks, electric circuits, scheduling, routing etc. It has considerable applications in physics, chemistry, computer science, electrical and civil engineering, genetics and communication science. Our concern is with the part of graph theory that is applied in chemistry known as chemical graph theory.

Graph Theory is used to model molecules mathematically, in order to get physical and chemical properties. Molecular structure can be represented as a graph known as molecular graph.

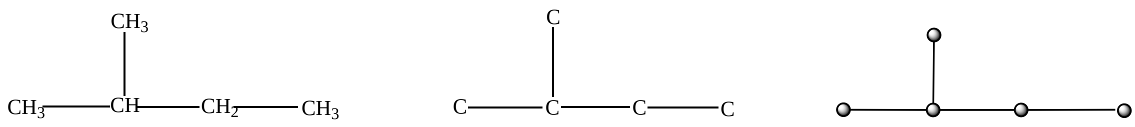

Figure 1.6: 2 methylebutane, its hydrogen depleted molecular graph and molecular graph

1.7 Molecular Graphs

A graph G is said to be molecular graph if vertices of G represents carbon atoms and edges of G represents bonds (covalent bond) between corresponding carbon atoms of an organic molecule. Usually, hydrogen atoms are not depicted in molecular graph of an organic compound. In this case, we said it hydrogen depleted molecular graph. In molecular graph maximum degree of graph is 4.

Chapter 2

Vertex-Degree Based Topological Indices

Molecular descriptor or topological index is a final result obtained by transforming the chemical information into a numerical number. The use of topological indices began in 1947, when Harold Weiner find boiling points of alkanes by using so called Weiner index [36]. After that, in order to explain physico-chemical properties, various topological indices have been introduced.

Molecular descriptors are generally divided into three kinds: degree-based indices [10, 17, 22, 33], distance based indices [13, 23, 30, 37] and spectrum-based indices [7, 26, 27, 28]. There are also some molecular descriptors based on both degrees and distances [6, 12].

Historically, the first vertex-degree based topological indices were Zagreb indices. But, initially these were used for completely different purpose and intended as molecular descriptors much later on.

First genuine vertex-degree based molecular descriptor was Randiȁ index, developed by Milan Randiȁ in 1975 [32]. Randic index of a graph G is

$$R(G) = \sum_{ef \in E(G)} (d_e d_f)^{-1/2}.$$

Later, Bollobás and Erdös generalized it for α, where $\alpha \in \mathbb{R}$ and is called generalized Randiȁ index [4]:

$$R_\alpha(G) = \sum_{ef \in E(G)} (d_e d_f)^{\alpha}.$$

The perticular case of general Randiȁ index for $\alpha = \frac{1}{2}$ is known as Reciprocal Randiȁ index, considered by Favaron et al. in [14]. RR index of any graph G is

$$RR(G) = \sum_{ef \in E(G)} (d_e d_f)^{1/2}.$$

In 2014, Gutman et al. established Reduced Reciprocal Randiȁ index in [19]. RRR index of any graph G is

$$RRR(G) = \sum_{ef \in E(G)} \sqrt{(d_e - 1)(d_f - 1)}.$$

First Zagreb index of G is defined by Gutman and Trinajstiȁ [21]:

$$M_1(G) = \sum_{ef \in E(G)} (d_e + d_f).$$

Second Zagreb index was think of by Gutman et al. in 1975 [20], defined as:

$$M_2(G) = \sum_{ef \in E(G)} (d_e d_f).$$

In 2003, Nikoliĉ et al. developed modified form of second Zagreb index [31]. Modified Zagreb index of a graph G is

$$M_2^*(G) = \sum_{ef \in E(G)} \frac{1}{(d_e d_f)}.$$

Li and Zhao established first generalized Zagreb index in [29] as:

$$M_\alpha(G) = \sum_{e \in V(G)} (d_e)^\alpha.$$

Albertson established a new index called Albertson index [2], defined as:

$$A(G) = \sum_{ef \in E(G)} |d_e - d_f|.$$

In 1987, Fajtlowicz established Harmonic index [9].

$$H(G) = \sum_{ef \in E(G)} \frac{2}{d_e + d_f - 2}.$$

In 2010, Fartula et al. established another molecular descriptor called Augmented Zagreb index [11].

$$AZI(G) = \sum_{ef \in E(G)} \frac{(d_e d_f)}{d_e + d_f}.$$

Zhou and Trinajstiĉ established general sum-connectivity index [39].

$$\chi_\alpha(G) = \sum_{ef \in E(G)} (d_e + d_f)^\alpha.$$

Estrada et al. established first member of an important class of indices named as atom-bond connectivity (ABC) indices in [8]. The first atom-bond connectivity index of a graph G is

$$ABC(G) = \sum_{ef \in E(G)} \sqrt{\frac{d_e + d_f - 2}{d_e d_f}}.$$

M. Ghorbani et al. established fourth member of the class of ABC index [16].

$$ABC_4(G) = \sum_{ef \in E(G)} \sqrt{\frac{S_e + S_f - 2}{S_e S_f}}.$$

In 2012, Xing and Zhou developed generalized form of atom bond connectivity index [38].

$$ABC(G) = \sum_{ef \in E(G)} \left(\frac{d_e + d_f - 2}{d_e d_f} \right)^{\alpha}.$$

D. Vukičeviȅ and B. Furtula established the first geometric-arithmetic (GA) index in [35]. The first geometric-arithmetic index of a graph G is

$$GA(G) = \sum_{ef \in E(G)} \frac{2\sqrt{d_e d_f}}{d_e + d_f}.$$

5th member of class geometric-arithmatic index established by Graovac et al. in [15] as:

$$GA_5(G) = \sum_{ef \in E(G)} \frac{2\sqrt{S_e S_f}}{S_e + S_f}.$$

Chapter 3

On topological indices of $HAC_5C_7[p,q]$ nanotube

3.1 Carbon Nanotubes

Ideally, carbon nanotubes (CNT's) can be defined as if one or more seamless cylindrical shells of graphitic sheets combine, a nanotube is form. These cylindrical sheets are closed at each end by half a fullerene. The carbon nanotubes containing only one cylinder are named as single-walled carbon nanotubes (SWCNT's) and carbon nanotubes containing two or more cylindrical shells are termed as multi-walled carbon nanotubes (MWCNT's).

First paper on formation of SWCNT was submitted by Iijima and Ichihashi belonging to NEC research laboratory in 1993 [24]. At the same time Bethune and his team from IBM also submit a paper on formation of SWCNT's [5]. Credit of discovery of SWCNT should be given to both Iijima and Bethune.

In 1991 Iijima made a report. This report enhance the interest of researchers on MWCNT's.
For more details on CNT's see reference [3, 34].

In this chapter we shall discuss the line graphs of $HAC_5C_7[p, q]$ nanotube constructed by joining left right side, as well as constructed by joining upside down. We shall also compute some well known vertex-degree based topological indices of the line graphs of $HAC_5C_7[p, q]$ nanotube.

3.2 $HAC_5C_7[p, q]$ nanotube constructed by joining left right side

$HAC_5C_7[p, q]$ $(p, q > 1)$ is a trivalent arrangement of alternating pentagons and heptagons. It can be either a cylinder or a torus. In the first row, the number of heptagons are represented by p, whereas q represents the repetition of vertices and edges in the first three rows. The number of vertices and edges in $HAC_5C_7[p, q]$ constructed by joining left right side are $8pq + p$ and $12pq$ respectively [25].

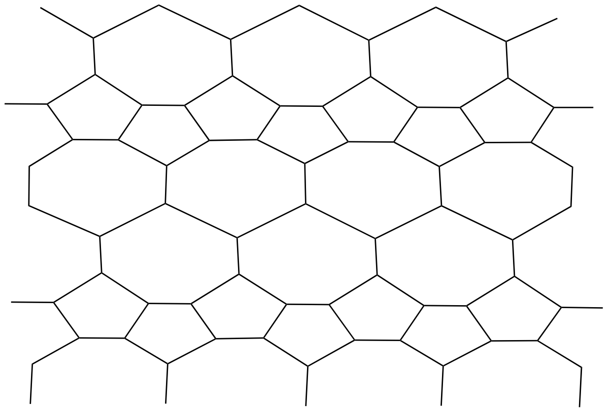

Figure 3.1: $HAC_5C_7[4,2]$ nanotube constructed by joining left right side

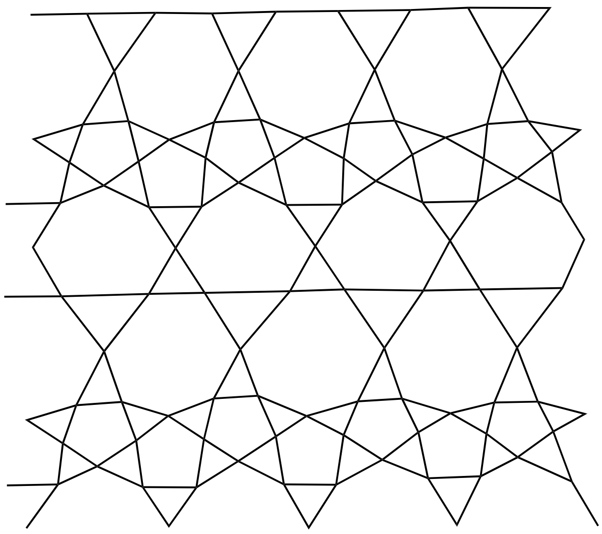

Figure 3.2: Line graph of $HAC_5C_7[4,2]$ nanotube constructed by joining left right side

Theorem 3.2.1. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then Randic index of G is equal to*

$$R_\alpha(G) = 24 \cdot 16^\alpha pq + 2 \cdot 8^\alpha p + 2 \cdot 9^\alpha p + 2 \cdot 12^\alpha p - 8 \cdot 16^\alpha p.$$

Proof. As we know that

$$R_\alpha(G) = \sum_{ef \in E(G)} (d_e d_f)^\alpha.$$

The order of graph G is $12pq$. The edge partition based on degree of the vertices of each edge is shown in Table 3.1.

(d_e, d_f)	$(2,4)$	$(3,3)$	$(3,4)$	$(4,4)$
$\lvert E \rvert$	$2p$	$2p$	$2p$	$24pq - 8p$

Table 3.1: The edge partition of the graph G

After substituting values in above formula, we get

$R_\alpha(G) = 24 \cdot 16^\alpha pq + 2 \cdot 8^\alpha p + 2 \cdot 9^\alpha p + 2 \cdot 12^\alpha p - 8 \cdot 16^\alpha p.$ □

Theorem 3.2.2. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then general Zagreb index of G is equal to*

$$M_\alpha(G) = 12 \cdot 4^\alpha pq + 2^\alpha p + 2 \cdot 3^\alpha p - 3 \cdot 4^\alpha p.$$

Proof. We know that

$$M_\alpha(G) = \sum_{e \in V(G)} (d_e)^\alpha.$$

The number of vertices in G are $12pq$, among which p vertices are of degree 2, $2p$ vertices are of degree 3 and remaining $12pq - 3p$ vertices are of degree 4. So,

$M_\alpha(G) = (p) \times (2)^\alpha + (2p) \times (3)^\alpha + (12pq - 3p) \times (4)^\alpha$

After simplifying, we get

$M_\alpha(G) = 12 \cdot 4^\alpha pq + 2^\alpha p + 2 \cdot 3^\alpha p - 3 \cdot 4^\alpha p.$ □

Theorem 3.2.3. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then general sum connectivity index is given by*

$$\chi_\alpha(G) = 24 \cdot 8^\alpha pq + 4 \cdot 6^\alpha p + 2 \cdot 7^\alpha p - 8 \cdot 8^\alpha p.$$

Proof. As we know that

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_e + d_f)^\alpha.$$

The edge partition is shown in Table 3.1. After substituting the values in above formula, the required result is obtained. □

Theorem 3.2.4. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then $ABC(G)$ index is given by*

$$ABC(G) = \sqrt{2}p + \tfrac{4}{3}\,p + \tfrac{\sqrt{15}}{3}\,p + 6\,\sqrt{6}pq - 2\,\sqrt{6}p.$$

Proof. As we know that, first ABC index is

$$ABC(G) = \sum_{ef \in E(G)} \sqrt{\frac{d_e + d_f - 2}{d_e d_f}}.$$

Using the values from Table 3.1:

$ABC(G) = (2p) \times \sqrt{\frac{2+4-2}{2.4}} + (2p) \times \sqrt{\frac{3+3-2}{3.3}} + (2p) \times \sqrt{\frac{3+4-2}{3.4}} + (24pq - 8p) \times \sqrt{\frac{4+4-2}{4.4}}$

After simplifying, we get

$ABC(G) = \sqrt{2}p + \tfrac{4}{3}\,p + \tfrac{\sqrt{15}}{3}\,p + 6\,\sqrt{6}pq - 2\,\sqrt{6}p.$ □

Theorem 3.2.5. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then $GA(G)$ index is given by*

$$GA(G) = \tfrac{4\sqrt{2}}{3}\,p - 6\,p + \tfrac{8\sqrt{3}}{7}\,p + 24\,pq.$$

Proof. As first geometric-arithmetic index is defined as

$$GA(G) = \sum_{ef \in E(G)} \frac{2\sqrt{d_e d_f}}{d_e + d_f}.$$

Using the values from Table 3.1:

$GA(G) = (2p) \times \frac{2\sqrt{2 \cdot 4}}{2+4} + (2p) \times \frac{2\sqrt{3 \cdot 3}}{3+3} + (2p) \times \frac{2\sqrt{3 \cdot 4}}{3+4} + (24pq - 8p) \times \frac{2\sqrt{4 \cdot 4}}{4+4}$

After simplifying, we get

$GA(G) = \tfrac{4\sqrt{2}}{3}\,p - 6\,p + \tfrac{8\sqrt{3}}{7}\,p + 24\,pq.$ □

Theorem 3.2.6. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then $ABC_4(G)$ index is given by*

$$ABC_4(G) = \tfrac{\sqrt{35}}{7}\,p + \tfrac{\sqrt{770}}{35}\,p + \tfrac{\sqrt{26}}{14}\,p + \tfrac{3}{\sqrt{2}}\,p + \tfrac{3\sqrt{30}}{2}\,pq - \tfrac{15\sqrt{30}}{16}\,p.$$

Proof. As we know that

$$ABC_4(G) = \sum_{ef \in E(G)} \sqrt{\frac{S_e + S_f - 2}{S_e S_f}}.$$

There are $12pq$ edges in G , if we partition the edge set into E_1, E_2, E_3, E_4 and E_5 as follows,

$E_1 = \{ef \in E(G) | (S_e, S_f) = (8, 14)\}$, $E_2 = \{ef \in E(G) | (S_e, S_f) = (10, 14)\}$

$E_3 = \{ef \in E(G) | (S_e, S_f) = (14, 14)\}$, $E_4 = \{ef \in E(G) | (S_e, S_f) = (14, 16)\}$

$E_5 = \{ef \in E(G) | (S_e, S_f) = (16, 16)\}$

E_1 contains $2p$ edges, E_2 contains $2p$ edges, E_3 contains p edges, E_4 contains $6p$ edges and E_5 contains $24pq - 13p$ edges. By putting the values in the formula of fourth ABC index, required result is obtained. □

Theorem 3.2.7. *Let G be the line graph of the $HAC_5C_7[p, q]$ nanotube. Then $GA_5(G)$ index is given by*

$$GA_5(G) = \tfrac{8\sqrt{7}}{11}\, p + \tfrac{\sqrt{35}}{3}\, p - 14\, p + \tfrac{8\sqrt{14}}{5}\, p + 24\, pq.$$

Proof. As we know that

$$GA_5(G) = \sum_{ef \in E(G)} \frac{2\sqrt{S_e S_f}}{S_e + S_f}.$$

There are $12pq$ edges in G , if we partition the edge set into E_1, E_2, E_3, E_4 and E_5 as follows,

$E_1 = \{ef \in E(G) | (S_e, S_f) = (8, 14)\}$, $E_2 = \{ef \in E(G) | (S_e, S_f) = (10, 14)\}$

$E_3 = \{ef \in E(G) | (S_e, S_f) = (14, 14)\}$, $E_4 = \{ef \in E(G) | (S_e, S_f) = (14, 16)\}$

$E_5 = \{ef \in E(G) | (S_e, S_f) = (16, 16)\}$

E_1 contains $2p$ edges, E_2 contains $2p$ edges, E_3 contains p edges, E_4 contains $6p$ edges and E_5 contains $24pq - 13p$ edges.

By putting the values in the formula of fifth GA index, the required result is obtained. □

3.3 $HAC_5C_7[p,q]$ nanotube constructed by joining upside down

$HAC_5C_7[p,q]$ $(p,q>1)$ nanotube constructed by joining upside down is shown in Figure 3.3. The order and size of $HAC_5C_7[p,q]$ is $8pq+6q$ and $12pq+6q$ respectively.

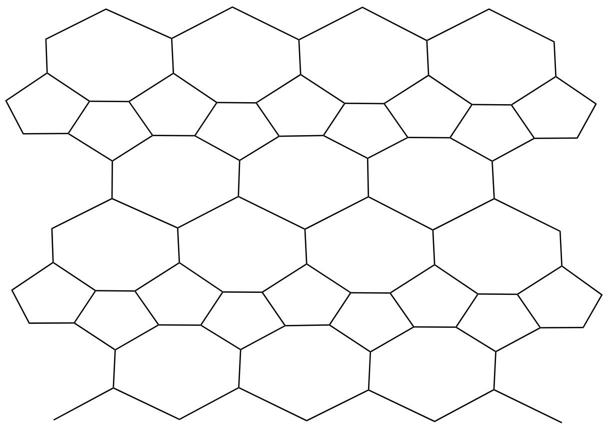

Figure 3.3: $HAC_5C_7[4,2]$ nanotube constructed by joining upside down

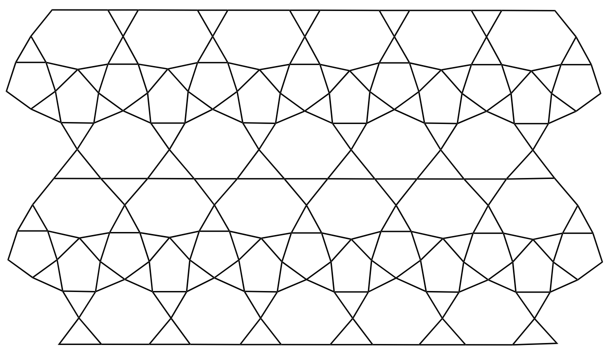

Figure 3.4: Line graph of $HAC_5C_7[4,2]$ nanotube constructed by joining upside down

Theorem 3.3.1. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then Randic index of G is equal to*

$$R_\alpha(G) = 24\cdot 16^\alpha pq + 4\cdot 6^\alpha q + 4\cdot 9^\alpha q + 12^{\alpha+1}q - 14\cdot 16^\alpha q.$$

Proof. As we know that

$$R_\alpha(G) = \sum_{ef \in E(G)} (d_e d_f)^\alpha.$$

The order of the graph G is $12pq + 6q$. The edge partition based on degree of the vertices of each edge is shown in Table 3.2.

(d_e, d_f)	$(2,3)$	$(3,3)$	$(3,4)$	$(4,4)$
$\lvert E \rvert$	$4q$	$4q$	$12q$	$24q - 14q$

Table 3.2: The edge partition of the graph G

After substituting values from Table 3.2 in above formula, the required result is obtained. ☐

Theorem 3.3.2. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then general Zagreb index of G is equal to*

$$M_\alpha(G) = 12 \cdot 4^\alpha pq + 2 \cdot 2^\alpha q + 8 \cdot 3^\alpha q - 4^{\alpha+1} q.$$

Proof. We know that

$$M_\alpha(G) = \sum_{e \in V(G)} (d_e)^\alpha.$$

In G, there are $2q$ vertices of degree 2, $8q$ vertices of degree 3 and $12pq - 4q$ vertices of degree 4, So,

$M_\alpha(G) = (2q) \times (2)^\alpha + (8q) \times (3)^\alpha + (12pq - 4q) \times (4)^\alpha$

After simplifying, we get

$M_\alpha(G) = 12 \cdot 4^\alpha pq + 2 \cdot 2^\alpha q + 8 \cdot 3^\alpha q - 4^{\alpha+1} q.$ ☐

Theorem 3.3.3. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then general sum connectivity index is given by*

$$\chi_\alpha(G) = 24 \cdot 8^\alpha pq + 4 \cdot 5^\alpha q + 4 \cdot 6^\alpha q + 12 \cdot 7^\alpha q - 14 \cdot 8^\alpha q.$$

Proof. As we know

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

The edge partition is shown in Table 3.2. After substituting the values in above formula, the required result is obtained. $\square$

Theorem 3.3.4. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then $ABC(G)$ index is given by*

$$ABC(G) = 2\sqrt{2}\,q + \tfrac{8}{3}\,q + 2\sqrt{15}\,q + 6\,\sqrt{6}pq - \tfrac{7\sqrt{6}}{2}\,q.$$

Proof. As we know that

$$ABC(G) = \sum_{ef \in E(G)} \sqrt{\frac{d_e + d_f - 2}{d_u d_v}}.$$

Using the values from Table 3.2:

$ABC(G) = (4q) \times \sqrt{\frac{2+3-2}{2.3}} + (4q) \times \sqrt{\frac{3+3-2}{3.3}} + (12q) \times \sqrt{\frac{3+4-2}{3.4}} + (24pq - 14q) \times \sqrt{\frac{4+4-2}{4.4}}$

After simplifying, we get

$ABC(G) = 2\sqrt{2}\,q + \frac{8}{3}\,q + 2\sqrt{15}\,q + 6\,\sqrt{6}pq - \frac{7\sqrt{6}}{2}\,q.$ $\square$

Theorem 3.3.5. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then $GA(G)$ index is given by*

$$GA(G) = \tfrac{8\sqrt{6}}{5}\,q - 10\,q + \tfrac{48\sqrt{3}}{7}\,q + 24\,pq.$$

Proof. As we know that

$$GA(G) = \sum_{ef \in E(G)} \frac{2\sqrt{d_e d_f}}{d_e + d_f}.$$

Using the values from Table 3.2:

$GA(G) = (4q) \times \frac{2\sqrt{2 \cdot 3}}{2+3} + (4q) \times \frac{2\sqrt{3 \cdot 3}}{3+3} + (12q) \times \frac{2\sqrt{3 \cdot 4}}{3+4} + (24pq - 14q) \times \frac{2\sqrt{4 \cdot 4}}{4+4}$

After simplifying, we get

$GA(G) = \frac{8\sqrt{6}}{5}\,q - 10\,q + \frac{48\sqrt{3}}{7}\,q + 24\,pq.$ $\square$

Theorem 3.3.6. *Let G be the line graph of the $HAC_5C_7[p,q]$ nanotube. Then $ABC_4(G)$ index is given by*

$$ABC_4(G)=$$

$$\begin{cases} \left(\frac{2\sqrt{435}}{15}+\frac{\sqrt{78}}{9}+\frac{\sqrt{170}}{15}+\frac{\sqrt{2090}}{55}+\frac{2\sqrt{138}}{15}+\frac{3\sqrt{70}}{35}+\frac{14\sqrt{7}}{15}\right. \\ \left.-\frac{33\sqrt{30}}{16}+\frac{8\sqrt{110}}{55}+\frac{\sqrt{210}}{15}+\frac{\sqrt{6}}{3}+\frac{\sqrt{770}}{35}+\frac{\sqrt{2}}{2}\right)q+\frac{3\sqrt{30}}{2}pq, & if \quad p=2\ ; \\ \left(\frac{\sqrt{78}}{9}+\frac{\sqrt{170}}{15}+\frac{\sqrt{2090}}{55}+\frac{2\sqrt{138}}{15}+\frac{3\sqrt{70}}{35}+\frac{4\sqrt{7}}{5}-\frac{17\sqrt{30}}{8}\right. \\ \left.+\frac{8\sqrt{110}}{55}+\frac{\sqrt{210}}{15}+\frac{\sqrt{6}}{3}+\frac{\sqrt{770}}{35}+\frac{\sqrt{2}}{2}+\frac{\sqrt{435}}{6}\right)q+\frac{3\sqrt{30}}{2}pq, & if \quad p>2\ ; \end{cases}$$

Proof. As fourth ABC index is defined as

$$ABC_4(G)=\sum_{ef\in E(G)}\sqrt{\frac{S_e+S_f-2}{S_eS_f}}.$$

First consider the graph G for $p=2$, the edge partition based on the degree sum of neighbor vertices of each vertex is shown in Table 3.3. We apply above formula to the Table 3.3 and get the required index. By Similar arguments we can obtain the expression of ABC_4 index of G for $p>2$ from Table 3.4.

(d_e, d_f)	Number of edges	(d_e, d_f)	Number of edges
$(6, 9)$	$2q$	$(6, 10)$	$2q$
$(9, 10)$	$2q$	$(9, 14)$	$2q$
$(10, 11)$	$2q$	$(10, 14)$	$2q$
$(10, 15)$	$4q$	$(11, 15)$	$4q$
$(14, 15)$	$2q$	$(14, 16)$	$2q$
$(15, 15)$	$7q$	$(15, 16)$	$8q$
$(16, 16)$	$24pq - 33q$		

Table 3.3: The edge partition of the graph G when $p = 2$

(d_e, d_f)	Number of edges	(d_e, d_f)	Number of edges
$(6, 9)$	$2q$	$(6, 10)$	$2q$
$(9, 10)$	$2q$	$(9, 14)$	$2q$
$(10, 11)$	$2q$	$(10, 14)$	$2q$
$(10, 15)$	$4q$	$(11, 15)$	$4q$
$(14, 15)$	$2q$	$(14, 16)$	$2q$
$(15, 15)$	$6q$	$(15, 16)$	$10q$
$(16, 16)$	$24pq - 34q$		

Table 3.4: The edge partition of the graph G when $p > 2$

$\square$

Theorem 3.3.7. *Let G be the line graph of the $HAC_5C_7[p, q]$ nanotube. Then $GA_5(G)$ index is given by*

$$GA_5(G)=$$

$$\begin{cases} \left(\frac{12\sqrt{6}}{5}+\frac{12\sqrt{10}}{19}+\frac{4\sqrt{110}}{21}+\frac{4\sqrt{210}}{29}-26+\frac{4\sqrt{165}}{13}+\frac{159\sqrt{15}}{62}\right. \\ \qquad\left.+\frac{364\sqrt{14}}{345}+\frac{\sqrt{35}}{3}\right)q+24\,pq, \qquad \textit{if} \quad p=2\ ; \\ \left(\frac{12\sqrt{6}}{5}+\frac{12\sqrt{10}}{19}+\frac{4\sqrt{110}}{21}+\frac{4\sqrt{210}}{29}-28+\frac{4\sqrt{165}}{13}+\frac{191\sqrt{15}}{62}\right. \\ \qquad\left.+\frac{364\sqrt{14}}{345}+\frac{\sqrt{35}}{3}\right)q+24\,pq, \qquad \textit{if} \quad p>2\ ; \end{cases}$$

Proof. The GA_5 index is defined as

$$GA_5(G)=\sum_{ef\in E(G)}\frac{2\sqrt{S_eS_f}}{S_e+S_f}.$$

First consider the graph G for $p=2$, the edge partition based on the degree sum of neighbor vertices of each vertex is shown in Table 3.3. We apply above formula to the Table 3.3 and get the required index. By Similar arguments we can obtain the expression of GS_5 index of G for $p>2$ from Table 3.4. $\square$

Chapter 4

On topological indices of $VC_5C_7[p,q]$ nanotube

4.1 Introduction

In this chapter, we shall discuss the line graphs of $VC_5C_7[p,q]$ nanotube constructed by joining left right side, as well as constructed by joining upside down. We shall also compute some well known vertex-degree based topological indices of the line graphs of $VC_5C_7[p,q]$ nanotubes.

4.2 $VC_5C_7[p,q]$ nanotube constructed by joining left side and right side

$VC_5C_7[p,q]$ $(p,q>1)$ is an arrangement of alternating pentagons and heptagons. In the first row, the number of pentagons are represented by p, whereas q represents the repetition of vertices and edges in the first four rows. The order and size of $VC_5C_7[p,q]$ is $16pq+3p$ and $24pq$ respectively. For further detail (see [23]). The 2-dimensional small lattice of $VC_5C_7[p,q]$ is shown in Figure 4.1.

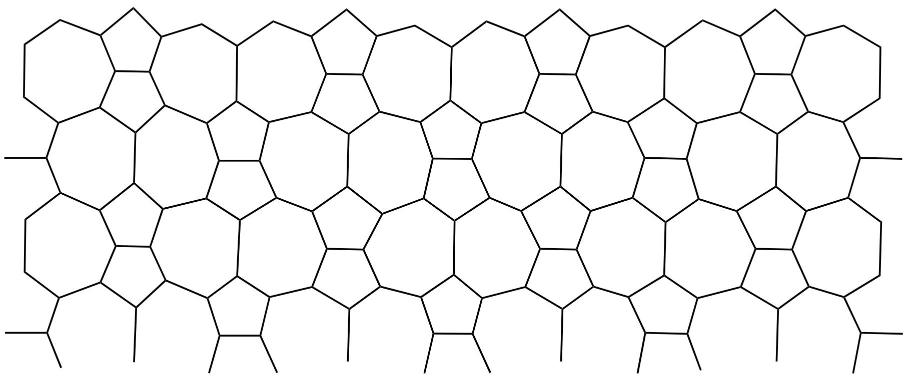

Figure 4.1: $VC_5C_7[4,2]$ nanotube constructed by joining left right side

The number of vertices and edges in $L\{VC_5C_7[p,q]\}$ are $24pq$ and $48pq-6p$ respectively.

Theorem 4.2.1. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $R_\alpha(G)$ index is given by*

$$R_\alpha(G) = 48\cdot 16^\alpha pq + 6\cdot 8^\alpha p + 6\cdot 9^\alpha p + 6\cdot 12^\alpha p - 24\cdot 16^\alpha p.$$

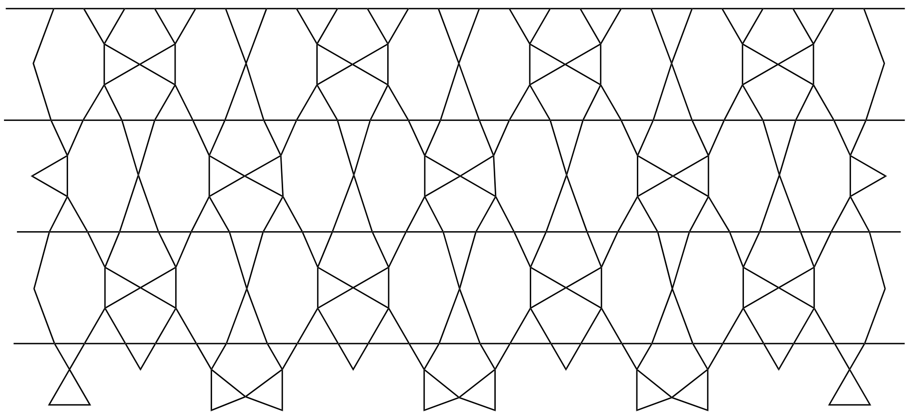

Figure 4.2: Line graph of $VC_5C_7[4,2]$ nanotube constructed by joining left right side

Proof. As we know that

$$R_\alpha(G) = \sum_{ef \in E(G)} (d_e d_f)^\alpha.$$

(d_e, d_f)	$(2,4)$	$(3,3)$	$(3,4)$	$(4,4)$
$\|E\|$	$6p$	$6p$	$6p$	$48pq - 24p$

Table 4.1: The edge partition of the graph G

Edge partition of the graph G is shown in Table 4.1. Using the edge partition from Table 4.1 in above formula, we obtain
$R_\alpha(G) = 48 \cdot 16^\alpha pq + 6 \cdot 8^\alpha p + 6 \cdot 9^\alpha p + 6 \cdot 12^\alpha p - 24 \cdot 16^\alpha p.$ □

Theorem 4.2.2. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $M_\alpha(G)$ index is given by*

$$M_\alpha(G) = 24 \cdot 4^\alpha pq + 3 \cdot 2^\alpha p + 6 \cdot 3^\alpha p - 9 \cdot 4^\alpha p.$$

Proof. As we know that

$$M_\alpha(G) = \sum_{e \in V(G)} (d_e)^\alpha.$$

The order of G is $24pq$. There are $3p$ vertices of degree 2, $6p$ vertices of degree 3 and $24pq - 9p$ vertices of degree 4 in G . So,
$M_\alpha(G) = (3p) \times (2)^\alpha + (6p) \times (3)^\alpha + (24pq - 9p) \times (4)^\alpha$
After simplifying, we obtain
$M_\alpha(G) = 24 \cdot 4^\alpha pq + 3 \cdot 2^\alpha p + 6 \cdot 3^\alpha p - 9 \cdot 4^\alpha p.$ □

Theorem 4.2.3. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $\chi_\alpha(G)$ index is given by*

$$\chi_\alpha(G) = 48 \cdot 8^\alpha pq + 12 \cdot 6^\alpha p + 6 \cdot 7^\alpha p - 24 \cdot 8^\alpha p.$$

Proof. As we know that

$$\chi_\alpha(G) = \sum_{ef \in E(G)} (d_e + d_f)^\alpha.$$

The edge partition is shown in Table 4.1. After substituting the values in above formula, the required result is obtained. □

Theorem 4.2.4. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $ABC(G)$ index is given by*

$$ABC(G) = 3\sqrt{2}\,p + 4\,p + \sqrt{15}\,p - 6\,\sqrt{6}\,p + 12\sqrt{6}\,pq.$$

Proof. As ABC index is defined as

$$ABC(G) = \sum_{ef \in E(G)} \sqrt{\frac{d_e + d_f - 2}{d_e d_f}}.$$

Using the values from Table 4.1:
$ABC(G) = (6p)\times\sqrt{\frac{2+4-2}{2.4}}+(6p)\times\sqrt{\frac{3+3-2}{3.3}}+(6p)\times\sqrt{\frac{3+4-2}{3.4}}+(48pq-24p)\times\sqrt{\frac{4+4-2}{4.4}}$
After simplifying, we obtain
$ABC(G) = 3\sqrt{2}\,p + 4\,p + \sqrt{15}\,p - 6\,\sqrt{6}\,p + 12\sqrt{6}\,pq.$ □

Theorem 4.2.5. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $GA(G)$ index is given by*

$$GA(G) = 4\sqrt{2}\,p - 18\,p + \tfrac{24\sqrt{3}}{7}\,p + 48\,pq.$$

Proof. As GA index is

$$GA(G) = \sum_{ef \in E(G)} \frac{2\sqrt{d_e d_f}}{d_e + d_f}.$$

Using the values from Table 4.1:
$GA(G) = (6p) \times \frac{2\sqrt{2\cdot 4}}{2+4} + (6p) \times \frac{2\sqrt{3\cdot 3}}{3+3} + (6p) \times \frac{2\sqrt{3\cdot 4}}{3+4} + (48pq - 24p) \times \frac{2\sqrt{4\cdot 4}}{4+4}$
After simplifying, we obtain
$GA(G) = 4\sqrt{2}\,p - 18\,p + \frac{24\sqrt{3}}{7}\,p + 48\,pq.$ □

Theorem 4.2.6. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $ABC_4(G)$ index is given by*

$$ABC_4(G) = \tfrac{\sqrt{3}}{2}\,p + \tfrac{2\sqrt{35}}{7}\,p + \tfrac{3\sqrt{770}}{35}\,p + \tfrac{2\sqrt{7}}{7}\,p + \tfrac{3\sqrt{2}}{2}\,p - \tfrac{13}{8}\,\sqrt{30}\,p + 3\,\sqrt{30}\,pq.$$

Proof. As we know that

$$ABC_4(G) = \sum_{ef \in E(G)} \sqrt{\frac{S_e + S_f - 2}{S_e S_f}}.$$

If we consider an edge partition based on degree sum of neighbors of end vertices then the edge set $E(G)$ can be divided into six edge partitions $E_i(G)$, $i = 1, 2, \ldots, 6$, i.e. $E(G) = \cup_{i=1}^{6} E_i(G)$. The edge partition $E_1(G)$ contains $2p$ edges ef, where $S_e = 8, S_f = 12$, the edge partition $E_2(G)$ contains $4p$ edges ef, where $S_e = 8$ and $S_f = 14$, the edge partition $E_3(G)$ contains $6p$ edges ef, where $S_e = 10, S_f = 14$, the edge partition $E_4(G)$ contains $2p$ edges ef, where $S_e = 12$ and $S_f = 14$, the edge partition $E_5(G)$ contains $6p$ edges uef, where $S_e = 14, S_f = 16$, and the edge partition $E_6(G)$ contains $48pq - 26p$ edges ef, where $S_e = S_f = 16$.
By substituting values in above formula, the required result is obtained. □

Theorem 4.2.7. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $GA_5(G)$ index is given by*

$$GA_5(G) = \tfrac{4\sqrt{6}}{5}\, p + \tfrac{16}{11}\, p\sqrt{7} + p\sqrt{35} + \tfrac{4}{13}\, p\sqrt{42} + \tfrac{8\sqrt{14}}{5}\, p - 26\, p + 48\, pq.$$

Proof. Fifth GA index is defined as

$$GA(G) = \sum_{ef \in E(G)} \frac{2\sqrt{d_e d_f}}{d_e + d_f}.$$

(S_e, S_f)	$(8, 12)$	$(8, 14)$	$(10, 14)$	$(12, 14)$	$(14, 16)$	$(16, 16)$
$\lvert E \rvert$	$2p$	$4p$	$6p$	$2p$	$6p$	$48pq - 26p$

Table 4.2: The edge partition of the graph G

Edge partition of the sum of neighbors of end vertices of G is shown in Table 4.2. After substituting values in above formula, we obtain the required result. □

4.3 $VC_5C_7[p,q]$ nanotube constructed by joining upside down

$VC_5C_7[p,q]$ $(p, q > 1)$ nanotube constructed by joining upside down is shown in Fig 4.3. The number of vertices and edges in $VC_5C_7[p,q]$ are $16pq + 8q$ and $24pq + 10q$ respectively.

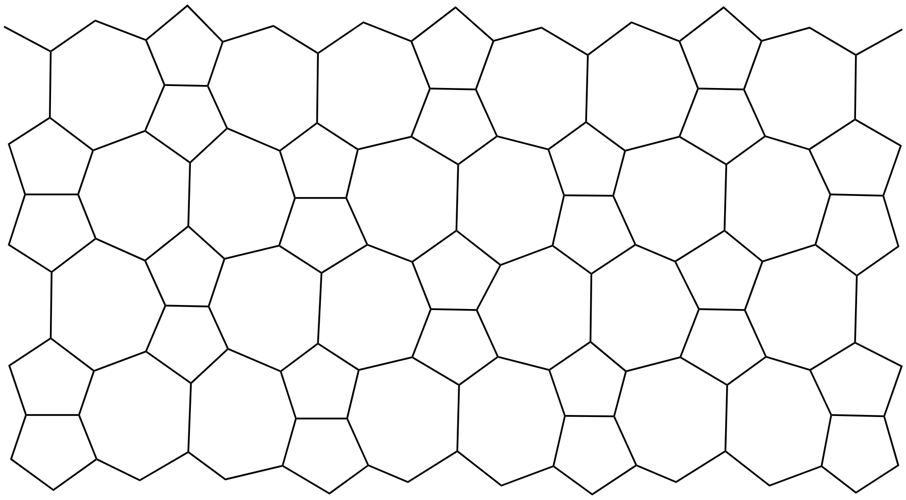

Figure 4.3: $VC_5C_7[3,2]$ nanotube constructed by joining upside down

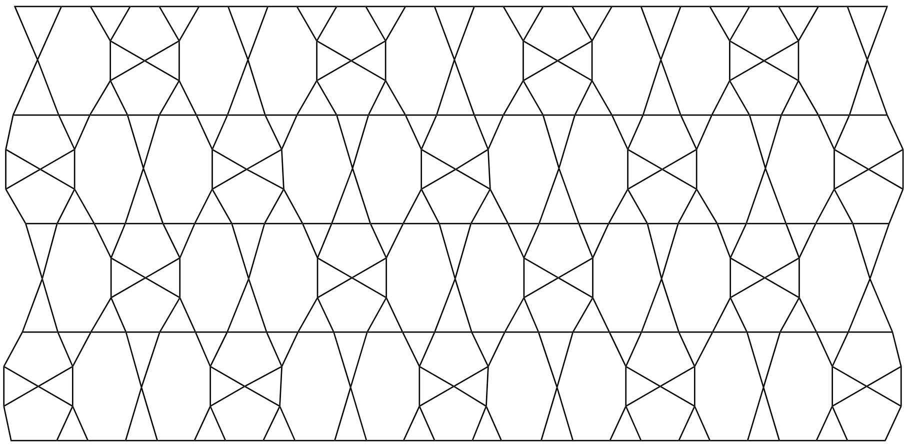

Figure 4.4: Line graph of $VC_5C_7[4,2]$ nanotube constructed by joining upside down

The number of vertices and edges in $L(VC_5C_7[p,q])$ are $24pq+10q$ and $48pq+16q$ respectively.

Theorem 4.3.1. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $R_\alpha(G)$ index is given by*

$$R_\alpha(G) = 48 \cdot 16^\alpha pq + 6 \cdot 9^\alpha q + 12 \cdot 12^\alpha q - 2 \cdot 16^\alpha q.$$

As we know that

Proof.

$$R_\alpha(G) = \sum_{ef \in E(G)} (d_e d_f)^\alpha.$$

The number of vertices of degree 3 and 4 are $8q$ and $24pq+2q$ respectively. If we partition the edge set, we have three partitions as shown in Table 4.3.

(d_e, d_f)	$(3,3)$	$(3,4)$	$(4,4)$
$\lvert E \rvert$	$6q$	$12q$	$48pq-2q$

Table 4.3: The edge partition of the graph G

After substituting the values in above formula, we get
$R_\alpha(G) = 48 \cdot 16^\alpha pq + 6 \cdot 9^\alpha q + 12 \cdot 12^\alpha q - 2 \cdot 16^\alpha q.$ □

Theorem 4.3.2. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $M_\alpha(G)$ index is given by*

$$M_\alpha(G) = 24 \cdot 4^\alpha pq + 8 \cdot 3^\alpha q + 2 \cdot 4^\alpha q.$$

Proof. We know that

$$M_\alpha(G) = \sum_{e \in V(G)} (d_e)^\alpha.$$

G contains $24pq+10q$ vertices, among of which $8q$ vertices are of degree 3 and remaining $24pq+2q$ vertices are of degree 4. So,
$M_\alpha(G) = (8q) \times (3)^\alpha + (24pq+2q) \times (4)^\alpha$
After simplifying, we obtain
$M_\alpha(G) = 24 \cdot 4^\alpha pq + 8 \cdot 3^\alpha q + 2 \cdot 4^\alpha q.$ □

Theorem 4.3.3. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $\chi_\alpha(G)$ index is given by*

$$\chi_\alpha(G) = 48 \cdot 8^\alpha pq + 6 \cdot 6^\alpha q + 12 \cdot 7^\alpha q - 2 \cdot 8^\alpha q.$$

Proof. As we know

$$\chi_\alpha(G) = \sum_{ef \in E(G)} (d_e + d_f)^\alpha.$$

The edge partition is shown in Table 4.3. After substituting the values in above formula, we obtain required result. □

Theorem 4.3.4. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $ABC(G)$ index is given by*

$$ABC(G) = 4\,q + 2\sqrt{15}\,q + 12\,\sqrt{6}pq - \tfrac{\sqrt{6}}{2}\,q.$$

Proof. As ABC index of G is

$$ABC(G) = \sum_{ef \in E(G)} \sqrt{\frac{d_e + d_f - 2}{d_e d_f}}.$$

Using the values from Table 4.3,
$ABC(G) = (6q) \times \sqrt{\frac{3+3-2}{3.3}} + (12q) \times \sqrt{\frac{3+4-2}{3.4}} + (48pq-2q) \times \sqrt{\frac{4+4-2}{4.4}}$
After simplifying, we obtain
$ABC(G) = 4\,q + 2\sqrt{15}\,q + 12\,\sqrt{6}pq - \frac{\sqrt{6}}{2}\,q.$ □

Theorem 4.3.5. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $GA(G)$ index is given by*

$$GA(G) = 4\,q + \tfrac{48\sqrt{3}}{7}\,q + 48\,pq.$$

Proof. As

$$GA(G) = \sum_{ef \in E(G)} \frac{2\sqrt{d_e d_f}}{d_e + d_f}.$$

Using the values from Table 4.3,
$GA(G) = (6q) \times \frac{2\sqrt{3\cdot 3}}{3+3} + (6q) \times \frac{2\sqrt{3\cdot 4}}{3+4} + (48pq - 2q) \times \frac{2\sqrt{4\cdot 4}}{4+4}$
After simplifying, we obtain
$GA(G) = 4\,q + \frac{48\sqrt{3}}{7}\,q + 48\,pq.$ □

Theorem 4.3.6. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then*

$$ABC_4(G) = 3\sqrt{30}pq + \left(\frac{13}{5}\sqrt{2} + \frac{8}{55}\sqrt{110} + \frac{1}{15}\sqrt{435} + \frac{2}{55}\sqrt{2090} + \frac{2}{35}\sqrt{770} - \frac{9}{8}\sqrt{30} + \frac{2}{77}\sqrt{3542} + \frac{6}{35}\sqrt{70}\right) q.$$

Proof. As we know that

$$ABC_4(G) = \sum_{ef \in E(G)} \sqrt{\frac{S_e + S_f - 2}{S_e S_f}}.$$

If we consider an edge partition based on degree sum of neighbors of end vertices then the edge set $E(G)$ can be divided into nine edge partitions $E_i(G)$, $i = 1, 2, \ldots, 9$, i.e. $E(G) = \cup_{i=1}^{9} E_i(G)$. The edge partition $E_1(G)$ contains $2q$ edges ef, where $S_e = 10, S_f = 11$, the edge partition $E_2(G)$ contains $4q$ edges ef, where $S_e = 10$ and $S_f = 11$, the edge partition $E_3(G)$ contains $4q$ edges ef, where $S_e = 10, S_f = 14$, the edge partition $E_4(G)$ contains $4q$ edges ef, where $S_e = 11$ and $S_f = 14$, the edge partition $E_5(G)$ contains $4q$ edges ef, where $S_e = 11, S_f = 15$, the edge partition $E_6(G)$ contains $4q$ edges ef, where $S_e = 14, S_f = 15$, the edge partition $E_7(G)$ contains $4q$ edges ef, where $S_e = 14, S_f = 16$, the edge partition $E_8(G)$ contains $8q$ edges ef, where $S_e = 15, S_f = 16$, and the edge partition $E_9(G)$ contains $48pq - 18q$ edges ef, where $S_e = S_f = 16$.
By substituting values in above formula, we obtain the required result. □

Theorem 4.3.7. *Let G represents the line graph of the $VC_5C_7[p,q]$ nanotube. Then $GA_5(G)$ index is given by*

$$GA_5(G) = 48\,pq + \left(-16 + \frac{4}{13}\sqrt{165} + \frac{32}{31}\sqrt{15} + \frac{8}{21}\sqrt{110} + \frac{2}{3}\sqrt{35} + \frac{8}{25}\sqrt{154} + \frac{8}{29}\sqrt{210} + \frac{32}{15}\sqrt{14}\right) q.$$

Proof. The GA_5 index of G is

$$GA_5(G) = \sum_{ef \in E(G)} \frac{2\sqrt{S_e S_f}}{S_e + S_f}.$$

(d_e, d_f)	Number of edges	(d_e, d_f)	Number of edges
$(10, 10)$	$2q$	$(10, 11)$	$4q$
$(10, 14)$	$4q$	$(11, 14)$	$4q$
$(11, 15)$	$4q$	$(14, 15)$	$4q$
$(15, 16)$	$4q$	$(14, 16)$	$8q$
$(16, 16)$	$48pq - 18q$		

Table 4.4: The edge partition of the graph G

Edge partition of the sum of neighbour vertices of G is shown in Table 4.4. After substituting values in above formula, the required result is obtained. □

Chapter 5

Conclusion and Open problems

5.1 Conclusions

This dissertation studied the construction of the line graphs of $HAC_5C_7[p,q]$ nanotube, constructed by joining left right side, as well as by joining upside down. We also compute some degree based molecular descriptors named general Randic index, general Zagreb index, general sum-connectivity index, first geometric-arithmetic index, fifth geometric-arithmetic index, first atom-bond connectivity index and fourth atom-bond connectivity index of the line graphs of $HAC_5C_7[p,q]$ nanotube.

Furthermore, this dissertation studied the construction of the line graphs of $VC_5C_7[p,q]$ nanotube, constructed by joining left right side, as well as by joining upside down. It also includes the computation of general Randic index, general Zagreb index, general sum-connectivity index, first geometric-arithmetic index, fifth geometric-arithmetic index, first atom-bond connectivity index and fourth atom-bond connectivity index of the line graphs of $VC_5C_7[p,q]$ nanotube.

Open Problem 1. Find the degree based topological indices of the para-line graph of the $HAC_5C_7[p,q]$ nanotube.

Open Problem 2. Compute various degree based topological indices of the paraline graph of the $VC_5C_7[p,q]$ nanotube.

Chapter 6

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