# On Topological Indices of Certain Graphs and Networks

by

**Sakander Hayat**

**Department of Mathematics**

School of Natural Sciences (SNS)

National University of Sciences and Technology (NUST)

Islamabad, Pakistan

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**Sakander Hayat**

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Supervised by

**Dr. Muhammad Imran**

**Department of Mathematics**
School of Natural Sciences (SNS)
National University of Sciences and Technology (NUST)
Islamabad, Pakistan

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**To the loving Memory of**

***My Mother (Late).***

## Abstract

In the study of Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships, physicochemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are used to predict bioactivity of the chemical compounds.

To compute and study topological indices of nanostructures is a respected problem in theoretical nanoscience. In this thesis, we compute and study certain degree based topological indices such as Randić, Zagreb, $ABC$, $GA$, $ABC_4$ and $GA_5$ for various nanostructures like nanotubes and nanocones. We give a characterization of $GA_5$ index for $k$-regular graphs which clear the way to compute this index for all nanotori. We calculate analytically closed results for some counting related polynomials like Omega, Sadhana and Padmakar-Ivan ($PI$) for certain nanotubes for the first time. We study degree based and counting related topological indices of certain networks like silicate networks, hexagonal networks, oxide networks and honeycomb networks.

We define a new class of silicate networks named as chain silicate networks and study certain degree based topological indices for them. These results provide a basis to understand the topology of these important networks.

## Acknowledgement

In the name of Almighty Allah, Who bestowed on me His blessings and gave me courage and vision to accomplish this work successfully. I invoke peace for Holy Prophet Hazrat Muhammad (PBUH) Who is forever a symbol of guidance for humanity.

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# Introduction

A graph can be recognized by a polynomial, a connection table, a sequence of numbers, a matrix and a numeric number (often called a topological index) which represents the whole graph and these representations are aimed to be uniquely defined for that graph. A topological index is a function $Top : \sum \to \mathbb{R}$ where "$\mathbb{R}$" is the set of real of real numbers and "$\sum$" is the set of finite simple graphs with the property that $Top(G) = Top(H)$ if both $G$ and $H$ are isomorphic. Obviously, the number of vertices and edges of a graph are also topological indices.

In the study of Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships, physicochemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are used to predict bioactivity of the chemical compounds. To compute and study topological indices of nanostructures is a respected problem in computational and theoretical nanoscience.

The first two chapters are devoted to some basic definitions and terminologies. In the first chapter, we give a brief introduction of graphs and basic concepts of graph parameters. The second chapter discusses about introduction to topological indices of graphs their significance, and some known results about them.

In the third chapter, we study topological indices of various nanotubes like H-naphtalenic, $VC_5C_7[p, q]$ nanotubes and $CNC_k[n]$ nanocones. Analytically closed results for certain degree based topological indices like Randić, Zagreb, $ABC$, $GA$, $ABC_4$ and $GA_5$ of these finite families of nanotubes are given. We also compute certain counting related polynomials named as Omega, Sadhana and PI for H-naphtalenic nanotubes, which are used to compute their corresponding topological indices. At the end of this chapter, we give a characterization of $GA_5$ index for $k$-regular graphs, which helps to compute this index for all types of nanotori.

In the fourth chapter, we study certain degree based topological indices for various interconnecting networks like silicate, hexagonal, oxide and honeycomb networks. We construct a new class of silicate networks named as chain silicate networks and then study their certain degree based topological indices. These results provide a basis to understand deep topology of these important networks.

A conclusion section highlighting the contribution made in this thesis with some possible open problems arising from the thesis is given at the end.

# Contents

# Chapter 1

# Preliminaries and basic concepts

This chapter gives a gentle yet concise introduction to most of the terminology used later in the thesis. The main concern of this section is to give brief introduction to basic concepts of graphs and is to familiarize about some special graph families. Some notable concepts in graphs like connectivity and planarity are also discussed at the end of this section.

## 1.1 History of graph theory and its branches

It is no coincidence that graph theory has been independently discovered many times, since it may quite properly be regarded as an area of *applied mathematics*.

The basic combinatorial nature of graph theory and a clue to its wide applicability are indicated in the words of Sylvester, "**The theory of ramification is one of pure colligation, for it takes no account of magnitude or position ; geometrical lines are used, but have no more real bearing on the matter than those employed in genealogical tables have in explaining the laws of procreation.**"

Indeed, the earliest recorded mention of the subject occurs in the works of Euler, and although the original problem he was considering might be regarded as a somewhat frivolous puzzle, it did arise from the physical world. Subsequent rediscoveries of graph theory by Kirchhoff and Cayley also had their roots in the physical world.

Kirchhoff's investigations of electric networks led to his development of the basic concepts and theorems concerning trees in graphs, while Cayley considered trees arising from the enumeration of organic chemical isomers. Another puzzle approach to graphs was proposed by Hamilton. After this, the celebrated four colour conjecture came into prominence and has been notorious ever since. In the present century, there have already been a great many rediscoveries of graph theory which we can only mention most briefly in this chronological account.

Euler (1707 − 1782) became the father of graph theory as well as topology. Graph theory is considered to have begun in 1736 with the publication of Eulers solution of the Königsberg bridge problem. The graph theory is one of the few fields of mathematics with a definite birth date by ore.

Generally speaking, graph theory is a branch of combinatorics but it is closely connected to applied mathematics, optimization theory and computer science. In reality, graph theory is cross-disciplinary between mathematics, computer science, electrical engineering and operations research. Here are some of the subjects within graph theory that are of interest to people in these disciplines:

1. **Optimization problems on graphs:** Problems of optimization on graphs generally treat a graph structure like a road network and attempt to maximize flow along that network while minimizing costs. There are many classical optimization problems associated to graphs and this field is sometimes considered a sub-discipline within combinatorial optimization.

2. **Topological graph theory:** Asks questions about methods of embedding graphs into topological spaces (like $\mathbb{R}^2$ or on the surface of a torus) so that certain graph-theoretic properties are maintained. For example, the question of planarity asks: Can a graph be drawn on the plane in such a way so that *no two edge cross*? Clearly, the bridges of Königsburg graph had that property, but not all graphs do.

3. **Graph coloring:** A question related both to optimization and to planarity asks how many colors does it take to color each vertex (or edge) of a graph so that no two adjacent vertices have the same color. Attempting to obtain a coloring of a graph has several applications to scheduling and computer science.

4. **Analytic graph theory:** Is the study of randomness and probability applied to graphs? Random graph theory is a subset of this study. In it, we assume that a graph is drawn from a probability distribution that returns graphs and we study the properties that certain distributions of graphs have.

5. **Algebraic graph theory:** Is the application of abstract algebra (sometimes associated with matrix groups) to graph theory. Many interesting results can be proved about graphs when using matrices and other algebraic properties.

6. **Spectral graph theory:** Spectral graph theory is the study of properties of a graph in relationship to the characteristic polynomial, eigenvalues, and eigenvectors of matrices associated to the graph, such as its adjacency matrix or Laplacian matrix.

7. **Chemical graph theory:** Chemical graph theory is the topology branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena.

Obviously this is not a complete list of all the various problems and applications of graph theory. However, this is a list of some of the major branches of this subject. Now, we proceed to the next section which deals with definitions and related concepts of graphs.

## 1.2 Graphs and related concepts

A *graph* is a tuple, $G = G(V, E)$ where $V = V(G)$, a finite nonempty set of $n$ points (i.e. vertices/nodes) and $E = E(G)$, the set of $m$ unordered pairs of distinct points of $V$. Each pair of points $(u_j, u_k)$ (or simply $(j, k)$) is a line (i.e. edge or link), $e_{j,k}$, of $G$ if and only if $(j, k) \in E(G)$.

In a graph $G(V, E)$, the number of vertices $|V|$ are called *order of G* denoted as $n$ while the number of edges $|E|$ are called *size of G* denoted as $m$. The main concepts and notation in this text are standard and mainly taken from books [14, 35, 60].

Two vertices are called *adjacent* if they have a connection by an edge. If two distinct edges are incident having a vertex in common then they are *adjacent edges*.

The set of all vertices having adjacency to $u$ in $G$ is called the *neighborhood* of $u$ and denoted as $N_G(u)$. The angle between edges as well as the length of an edge are disregarded.

A *directed graph* or *digraph* consists of a finite nonempty set $V$ of vertices along with a collection of ordered pairs of distinct vertices i.e. directed edges. The elements of $E$ are directed lines or arcs. In a *multigraph* two vertices may have more than one edge joining them. Figure 1.1 depicts the graph, digraph and a multigraph.

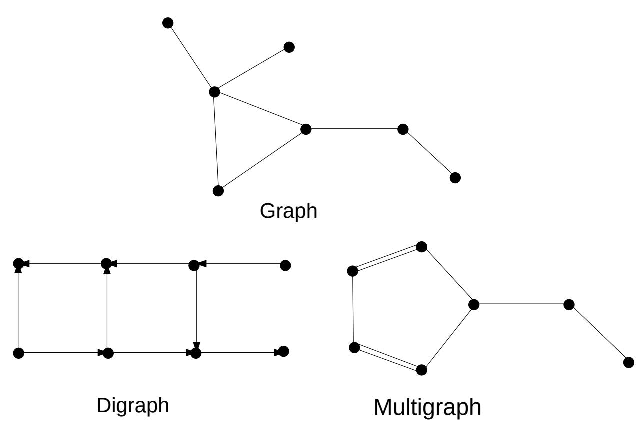


Figure 1.1: A representation of graph, digraph and multigraph

The number of vertices adjacent to a vertex $u$ is called the *degree* of the vertex $u$, denoted as $d_G(u)$ or simply $d_u$. An isolated vertex in a graph $G$ is the vertex of degree 0 while an end vertex (or a leaf) is a vertex of degree 1. Each loop counts to two edges.

A graph $G$ is said to be *finite*, if the number of edges and vertices of $G$ are finite, otherwise $G$ will be an *infinite graph*.

A *walk* is a finite string, $w_{1,n} = (u_j)_{1\leq j\leq n}$, $u_j \in V(G)$ such that any pair $(u_{j-1}, u_j) \in E(G)$, $j = 2, ..., n$. In a walk, we can visit vertices and edges more than once. If $u_1 = u_n$ then the walk is said to be closed and is open if $u_1 \neq u_n$, where $u_1$ and $u_n$ are the first and last vertex of the walk. A closed walk is also called a *self -returning walk*. The set of all walks in $G$ is denoted by $\widetilde{W}(G)$ . The length of a walk $w_{1,n} = (u_j)_{1\leq j\leq n}$ equals the number of edges traveled in it.

A *trail* is a walk in which all its edges are distinct. The vertices can be revisited.

A *path* (i.e. self -avoiding walk) in a graph is a finite or infinite sequence of edges which connect a sequence of vertices. Revisiting of vertices and edges is prohibited. A path is closed if its initial and terminal vertices are same. The set of all paths in $G$ is denoted by $P(G)$.

A graph is *connected* if there exist a path between any pair of vertices. A maximal connected subgraph of $G$ is called a component. A graph is called *disconnected* graph, if it has at least two components.

A *cycle* is a closed path. The *girth* of a graph, $g(G)$, is the length of a shortest cycle (if any) in $G$. The *circumference*, $c(G)$ is the length of a largest cycle. A cycle is both a self-returning and a self-avoiding walk.

A *Hamiltonian path* visits once all the vertices in $G$. A closed hamiltonian path is called a *Hamiltonian circuit*. Figure 1.2 illustrate each type of above discussed walk.

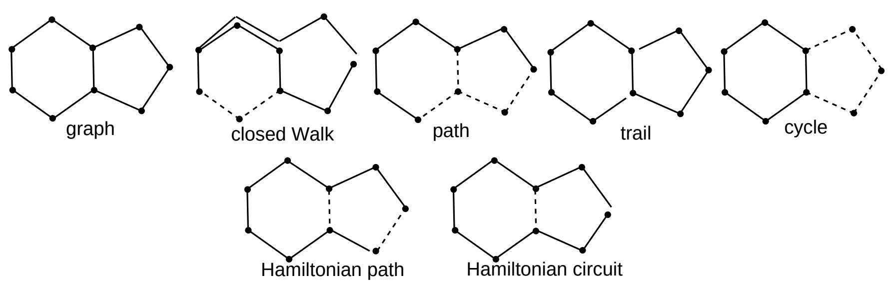


Figure 1.2: Representation of a graph and closed walk, path, trail, cycle, Hamiltonian path and Hamiltonian circuit in it.

Now we discuss some special families of graphs which play an important role in the theory of graphs.

A *path graph*, is a simple graph whose vertices can be arranged so that two vertices are adjacent iff they are consecutive in a list, a path consisting of $n$ vertices is denoted by $P_n$. A *tree*, $T_n$, is an acyclic connected graph of $n$ vertices. A *star* is a set of vertices joined by a common vertex; it is denoted by $S_{n'}$, with $n' = n - 1$, where $n$ is the number of vertices in star. An $n$-dimensional *cycle*, $C_n$, is a chain of $n$ vertices, having same starting and ending vertex. In a cycle graph, every vertex is of degree two. Examples of above discussed graphs are depicted in Figure 1.3.

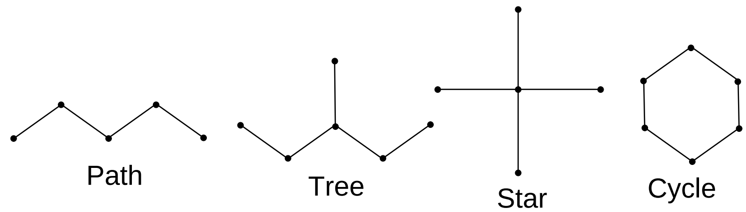


Figure 1.3: Examples of path graph, tree graph, star graph and cycle graphs.

A *complete graph*, $K_n$, is an $n$-ordered graph with any two vertices adjacent. The number of edges in a complete graph is $\binom{n}{2} = n(n-1)/2$. In Figure 1.4, complete graphs with $n = 1$ to 5 are depicted.

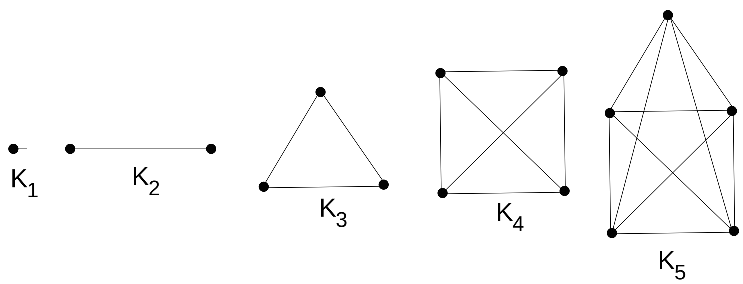


Figure 1.4: Complete graphs of different dimensions.

A *bipartite graph* is a graph whose vertex set $V$ can be decomposed into two disjoint subsets $X, Y \subseteq V$ with $X \cup Y = V$; $X \cap Y = \varnothing$ such that the vertices in $X$ are only adjacent to the vertices in $Y$.

In a bipartite graph $G$ with partite sets $X$ and $Y$, if any vertex $u \in X$ is adjacent to any vertex $v \in Y$ then $G$ is a *complete bipartite graph* and is symbolized by $K_{m,n}$, with $m = |X|$ and $n = |Y|$. A star is a complete bipartite graph $K_{1,n}$. It is clear that $K_{m,n}$ has $m + n$ vertices and $mn$ edges. Figure 1.5 presents some bipartite graphs with their bipartition.

A *rooted graph* is a graph in which heteroatoms or carbons with an unshared electron are specified. Equivalently, a rooted graph is a graph in which one vertex is labeled in a special way to distinguish it from other vertices of graph. This labeled vertex is called the *root of the graph* (Figure 1.6).

A *homeomorph* of a graph $G$ is a graph resulted by inserting vertices of degree 2

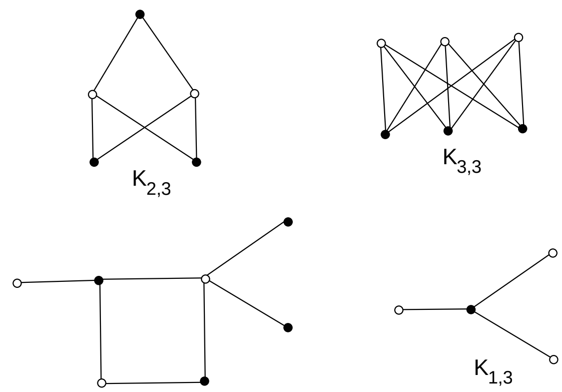


Figure 1.5: Different bipartite graphs with bipartition as hole vertices in one partite set and black vertices in other.

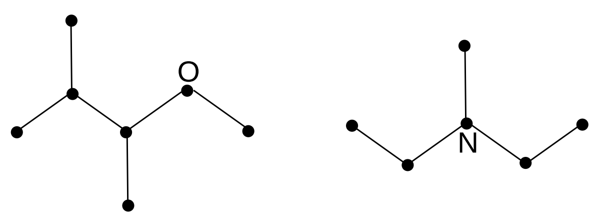


Figure 1.6: Rooted graphs.

(Figure 1.7). The *line graph* of a graph $G$, denoted by $L(G)$, such that its vertices represent edges of $G$ and two vertices of $L(G)$ are adjacent if the corresponding edges of $G$ are incident to a common vertex. Figure 1.8 illustrate such a derivation.

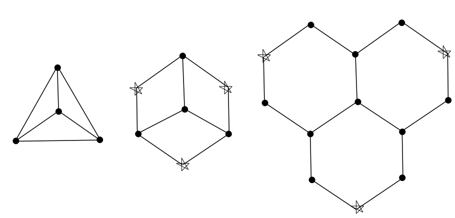

Figure 1.7: Homeomorphs of tetrahedron.

Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic (written $G_1 \cong G_2$) if there exists a mapping $f : V_1 \to V_2$ which obeys the following conditions:

1. $f$ is a bijective function (one-to-one and onto),

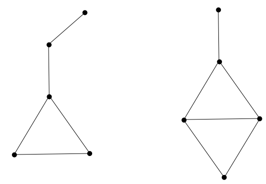

Figure 1.8: A graph and its line graph.

2. for all vertices $u, v \in V$; $(u, v) \in E_1 \Leftrightarrow (f(u), f(v)) \in E_2$.

The function $f$ is called an isomorphism.

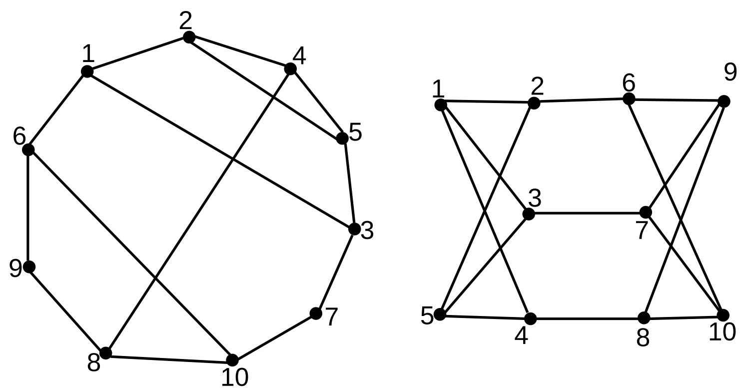


Figure 1.9: Two isomorphic graphs.

An *induced subgraph* of a graph $G$ is a graph $G_1 = (V_1, E_1)$ having $V_1 \subseteq V$ and $E_1 \subseteq E$ (Figure 1.10). A *spanning subgraph* is a subgraph $G_1 = (V, E_1)$ containing all the vertices of $G$ but $E_1 \subseteq E$ (Figure 1.11).

Now we discuss the concept of distance and degree in graphs.

The *distance* between two vertices $u$ and $v$, is denoted as $d(u, v)$, is the length of a *shortest* path joining them : $d(u, v) = \min l(p_{u,v})$, where $l(p_{u,v})$ denotes the length of any path between $u$ and $v$; and if there is no path between $u$ and $v$ then $d(u, v) = \infty$. A shortest path is also called a *geodesic*. The *eccentricity* of a vertex $u$, denoted as $ecc_u$, in a connected graph $G$ is the maximum distance between $u$ and any vertex $v$ of $G$: $ecc_u = \max d(u, v)$ while the *radius* of a graph $G$, denoted as $r(G)$, is the minimum eccentricity among all vertices $u$ in $G$: $r(G) = \min ecc_u = \min \max d(u, v)$. Conversely, the *diameter* of a graph $G$, denoted as $d(G)$, is the maximum eccentricity

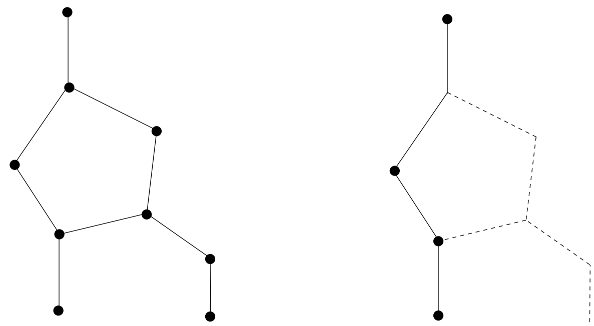

Figure 1.10: A graph and its induced subgraph.

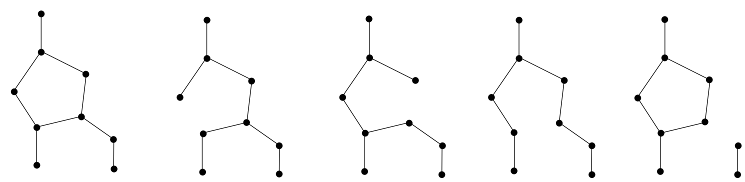

Figure 1.11: A graph and its spanning subgraphs.

in $G$: $d(G) = \max ecc_u = \max \max d(u,v)$.

In a connected graph, the distance is a *metric*, that is, for all vertices $u$ , $v$ and $w$,

1. $m(u,v) \geq 0$, with $m(u,v) = 0$ if and only if $u = v$.

2. $m(u,v) = m(v,u)$

3. $m(u,v) + m(u,w) \geq m(v,w)$

When $l(p_{u,v})$ is expressed in number of edges, the distance is called *topological distance*; when it is measured in meters or submultiples:$(nm, pm)$ it is a *metric distance*. Table 1.1 illustrates the two types of distances.

An *invariant* of a graph is a graph theoretical property, which is preserved by isomorphism. In other words, it remains unchanged, irrespective of the numbering or pictorial representation of $G$.

The *degree*, $d_u$, (i.e. valency), sometimes denoted by $k$) of a vertex $u$ in $G$ is the number of edges incident with $u$ or the cardinality of $N_G(u)$. Since any edge has two

| Chemical Compound | Topological Distance | Metric Distance ($pm$) |
|---|---|---|
| $CH_3 - CH_3$ | 1 | 154 |
| $CH_2 = CH_2$ | 1 | 134 |
| $CH \equiv CH$ | 1 | 121 |

Table 1.1: Topological and Metric Distances

terminal vertices, it contributes twice to the sum of degrees of vertices in $G$, such that $\sum u \in E \; d_u = 2m$, a result which was the first theorem of graph theory (Euler, 1736). In a $(n, m)$ graph, $0 \leq d_u \leq n - 1$, for any vertex $u$. If all vertices have the same degree, $k$, the graph is called *k-regular*; otherwise it is *irregular* (Figure 1.12).

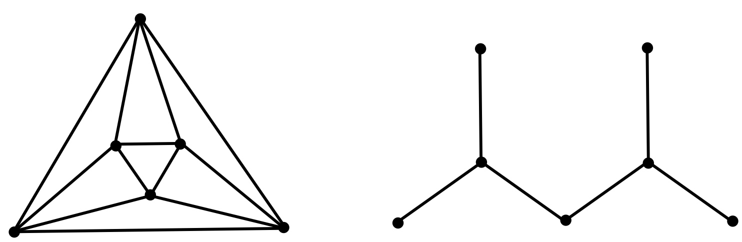

Figure 1.12: A regular and an irregular graph.

## 1.3 Chemical graphs

A *chemical graph* is a model of a chemical system, used to characterize the interactions among its components: atoms, bonds, groups of atoms or molecules. A structural formula of a chemical compound can be represented by a molecular graph, its vertices being atoms and edges corresponding to covalent bonds. Usually hydrogen atoms are not depicted in which case we speak of hydrogen suppressed molecular graphs (Figure 1.13).

The heavy atoms different from carbon (i.e. heteroatoms) can be represented, as shown in Figure 1.6. Similarly, a transform of a molecule (e.g. a chemical reaction) can be visualized by a reaction graph, whose vertices are chemical species and edges reaction pathways.

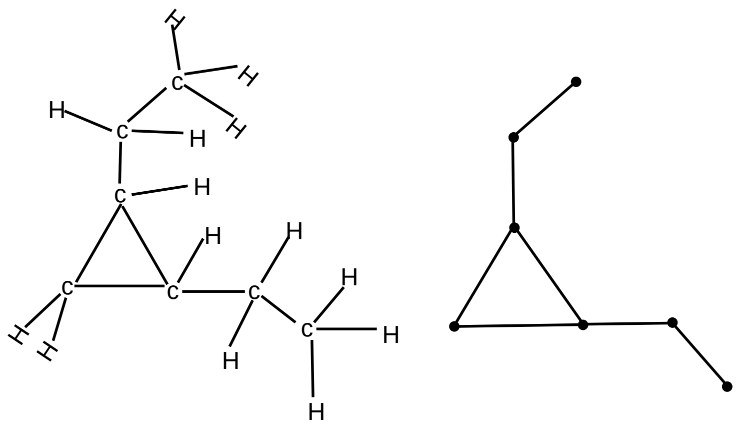


Figure 1.13: A chemical structure and its hydrogen depleted representation (molecular graph).

## 1.4 Planarity and connectivity in graphs

In this section we present some basic concept of planarity in graphs. Concept of connectivity that are useful in measuring connectedness of graphs is also presented at the end of this section.

A *planar graph* usually represented as $G = (V, E, F)$, with vertex set $V$, edge set $E$ and $F$ is being the set of all regions/faces, is a graph, which can be drawn in the plane without crossing any edge. The plane drawing of a graph is called its plane graph. The regions in a plane graph are called faces, $F$, the outer region being the unbounded/exterior face (e.g. $f_4$ in Figure 1.14). For any plane graph with $n$ vertices, $m$ edges and $f$ faces the Euler formula [23] is true: $V - E + F = 2$. A graph is planar if and only if it has no subgraphs homeomorphic to $K_5$ or $K_{3,3}$ (Kuratowski's theorem) [47].

Now we present an important concept in graphs which explains the concept that how much a graph is connected?

Let $G$ be a connected graph and $S \subseteq V(G)$, if $G \setminus S$ is disconnected, then $S$ is referred to as a *vertex cut* of $G$.

A vertex cut of $G$ with minimum cardinality is called a *minimum vertex cut* and the cardinality of that minimum vertex cut is recognized as *connectivity number*,

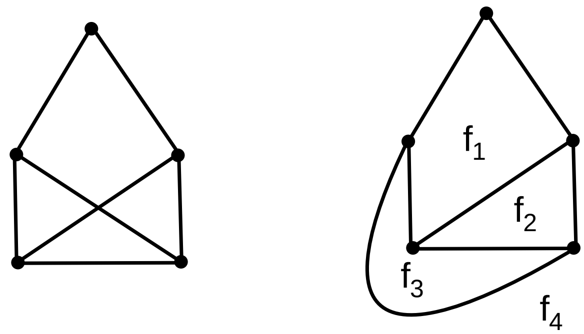


Figure 1.14: A planar graph and its faces.

denoted by $\kappa(G)$. If $G$ is a complete graph, then $\kappa(G)$ is defined to be $n-1$. For a complete graph $G$, connectivity number $\kappa(G)$ is defined to be $n-1$. Thus, $\kappa(G) = 0$ if $G$ is either trivial or disconnected. In a graph $G$, if $\kappa(G) \geq k$ then $G$ is said to be *$k$-connected*.

A cycle $C_n$, where $n \geq 4$ is 2-connected and a path of length two or more is 1-connected. A 3-connected graph $G$ and 1-connected graph $H$ are shown in Figure 1.15.

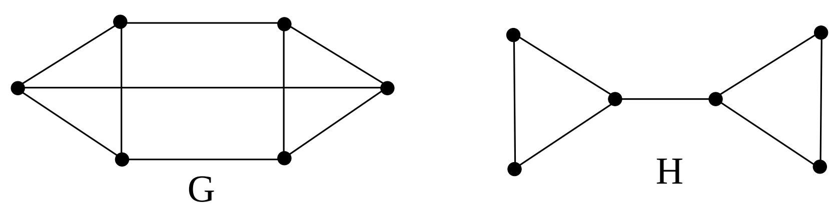


Figure 1.15: Graph

Let $G$ be a connected graph and $S \subseteq E(G)$, if $G \setminus S$ is disconnected then $S$ is referred as an *edge cut* of $G$.

An edge cut of minimum cardinality in $G$ is called a *minimum edge cut* and the cardinality of that minimum edge cut is referred as *edge connectivity number*, denoted by $\kappa'(G)$.

Let $G$ be a non trivial graph then $\kappa'(G) = 0$ if and only if $G$ is disconnected. The edge connectivity number of a trivial graph is also zero. For a connected graph

$G$, $\kappa'(G) = 1$ if and only if $G$ contains a bridge. Furthermore, if $G \cong K_n$ then $\kappa'(G) = n - 1$. A graph $G$ is said to be *k-edge-connected* if $\kappa'(G) \geq k$.
Consider the graph $G$ in figure 1.15, the graph $G$ has $\kappa(G) = \kappa'(G) = 3$.

*Subdividing a graph G* means performing a sequence of edge subdivision operations. The resulting graph is known as *subdivision of the graph G*. We can convert a general graph into a simple graph by the use of subdivision operation.

The *barycentric subdivision* of a graph $G$ is the subdivision in which a new vertex of degree two is added in the interior of each edge. It can be noted that the resulting graph after applying barycentric subdivision is loopless and moreover a loopless graph can be converted into a simple graph by performing barycentric subdivision operation.

Consider the graphs of Figure 1.16, where $G$ is a graph having loop and parallel edges but barycentric subdivision yields a loopless graph and further becomes a simple graph when we again apply barycentric subdivision. $H$ is a cycle of length 5 but its barycentric subdivision yields a cycle of length 10.

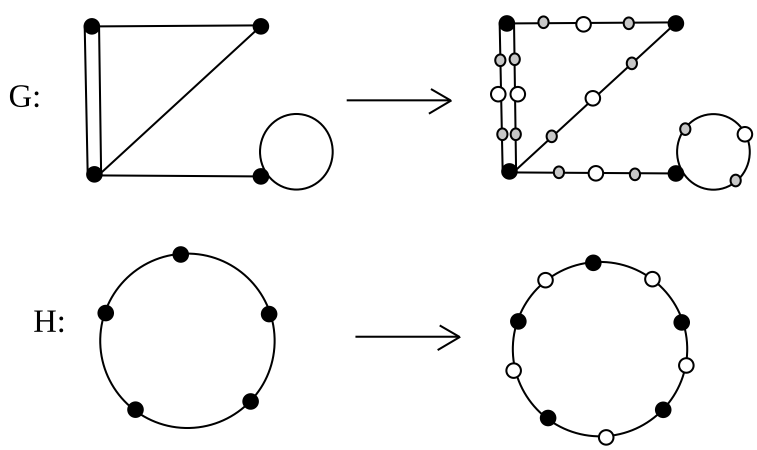


Figure 1.16: Barycentric subdivision of some graphs

# Chapter 2

# Topological indices of graphs and known results

This chapter deals with the concept of topological indices and their major types based on different graph parameters such as distance, degree etc. Moreover, we discuss some known results about these topological indices.

## 2.1 Introduction to topological indices

In graph-theoretical terms, a single numeric number representing a chemical structure is called a *topological descriptor*. It does not depend on the labeling or the pictorial representation of a graph because of being a structural invariant. Despite the considerable loss of information by the projection in a single numeric number of a structure, such descriptors found broad applications in the correlation and prediction of several molecular properties and also in tests of similarity and isomorphism. When a topological descriptor correlates with a molecular property, it can be denominated as molecular index or topological index (TI).

There are hundreds of topological indices which are reported so far. Randić has outlined some desirable attributes for the topological indices in the view of preventing their hazardous proliferation.

List of desirable attributes for a topological index.

- Direct structural interpretation
- Good correlation with at least one property
- Good discrimination of isomers
- Locally defined
- Generalizable to higher analogues
- Linearly independent
- Simplicity
- Not based on physico-chemical properties
- Not trivially related to other indices
- Efficiency of construction
- Based on familiar structural concepts
- Show a correct size-dependence
- Gradual change with gradual change in structures

Only an index having a direct and clear structural interpretation can help to the interpretation of a complex molecular property. If the index correlates with a single molecular property it could indicate the structural composition of that property.

If it is sensible to gradual structural changes (e.g., within a set of isomers) then the index could give information about the molecular shape. If it is locally defined, the index could describe local contributions to a given property. If the index can be generalized to higher analogues or it can be built up on various bases (e.g., on various matrices) it could offer a larger pool of descriptors for the regression analysis.

Among the molecular properties, good correlation with the structure was found for: thermodynamic properties (e.g., boiling points, heat of combustion, enthalpy of formation, etc.), chromatographic retention indices, octane number and various biological properties.

Thus, a topological index converts a chemical structure into a single number, useful in QSPR/QSAR studies. More than a hundred of topological descriptors were proposed so far and tested for correlation with physico-chemical (QSPR) or biological activity (QSAR) of the molecules.

There are two types of invariants, named as Local Invariants (LOIs) and Global Invariants (GLIs). LOIs are defined locally for any atom/vertex whereas GLIs are defined for the whole chemical structure/graph. When a TI shows one and the same value for two or more structures, it is said that TI is degenerated. The degeneracy may appear both in the assignment and the operational stages. The assignment degeneracy appears when non-equivalent subgraphs (i.e., vertices) receive identical LOIs or when non-isomorphic graphs show the same ordered LOIs. The operational degeneracy is seldom encountered (e.g., when simple operations act on weakly differentiated LOIs) and leads to the same value of TI for non-isomorphic graphs which do not show assignment degeneracy.

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph. A TI is actually a numeric quantity associated with chemical constitution purporting for correlation of chemical structure with many physio-chemical properties, chemical reactivity or you can say that biological activity. Mathematically a topological index is a function $Top : \sum \rightarrow \mathbb{R}$ where "$\mathbb{R}$" is the set of real of real numbers and "$\sum$" is the set of finite simple graphs with the property that $Top(G) = Top(H)$ if both $G$ and $H$ are isomorphic. In other words, these numeric numbers are unique under graph isomorphism.

Why do we name these numeric numbers for a graph as topological indices

? In mathematics, a topology is a the study of geometrical properties and spatial (related to space) relations unaffected by the continuous change of shape or size of figures. In other words a topology is a geometrical/structural study of mathematical objects which remains unaffected by doing some change in size or shape. A topological index also study the structural properties of underlying structure/graph (i.e. mathematical object) and remains unchanged/unaffected by doing a continuous change in shape of underlying structure/graph. In topology, a topological space actually studies the geometrical/structural properties of given space, while in graph theory a topological index studies geometrical/structural properties of underlying graph by giving important information about the graph. Furthermore, we usually define a space on the set of vertices of a graph satisfying some axioms. On vertex set of a graph, we define a topology which satisfy the axioms of a topological space as like we define a metric space. Due to these reasons, we call these numbers as topological numbers/indices.

Obviously, the number of vertices and edges of a graph are trivially topological indices. Other common examples of topological indices in a graph which trivially satisfy the definition of a topological index are radius, diameter and chromatic number etc. The theory of topological indices was started by the theoretical chemists and these numbers found to be much significant because of their chemical significance and importance. We do not call number of edges and vertices, radius, diameter etc as topological indices due to the reason because they do not have any chemical significance.

Topological descriptors play a vital role in Quantitative structure-activity (QSAR) and structure-property (QSPR) study. They correlate certain physico-chemical properties (boiling point, melting point, strain energy, enthalpy of vaporization, enthalpy of formation etc.) of certain chemical compounds especially carbon containing compounds (hydrocarbons, nanotubes, nanocones, nanostar, dendrimers, graphite sheets, diamonds, fullerenes etc). Due to this specific property, these descriptors found diverse application in organic chemistry, nanotechnology and biotechnology.

If it is required to find a result for a chemical compound which correlates its specific physico-chemical property, then we construct its chemical graph and by applying various graph-theoretic tools, we find a numeric number which correlates with the value of that particular physico-chemical property. For example, we want to find the value that correlates the boiling point of any member of alkane family, then by drawing its hydrogen depleted graph, we find its Wiener index that correlates its exact value of boiling point. In a similar fashion, if we want to calculate the correlating value of strain energy of branched or cyclo-alkanes, we just calculate its atom-bond connectivity ($ABC$) index (to be discussed in the later part).

This is not the enough introduction to these so-called descriptors, but we must stop here. Now, we discuss some major classes of topological indices, their minor introduction and some well-known results which motivate us to work in this prestigious area of research.

## 2.2 Some major classes of topological indices

As we have already mentioned that, there are hundreds of topological indices which has been reported so far. So, it is not possible to discuss all of them in this short text. We classify them with respect to some graph parameters such as degree and distance etc. In this section, we introduce some distance based, degree based and counting related topological indices. Distance based indices are purely defined using distances in graph, degree based indices are constructed using concept of a valency or degree of vertex and counting related are based on counting the edges in graph, which are topologically parallel. Not all of the indices can be covered in these classes because there are some indices which are defined using both degree and distance of graphs e.g., degree distance index.

In this thesis, $G$ is considered to be simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Distance between vertices $u$ and $v$ is denoted as $d_G(u,v) = d(u,v)$ while $d_G(u) = d_u$ is the degree of vertex $u \in V(G)$. The quantity $\delta_G(u) = S_u = \sum\limits_{v \in N_G(u)} d(v)$, where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

Now, we discuss those classes by taking their examples and known results.

## 2.3 Distance based topological indices

These topological indices are based on distance between two vertices in a graph. Some examples of these indices are following.

- Wiener index
- Harary index
- Szeged index

- Balaban index
- Schultz Molecular Topological Index (MTI) , etc

Now, we define and introduce some of the above mentioned indices.

### 2.3.1 Wiener index

The concept of topological index came from work of *Harold Wiener* in 1947, while he was working on boiling point of paraffin. He named this index as *path number*. Later on, this concept was changed and path number was named as Wiener index [62] and then theory of topological index started. The Wiener index is defined as

$$W(G) = \frac{1}{2} \sum_{(u,v)} d(u,v),$$

where $(u,v)$ is any ordered pair of vertices in $G$ and $d(u,v)$ is the distance between vertices $u$ and $v$.

Its not easy to calculate all distances in a graph having large number of vertices and edges, so researchers construct some ad hoc techniques to compute these indices which reduces the computational complexity of these indices. Now, we present some known results for Wiener index which motivate us to work on nanostructures. To compute and study the topological indices of nanostructures is a respected problem in theoretical nanoscience.

Diedea et al. [15] calculated the analytically closed result of Wiener index for armchair polyhex nanotube $TUVC_6[p,q]$, where $p$ and $q$ are defined in a way such as $p$ is the number of pairs of hexagons in any row and $q$ is the number of vertices in first column. In Figure 2.1, a $TUVC_6[p,q]$ nanotube with $p = 3$ and $q = 8$ is depicted.

**Theorem 2.3.1.** [15] *Consider the armchair polyhex nanotube* $TUVC_6[p,q]$*,* $p, q > 1$

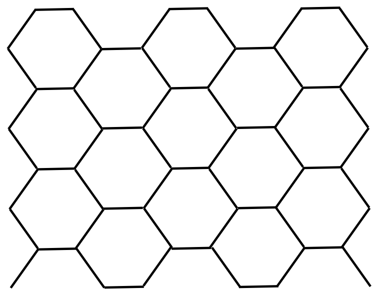

Figure 2.1: $TUVC_6[p,q]$ nanotube with $p=3$ and $q=8$.

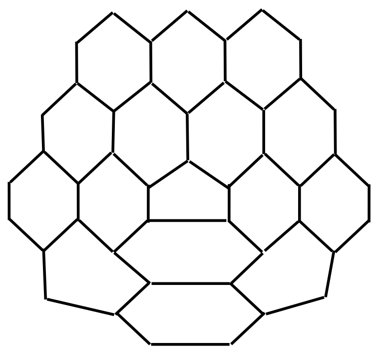

Figure 2.2: A $CNC_5[2]$ nanocone.

*and* $z \equiv p(mod 2)$*, then its Wiener index is equal to*

$$\begin{aligned} W_{TUVC_6}(p,q,z) &= 12(-1)^{p-z}pq + 3(-1)^{p-z+1} + 3(-1)^{-z} - 12q^2z^2 + 12q^2z + \\ &\quad 12(-1)^{p-z}p + 12z^2q + 6(-1)^{p-z+1}p^2 + 8pq^3 - 28pq + 6q^2 + \\ &\quad 18q + 8p^3q + 12p^2q^2 + 12(-1)^{p-z}q + 6(-1)^{p-z+1}q^2 - 24qz - \\ &\quad 12p + 14p^2 + 6(-1)^{1-z}q - 2p^4. \end{aligned}$$

Alipour et al. [2] computed the Wiener index of one-pentagonal nanocone, $CNC_5[n]$, having pentagon at its core and hexagonal layers on its conical surface and $n$ is the number of hexagonal layers on its conical surface. A $CNC_5[2]$ nanocone is depicted in Figure 2.2.

**Theorem 2.3.2.** [2] *Consider the graph of one-pentagonal nanocone,* $CNC_5[n]$*, then its Wiener index is equal to*

$$W(CNC_5[n]) = an^5 + bn^4 + cn^3 + dn^2 + en + f$$

where $a = 20.6666666666671,\ b = -1.63759458326337 \times 10^{-11}$,
$c = -5.83333333311,\ d = -1.28391164496 \times 10^{-09}$,
$e = 0.166666669517,\ f = -1.75858629993 \times 10^{-09}$.

Yousefi et al. [66] computed the exact expression of Wiener index for an arbitrary polyhex nanotorus presented in following theorem.

**Theorem 2.3.3.** [66] *Consider the graph of an arbitrary polyhex nanotorus $T = T[p, q]$, where $p$ and $q$ are defining parameters, then its Wiener index is equal to*

$$W(T) = \begin{cases} \frac{pq^2}{24}(6p^2 + q^2 - 4), & q < p; \\ \\ \frac{p^2q}{24}(3q^2 + 3pq + p^2 - 4), & q \geq p. \end{cases}$$

Harary index is the sum of reciprocal distances in a graph. In other words, we can say that Harary index is the reciprocal extension of a Wiener index. We omit to discuss this index and we now discuss Szeged index. Which is significantly more powerful than Wiener index in a way that Wiener index only correlate the boiling point of branched alkanes, whereas the Szeged index correlate this important physico-chemical property for both branched and cyclo-alkanes.

### 2.3.2 Szeged index

Let $u$ and $v$ be two adjacent vertices of the graph $G$ and $e = uv$ be the edge between them. Let $B_u(e)$ be the set of all vertices of $G$ lying closer to $u$ than to $v$ and $B_v(e)$ be the set of all vertices of $G$ lying closer to $v$ than to $u$, that is,

$$toremovenumbering(beforeeachequation)B_u(e) = \{x|x \in V(G), d(x,u) < d(x,v)\},$$
$$B_v(e) = \{x|x \in V(G), d(x,v) < d(x,u)\}.$$

Let $n_u(e) = |B_u(e)|$, $n_v(e) = |B_v(e)|$. The Szeged index of $G$ is defined as

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e)n_v(e).$$

There is a lot of calculation, which is required to calculate the exact expression of this index. Eliasi et al. [21] calculate the exact expression of the Szeged index for armchair polyhex nanotube defined above and depicted in Figure 2.1.

**Theorem 2.3.4.** [21] *The Szeged index of* $G = TUVC_6[2p, q]$ *is equal to*
***Case I:*** *If* $p$ *is even, then*

$$Sz(G) = \begin{cases} -\frac{p}{12}\Big( - 36p^2q^3 + 24p^2q^2 - 3q + 6q^2 + 6q^5 - \\ 6(-1)^q q^2 + 4q^3 - 3 + 3(-1)^q q + 3(-1)^q - 6q^4\Big), & \text{if } q \le p; \\ \\ \frac{p}{60}\Big(12p^5 + 30p^4 - 80qp^4 - 120qp^3 + 160q^2p^3 + \\ 60q^3p^2 + 80p^2q - 120pq^2 + 30p(-1)^q + \\ 18p + 24q^4p - 33q - 2q^5 + \\ 15(-1)^{q+1}q + 20q^3\Big), & \text{if } p < q < 2p-2; \\ \\ -\frac{p^2}{30}\big( - 70pq^3 + 24 - 26p^4 - 80p^2 - 15p^3 + 60p^2q - \\ 40p^3q + 80pq\big), & \text{if } q \ge 2p-2. \end{cases}$$

***Case II:*** *If* $p$ *is odd, then*

$$Sz(G) = \begin{cases} -\frac{p}{12}\Big( - 36p^2q^3 + 24p^2q^2 + 9q - 6q^2 + 2q^5 - \\ 9(-1)^q q^2 - 3 + 4q^3 - 9(-1)^q q + 3(-1)^q - 6q^4\Big), & \text{if } q \le p; \\ \\ \frac{p}{60}\Big(30 - 80qp^4 - 120qp^3 + 160q^2p^3 + 60q^3p^2 + \\ 80p^2q - 20q^4p + 120pq^2 + 30p(-1)^q + 12p^5 + \\ 30p^4 + 20q^3 - 42p + 120pq + 2q^5 - 33q - 2q^5 + \\ 15(-1)^{q+1}q + 20q^3\Big), & \text{if } p < q < 2p-2; \\ \\ -\frac{p^2}{30}\big( - 60pq + 54p + 30p^2 - 15 - 15p^4 - 80p^3 - \\ 70p^2q^3 - 40p^4q + 60p^3q + 80p^2 + 26p^5\big), & \text{if } q \ge 2p-2. \end{cases}$$

Yazdani et al. [65] computed the Szeged index of H-naphtalenic nanotubes as following. This nanotube is defined and discussed with detail in Section 1 of Chapter 3.

**Theorem 2.3.5.** [65] *The Szeged index of H-naphtalenic nanotube* $T = NPHX[2m, 2n]$ *is equal to*

$$\begin{aligned} Sz(T) &= 2400n^3 - 10000n^3m - 400n^2m^2 + 1200m^3n^2 + 8200m^4n^2 + 24\mu^2m + \\ &\quad 960\mu m^2n(n-m)^2 + 480\mu m^2|n-m|n + 7200n^3m^2 + 6400n^3m^3 - \\ &\quad 480\mu m^2n - 8\mu^2m|n-m| - 4\mu^2m(n-m)^2 - 64\mu^2m(n-m)^3, \end{aligned}$$

*where,*

$$\mu = \begin{cases} 2mn, & \text{if } m \geq n; \\ 2mn - 1, & \text{if } m < n. \end{cases}$$

We now discuss the Balaban index or in short $J$ index, which has low degeneracy than Wiener index.

### 2.3.3 Balaban index

The *Balaban index* is a topological index introduced by *Balaban* near to 30 years ago. The Balaban index of a graph $G$ is the first simple index of very low degeneracy. This is also called the $J$ index. It is defined as

$$J(G) = \frac{E(G)}{\mu + 1} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma_u \sigma_v}},$$

where $\sigma_u = \sum_{w \in V(G)} d(u, w)$ and $\mu = m - n + 1$ is called the cyclomatic number of $G$.

Balaban index has been used in various QSAR and QSPR studies [8]. The Balaban index and Wiener index are two kinds of important topological indices based on the distance. Balaban et al. [9] compare the sequence of the isomers of alkane with $k$ carbon atoms, where $6 \leq k \leq 9$. The result shows that the sequence of the isomers of alkane based on the Balaban index is parallel with that based on the Wiener index. Moreover, the former has smaller degeneracy than latter, which means that using the Balaban index to characterize molecular structure is better than the Wiener index [10]. Now, we discuss the result, in which Balaban index is computed for infinite class of dendrimers $D_k$, where parameter $k$ is defined in a special way.

The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macrocapsules, nanolatex, coloured glasses, chemical sensors, modified electrodes and so on [7, 20]. Figure 2.3 shows the nanostar dendrimer $D_k$ with $k = 2$.

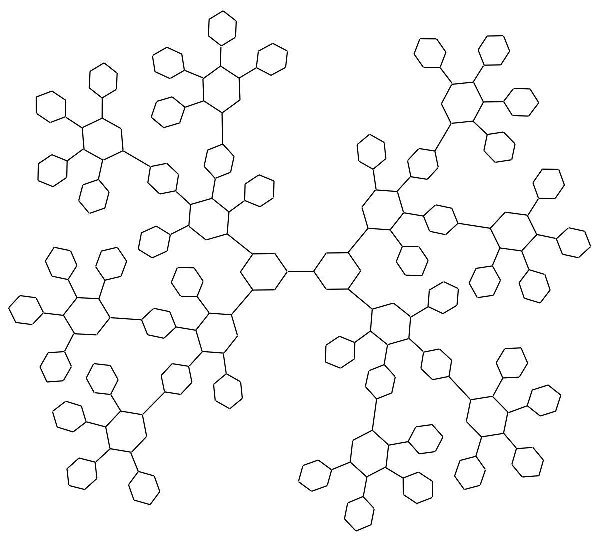

Figure 2.3: The nanostar dendrimer $D_k$ with $k = 2$.

**Theorem 2.3.6.** [57] *Let $D_k$ be the infinite dendrimer, then its Balaban index is equal to*

$$J(D_k) = \frac{1}{2}\big(3 + 2^{k+2} + (3k-7)2^k\big) + \sum_{i=1}^{k}\big[3.2^{i-1}(3 + 2^{k-i+2} + (3k+3i-7)2^k)\big].$$

A $TUC_4C_8(R)[p, q]$ nanotube is parameterized in this manner that $p$ is the number of octagons in any fixed row and $q$ is the number of octagons in any fixed column as shown in Figure 2.4. If we wrap it up so that each dangling edge is connected to rightmost vertex of the same row we get this nanotube. The Balaban index for $TUC_4C_8(R)$ nanotori is discussed by Yousefi-Azari et al. [67].

**Theorem 2.3.7.** [67] *The Balaban index of $T = TUC_4C_8(R)[m, n]$ nanotori is equal*

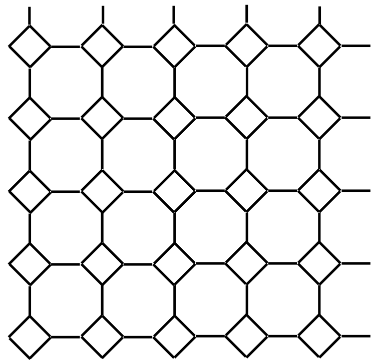

Figure 2.4: The graph of $TUC4C8(R)[p,q]$ nanotube with $p = 5$ and $q = 4$.

*to*

$$J(T) = \begin{cases} \frac{54mn^2}{(mn+2)(6n^2+3mn+m^2-4)}, & n \leq m; \\ \\ \frac{54mn^2}{(mn+2)(6m^2+3mn+n^2-4)}, & n > m. \end{cases}$$

Now, we move on to the degree based topological indices, their minor introduction and some known results. Since, our main concern in this research is on degree based topological indices, so they need special attention.

## 2.4 Degree based topological indices

These topological indices are defined on the ground of degree of a vertex. These indices are of special importance because of their unique chemical significance. They correlate various physico-chemical properties such as, boiling point, strain energy, resonance energy and Kovat's constant in a more efficient way with more prediction power. The examples of famous degree based topological indices are following.

- Randić index
- Sum-connectivity index
- Zagreb index
- Atom-Bond Connectivity index

- Geometric-Arithmetic index, etc

Now, we introduce, define and give some known results of these topological indices.

### 2.4.1 Randić index

The very first and oldest degree based topological index is *Randić* index denoted by $\chi(G)$ and introduced by Milan Randić [54] in 1975. The Randić index of graph $G$ is defined as

$$R_{-\frac{1}{2}}(G) = \chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The general Randić index was proposed by Bollobás and Erdös [11] and Amic et al. [4] independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists [42]. Many important mathematical properties have been established [12]. For a survey of results, we refer to the new book by Li and Gutman [49].

The general Randić index $R_\alpha(G)$ is the sum of $(d_u d_v)^\alpha$ over all edges $e = uv \in E(G)$ defined as

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

Obviously $R_{-\frac{1}{2}}(G)$ is the particular case of $R_\alpha(G)$ when $\alpha = -\frac{1}{2}$.

For a connected graph $G$, the sum connectivity index is defined as following.

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

We present some known motivating results of this Randić index and sum connectivity index.

An $HAC_5C_7[p, q]$ is a $C_5C_7$ net and constructed by alternating $C_5$ and $C_7$ following the trivalent decoration as shown in Figure 2.6. This type of tiling can cover a cylinder and a torus also. The 2-dimensional lattice of $HAC_5C_7[p, q]$, in which $p$ is the number of heptagons in one row and $q$ is the number of periods in whole lattice is discussed in [52]. A period consist of three rows as in Figure 2.5 in which $m$-th period is shown. Farahani [25] computed the Randić index and sum connectivity index of $HC_5C_7[p, q]$ nanotubes.

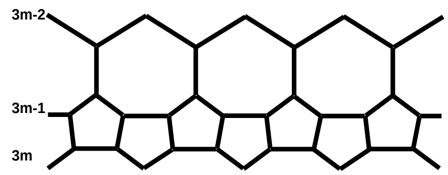


Figure 2.5: $m$-th period of $HAC_5C_7$ nanotube.

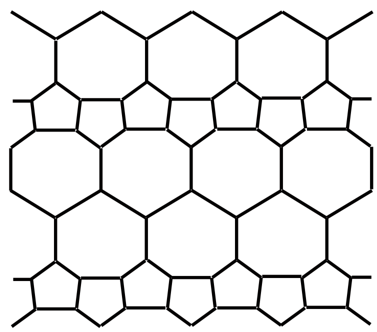

Figure 2.6: The graph of $HAC_5C_7[p, q]$ nanotube with $p = 4$ and $q = 2$.

**Theorem 2.4.1.** [25] *Let $G$ be the $HC_5C_7[p, q]$, $\forall p, q \in \mathbb{N}$ nanotube, then its Randić index is*

$$\chi(G) = 4pq + 2\left(\frac{8\sqrt{6} - 5}{6}\right)p.$$

Sum connectivity index for $G$ is equal to

$$X(G) = 2\sqrt{6}pq + \left(\frac{8\sqrt{5}}{5} - \frac{2\sqrt{6}}{3} + \frac{1}{2}\right)p.$$

To compute and study the topological indices of networks is an important and respected problem in network analysis. These results are significant contribution in network sciences and play an important role to discuss the deep topologies of underlying networks. Rajan et al. [53] studied and computed certain degree based topological indices of silicate, hexagonal and honeycomb networks which are defined and discussed in chapter 4.

**Theorem 2.4.2.** [53] *For an n-dimensional silicate network $SL_n$, the Randić index is equal to*

$$R_{\frac{1}{2}}(SL_n) = (3 + 3\sqrt{2})n^2 + \sqrt{2}n.$$

For an $n$-dimensional hexagonal network $HX_n$, the Randić index is

$$R_{\frac{1}{2}}(HX_n) = \frac{3}{2}n^2 + (\sqrt{6} - 4)n + 2\sqrt{3}(1 - \sqrt{2}) + \frac{1}{2}.$$

For an $n$-dimensional honeycomb network $HC_n$, the Randić index is

$$R_{\frac{1}{2}}(HC_n) = 3n^2 + (2\sqrt{6} - 5)n + 5 - 2\sqrt{6}.$$

Now we discuss the Zagreb indices.

### 2.4.2 Zagreb index

An important topological index introduced about forty years ago by Ivan Gutman and Trinajstić [33] is the *Zagreb index* or more precisely first zagreb index denoted by $M_1(G)$ and was defined as the sum of degrees of end vertices of all edges of $G$. Consider a graph $G$, then first zagreb index is defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

The second version of Zagreb index is proposed late on. It is defined as the product of degrees of end vertices of all edges of $G$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

There is a lot research, which has been done on this index. Lot of papers have been published in different fields of theoretical chemistry by researchers of this interesting interdisciplinary field. We discuss some of the important results of Zagreb index. Farahani et al. [26] computed the zagreb index and Zegreb polynomial of circumcoronene series of benzenoid which are benzenoid structures of special type. A 3-dimensional circumcoronene series of benzenoid graph is depicted in Figure 2.7.

**Theorem 2.4.3.** [26] *Let $G = H_k$, $k > 1$ be the circumcoronene series of benzenoid. Then its first Zagreb index is equal to*

$$M_1(G) = 54k^2 - 30k.$$

Its second Zagreb index is equal to

$$M_2(G) = 81k^2 - 63k + 6.$$

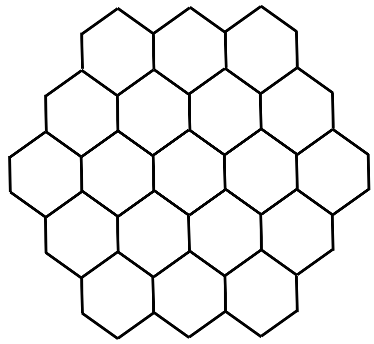

Figure 2.7: A 3-dimensional circumcoronene series of benzenoid graph.

Ilić et al. [43] gave lower bounds for first and second Zagreb indices.

**Theorem 2.4.4.** [43] *For an $n$-ordered simple, connected graph, $M_1$ is bounded below by*

$$M_1 \geq \frac{4m^2}{n}.$$

Its second Zagreb index is bounded below by

$$M_2 \leq \frac{4m^3}{n^2}.$$

### 2.4.3 Atom-bond connectivity index

One of the well-known connectivity topological index is *atom-bond connectivity* ($ABC$) index introduced by Estrada et al. [22]. For a graph $G$, the $ABC$ index is defined as

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

This topological index is very efficient in correlating some important physico-chemical properties like strain energy as well as stability of both branched and cyclo-alkanes.

There are subsequent versions of $ABC$ index, which have been defined later on. The generalized $ABC$ index is defined in the following manner:

$$ABC_k(G) = \sum_{uv \in E(G)} \sqrt{\frac{Q_u + Q_v - 2}{Q_u Q_v}}.$$

where $k \in \mathbb{N}$ and $Q_u$ is the quantity which is uniquely related to the vertex $u$.

- When $Q_u = d_u$ then $k = 1$ and $d_u$ is the degree of vertex $u$ and $d_v$ is defined analogously.

- When $Q_u = n_u$ then $k = 2$ and $n_u$ denotes the number of vertices of $G$ whose distances to vertex $u$ are smaller than those to other vertex $v$ of the edge $e = uv$.

- When $Q_u = m_u$ then $k = 3$ and $m_u$ denotes the number of edges of $G$ lying closer to vertex $u$ than to $v$ of the edge $e = uv$.

- When $Q_u = S_u$ then $k = 4$ and $S_u = \sum_{v \in N_G(u)} d(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

- When $Q_u = \xi_u$ then $k = 5$ and $\xi_u = \max_{v \in V(G)} d(u, v)$.

Now, we exhibit some known and motivating results for $ABC_k$ index.

A $TUC_4C_8(S)[p, q]$ nanotube is parameterized in this manner that $p$ is the number of octagons in any fixed row and $q$ is the number of octagons in any fixed column as shown in Figure 2.8. Asadpour et al. [5] computed the $ABC$ index of

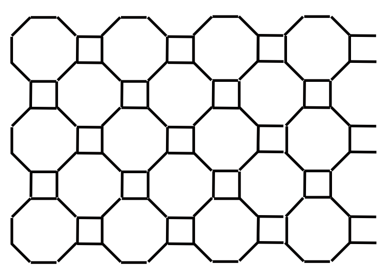

Figure 2.8: A $TUC_4C_8(S)[p, q]$ nanotube with $p = 4$ and $q = 3$.

$TUC_4C_8(S)[p, q]$ nanotube.

**Theorem 2.4.5.** [5] *Let $G$ be the graph of $TUC_4C_8(S)[p, q]$ nanotube, then its ABC index is equal to*

$$ABC(G) = \sqrt{2}(8pq - 3p - 3q + 4) + 4\sqrt{\frac{3}{5}}(p + q - 2).$$

The fourth version of $ABC$ index is introduced by Ghorbani et al. [28] in 2010. They computed it for nanostar dendrimers defined in section 2.3.3 and depicted in Figure 2.3.

**Theorem 2.4.6.** [28] *Let $G_n$ be the graph of nanostar dendrimers. Then*

$$\begin{aligned} ABC_4(G_n) &= \left(\frac{1}{2}\sqrt{6}+\frac{2}{7}\sqrt{3}+\frac{13}{5}\sqrt{2}+\sqrt{\frac{7}{5}}+10\sqrt{\frac{2}{7}}\right)n+ \\ &\left(\sqrt{6}-\frac{2}{7}\sqrt{3}-\frac{8}{5}\sqrt{2}+2\sqrt{\frac{7}{5}}-4\sqrt{\frac{2}{7}}\right). \end{aligned}$$

Farahani computed the $ABC_4$ for V-phenylic nanotube and nanotori.

**Theorem 2.4.7.** [27] *Consider the graph of V-phenylic nanotube $VPHX[m,n]$ $m,n>1$, then its $ABC_4$ index is equal to*

$$ABC_4(VPHX[m,n]) = \left(4n+\sqrt{\frac{5}{6}}+\sqrt{\frac{7}{6}}-2\right)m$$

Consider the graph of V-phenylic nanotorus $VPH[m,n]$ $m,n>1$,. Then its $ABC_4$ index is

$$ABC_4(VPH[m,n]) = 4mn$$

Now, we study geometric-arithmetic ($GA$) index, which has more predictive power than Randić index.

### 2.4.4 Geometric-arithmetic index

Another well-known topological descriptor is *Geometric-Arithmetic* ($GA$) index which was introduced by *Vukičević* et al. [61]. Consider a graph $G$, then its $GA$ index is defined as

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

For physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and a centric factor. The predictive power of GA index is somewhat better than predictive power of the Randić connectivity index.

There are some version of $GA$ index, which are defined subsequently. The generalized $GA$ index is defined in the form:

$$GA_k(G) = \sum_{uv\in E(G)} \frac{2\sqrt{Q_u Q_v}}{(Q_u + Q_v)}.$$

where $k \in \mathbb{N}$ and $Q_u$ is the quantity which is uniquely related to the vertex $u$.

- When $Q_u = d_u$ then $k = 1$ and $d_u$ is the degree of vertex $u$ and $d_v$ is defined analogously.

- When $Q_u = n_u$ then $k = 2$ and $n_u$ denotes the number of vertices of $G$ whose distances to vertex $u$ are smaller than those to other vertex $v$ of the edge $e = uv$.

- When $Q_u = m_u$ then $k = 3$ and $m_u$ denotes the number of edges of $G$ lying closer to vertex $u$ than to $v$ of the edge $e = uv$.

- When $Q_u = \xi_u$ then $k = 4$ and $\xi_u = \max\limits_{v\in V(G)} d(u, v)$.

- When $Q_u = S_u$ then $k = 5$ and $S_u = \sum\limits_{v\in N_G(u)} d(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

Now, we present some known results for $GA$ index and its version.

A $HAC_5C_6C_7[p, q]$ nanotube is a $C_5C_6C_7$ net and constructed by alternating $C_5, C_6$ and $C_7$ following the trivalent decoration as shown in Figure 2.10. This tessellation of $C_5, C_6$ and $C_7$ can either cover a cylinder or a torus. The 2-dimensional lattice of $HAC_5C_6C_7[p, q]$, in which $p$ is the number of pentagons in one row and $q$ is the number of periods in whole lattice. A period consist of three rows as in Figure 2.9 in which $m$-th period is shown. Iranmenash et al. [45] computed the $GA$ index for $HAC_5C_6C_7[p, q]$ nanotubes.

**Theorem 2.4.8.** [45] *For graph of $HAC_5C_6C_7[p, q]$ nanotube, the GA index is*

$$GA(HAC_5C_6C_7[p, q]) = \left(24q + \frac{8\sqrt{6}}{5} + \sqrt{3} - 6\right)p.$$

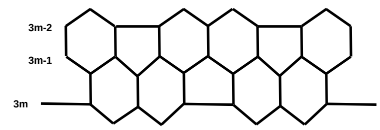


Figure 2.9: $m$-th period of $HAC_5C_6C_7$ nanotube.

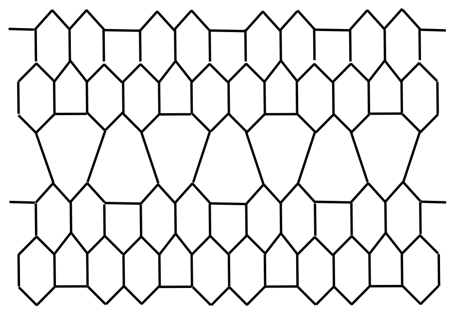

Figure 2.10: The graph of $HAC_5C_6C_7[p, q]$ nanotube with $p = 4$ and $q = 2$.

Farahani [24] computed the $GA_5$ index of $TUC_4C_8(S)[p, q]$ nanotubes depicted in Figure 2.8.

**Theorem 2.4.9.** [24] *For graph of $TUC_4C_8(S)[p, q]$ nanotube, the $GA_5$ index is*

$$GA_5(TUC_4C_8(S)[p, q]) = \left(12q + \frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} - 7\right)p.$$

There are hundreds of papers which have been published on these so-called degree based topological indices so far. Lot of research is done on these numbers so far and progress is doing so. So this is not an enough introduction to these indices, but we must stop here.

## 2.5 Counting related polynomials and topological indices

*Counting polynomials* are those polynomials having at exponent the extent of a property partition and coefficients the multiplicity/occurrence of the corresponding partition. A counting polynomial is defined as:

$$P(G, x) = \sum_k m(G, k)x^k, \tag{2.5.1}$$

where the coefficient $m(G, k)$ are calculable by various methods, techniques and algorithms. The expression (1) was found independently by Sachs, Harary, Milić, Spialter, Hosoya, etc [14]. The corresponding topological index $P(G)$ is defined in this way:

$$P(G) = P'(G, x)|_{x=1} = \sum_k m(G, k) \times k.$$

Two edges $e = uv$ and $f = xy$ in $E(G)$ are said to be *codistant*, usually denoted by $e\ co\ f$, if

$$d(x, u) = d(y, v)$$

and

$$d(x, v) = d(y, u) = d(x, u) + 1 = d(y, v) + 1.$$

The relation "*co*" is reflexive as $e\ co\ e$ is true for all edges in $G$, also symmetric as if $e\ co\ f$ then $f\ co\ e$ for all $e, f \in E(G)$ but the relation "*co*" is not necessarily transitive. Consider

$$C(e) = \{f \in E(G) : f\ co\ e\}.$$

If the relation is transitive on $C(e)$ also, then $C(e)$ is called an *orthogonal cut* "*co*" of the graph $G$. Let $e = uv$ and $f = xy$ be two edges of a graph $G$, which are opposite or topological parallel, and this relation is denoted by $e\ op\ f$. A set of opposite edges, within the same face or ring, eventually forming a strip of adjacent faces/rings, is called an opposite edge strip ops, which is a quasi-orthogonal cut qoc (i.e. the transitivity relation is not necessarily obeyed). Note that "*co*" relation is defined in the whole graph while "*op*" is defined only in a face/ring.

The following indices are examples of counting related topological indices.

- Omega index
- Sadhana index
- Padmakar-Ivan (PI) index
- Non-Equidistance index, etc

The construction is almost same for all indices which are shown above. All of them are defined on the base of counting the opposite edge strips ops defined above. We discuss two famous among them which Omega, Sadhana and PI polynomials and indices.

### 2.5.1 Omega index

The omega polynomial was introduced by Diudea [17] in 2006 on the ground of op strips. The Omega polynomial is proposed to describe cycle-containing molecular structures, particularly those associated with nanostructures. Let $G$ be a graph, then its Omega polynomial denoted by $\Omega(G, x)$ in $x$ is defined as

$$\Omega(G, x) = \sum_{k} m(G, k) \times x^k,$$

where $m(G, k)$ be the number of ops of length $k$.

The corresponding Omega index $\Omega(G)$ is defined as

$$\Omega(G) = \Omega'(G, x)|_{x=1} = \sum_{k} m(G, k) \times k.$$

Now, we discuss some known results for Omega polynomial and Omega index for different families of chemically interesting graphs. A $k$-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells [48]. In Figure 2.11, a zig-zag chain of 8-cycles with $n = 2$ is depicted. Ghorbani

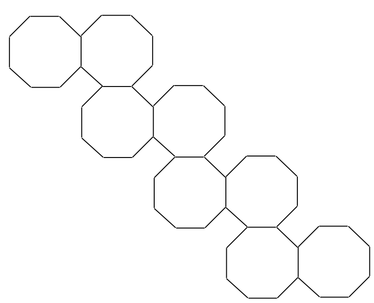

Figure 2.11: A zig-zag chain of 8-cycles with $n = 2$.

et al. [30] computed the Omega polynomial of 2-polyomino and triangular benzenoid systems.

**Theorem 2.5.1.** [30] *Consider the graph of 2-polyomino systems $G_n$, then its Omega polynomial is equal to*

$$\Omega(G_n, x) = (4n-1)x^3 + (8n+2)x^2.$$

Triangular benzenoid are the benzenoid structures in which hexagons are arranged in a manner that they form triangle like structures. In 2.12, triangular benzenoid of dimension $n$ is shown.

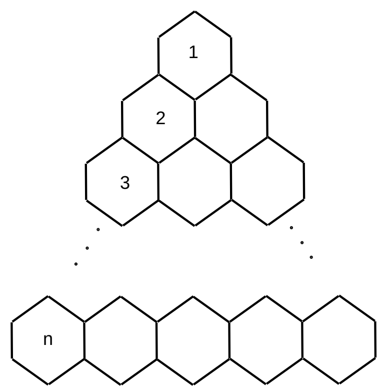


Figure 2.12: A triangular benzenoid structure.

**Theorem 2.5.2.** [30] *Consider the graph of triangular benzenoid systems $G[n]$, then its Omega polynomial is equal to*

$$\Omega(G[n], x) = 3(x^2 + x^3 + ... + x^{n+1}).$$

Ghorbani et al. [31] computed the Omega polynomial of an infinite class of fullerenes.

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. The discovery of $C_{60}$ bucky-ball, which has a nanometer-scale hollow spherical structure in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon. $F_{4\times3^n}$ is an infinite family of fullerenes with $4 \times 3^n$ carbon atoms and $2 \times 3^{n+1}$ bonds. A $F_{4\times3^1}$ fullerene is depicted in Figure 2.13.

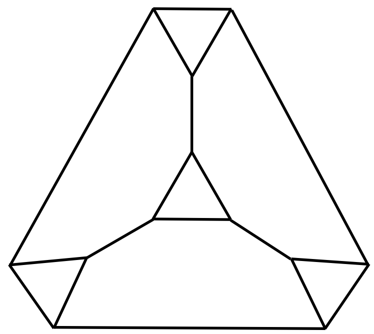

Figure 2.13: A $F_{4\times 3^1}$ fullerene.

**Theorem 2.5.3.** [31] *Consider the graph of infinite class of fullerenes, $F_{4\times 3^n}$, then*

$$\Omega(F_{4\times 3^n}, x) = \begin{cases} 6x^{3^{\frac{n+1}{2}}} + \left(\sum_{k=1}^{\frac{n-1}{2}} 6\times 3^k\right) x^{6\times 3^{\frac{n-1}{2}}}, & 2 \nmid n; \\ \\ 6x^{3^{\frac{n}{2}+1}} + \left(\sum_{k=1}^{\frac{n}{2}-1} 6\times 3^k\right) x^{6\times 3^{\frac{n}{2}}}, & 2 \mid n. \end{cases}$$

Now we discuss Sadhana polynomial and its index by defining it and giving some known results.

### 2.5.2 Sadhana index

The Sadhana polynomial is defined based on counting opposite edge strips in any graph. This polynomial counts equidistant edges in $G$ [16]. Let $G$ be a graph, then Sadhana polynomial denoted by $Sd(G, x)$ is defined as

$$Sd(G, x) = \sum_k m(G, k) \times x^{e-k},$$

where $m(G, k)$ be the number of ops of length $k$ and $e = E(G)$ is the edge set cardinality of $G$.

The corresponding Sadhana index $\Omega(G)$ is defined as

$$Sd(G) = Sd'(G, x)|_{x=1} = \sum_k m(G, k) \times e - k.$$

We give some known results on Sadhana polynomial.

In Figure 2.11, a zig-zag chain of 8-cycles with $n = 2$ is depicted. Ghorbani et al. [30] computed the Sadhana polynomial of 2-polyomino systems.

**Theorem 2.5.4.** [30] *Consider the graph of 2-polyomino systems $G_n$, then its Omega polynomial is equal to*

$$Sd(G_n, x) = (4n-1)x^{28n-2} + (8n+2)x^{28n-1}.$$

A $F_{4\times 3^1}$ fullerene is depicted in Figure 2.13. Ghorbani et al. [31] computed the Sadhana polynomial of an infinite class of fullerenes.

**Theorem 2.5.5.** [31] *Consider the graph of infinite class of fullerenes, $F_{4\times 3^n}$, then*

$$Sd(F_{4\times 3^n}, x) = \begin{cases} 6x^{2\times 3^{n+1}-3^{\frac{n+1}{2}}} + \left(\sum_{k=1}^{\frac{n-1}{2}} 2\times 3^{n+1} - 6\times 3^k\right)x^{6\times 3^{\frac{n-1}{2}}}, & 2 \nmid n; \\ 6x^{2\times 3^{n+1}-3^{\frac{n}{2}+1}} + \left(\sum_{k=1}^{\frac{n}{2}-1} 2\times 3^{n+1} - 6\times 3^k\right)x^{6\times 3^{\frac{n}{2}}}, & 2 \mid n. \end{cases}$$

Now we study PI polynomial and its index.

### 2.5.3 PI index

The PI polynomial is also defined based on counting opposite edge strips in any graph. This polynomial counts non-equidistant edges in $G$ [16]. Let $G$ be a graph, then PI polynomial denoted by $PI(G, x)$ is defined as

$$PI(G, x) = \sum_k m(G, k) \times k \times x^{e-k}.$$

The corresponding PI index $PI(G)$ is defined as

$$PI(G) = PI'(G, x)|_{x=1} = \sum_k m(G, k) \times k \times e - k.$$

Yazdani et al. [64] determined Padmakar-Ivan (PI) polynomials of $HAC_5C_6C_7[4p, 2q]$ nanotubes defined in 2.10.

**Theorem 2.5.6.** [64] *Let $G$ be the $HAC_5C_6C_7$ nanotube, then PI polynomial of $G$ is*

$$PI(G,x) = qx^{9pq-\frac{p}{4}} + px^{9pq+\frac{p}{4}6q} + 4qx^{9pq-\frac{15}{4}p+2} - 9pq - \frac{p}{4} + \binom{|V(G)|+1}{2},$$

*where* $|V(G)| = \frac{3}{2}p^2q + \frac{7}{2}q + p$.

In Figure 2.11, a zig-zag chain of 8-cycles with $n = 2$ is depicted. In Figure 2.12 triangular benzenoid of dimension $n$ is depicted. Ghorbani at et. [30] calculated the PI polynomial of 2-polyomino and triangular benzenoid systems.

**Theorem 2.5.7.** [30] *Consider the graph of 2-polyomino systems $G_n$, then its PI polynomial is equal to*

$$PI(G_n,x) = 4nx^{35n-3} + 3(3n-1)x^{35n-2} + 2(11n+2)x^{35n-1}.$$

For graph of triangular benzenoid systems $G[n]$, the PI polynomial is

$$PI(G[n],x) = 3(2x^{e-2} + 3x^{e-3} + ... + (n+1)x^{e-n-1}),$$

*where* $e = 28n + 1$.

The non-equidistance index is defined on the same lines with slightly difference in summation.

That is the end of this chapter. In this chapter, we discussed and studied the introduction to topological indices, their major classes with respect to some graph parameters like distance, degree and counting the equi and non-equidistant edges in a graph. We then briefly studied the topological indices of these classes by giving some known results on them for different chemically interesting families of graphs like nanotubes, nanocones, nanostars, fullerenes, polyomino systems and benzenoid structures.

# Chapter 3

# Topological indices of certain nanostructures

To compute and study the topological indices of nanostructures like nanotubes and nanostars and nanocones is a respected problem in theoretical and computational nanoscience. Diudea was the first chemist which considered the problem of computing topological indices of nanostructures see [15, 18, 19].

In this chapter, we compute certain degree based topological indices like Randić, Zagreb, $ABC$, $GA$, $ABC_4$ and $GA_5$ for certain nanotubes named as H-naphtalenic, $TUC_4[p, q]$ and $VC_5C_7[p, q]$ nanotubes. We also compute certain counting related polynomials such as Omega, Sadhana and PI for H-naphtalenic nanotubes and $TUC_4[p, q]$. Since, graphs of all nanotori are $k$-regular so we give a characterization of $GA_5$ index for $k$-regular graphs, which helps us to compute this index for all types of nanotori.

## 3.1 Results for H-naphtalenic nanotubes

In this section, we compute the certain topological indices for H-Naphtalenic nanotubes. This nanotube is a trivalent decoration having sequence of $C_6, C_6, C_4$,$C_6, C_6$, $C_4$... in first row and a sequence of $C_6, C_8, C_6, C_8, ...$ in other row. In other words, the whole lattice is a plane tiling of $C_4$, $C_6$ and $C_8$ and this type of tiling can either

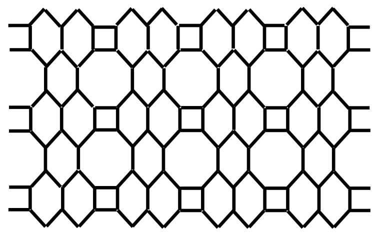

Figure 3.1: $NPHX[m,n]$ nanotube with $m=4$ and $n=3$.

| $(d_a, d_b)$ where $ab \in E(H)$ | $(2,3)$ | $(3,3)$ |
|---|---|---|
| Number of edges | $8m$ | $15mn-10m$ |

Table 3.1: Edge partition of $2D$-lattice of H-Naphtalenic nanotubes based on degrees of end vertices of each edge.

cover a cylinder or a torus. These nanotubes usually symbolized as $NPHX[m,n]$, in which $m$ is the number of pairs of hexagons in first row and $n$ is the number of alternative hexagons in a column as depicted in Figure 3.1.

**Lemma 3.1.1.** [39] *Let $NPHX[m,n]$ be the graph of H-Naphtalenic nanotubes with $(m,n>1)$, then its vertex set cardinality is*

$$|V(NPHX[m,n])| = 10mn.$$

**Lemma 3.1.2.** [39] *Consider the graph of H-Naphtalenic nanotubes $NPHX[m,n]$ with $(m,n>1)$, then its edge set cardinality is*

$$|E(NPHX[m,n])| = 15mn-2m.$$

Now we compute certain degree based topological indices for this class of nanotubes. We can clearly see that, there are two type of edges in $2D$-lattice of this nanotube as shown in Figure 3.1. Table 3.1 shows this partition of $NPHX[m,n]$ nanotube.

In the following theorem, we compute the $ABC$ index of $NPHX[m,n]$ nanotubes.

**Theorem 3.1.3.** *Consider the graph of $NPHX[m,n]$ nanotubes, then its ABC index is equal to*

$$ABC(NPHX[m,n]) = \left(5n - \frac{20+12\sqrt{2}}{3}\right)m.$$

*Proof.* Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices of each edge of graph of $NPHX[m,n]$ nanotube given in table 3.1, we compute the $ABC$ index of $NPHX[m,n]$ nanotube. Since

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

This gives that
$ABC(NPHX[m,n]) = (8m)\sqrt{\frac{2+3-2}{2\times3}} + (15mn - 10m)\sqrt{\frac{3+3-2}{3\times3}}$.
After simplification, we get

$$ABC(NPHX[m,n]) = \left(5n - \frac{20+12\sqrt{2}}{3}\right)m. \quad \square$$

The $GA$ index for $NPHX[m,n]$ nanotubes is computed in the following theorem.

**Theorem 3.1.4.** *Consider the graph of $NPHX[m,n]$ nanotubes, then its GA index is equal to*

$$ABC(NPHX[m,n]) = \big(15n - \frac{50+16\sqrt{6}}{5}\big)m.$$

*Proof.* Consider the graph of $NPHX[m,n]$. Since

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

This implies that
$GA(NPHX[m,n]) = (8m)\frac{2\sqrt{2\times3}}{2+3} + (15mn - 10m)\frac{2\sqrt{3\times3}}{3+3}$.
After simplification, we get

$$GA(NPHX[m,n]) = \big(15n - \frac{50+16\sqrt{6}}{5}\big)m. \quad \square$$

Now we compute Randić index for this family of nanotubes.

| $(S_u, S_v)$ where $uv \in E(G)$ | $(6,7)$ | $(6,8)$ | $(8,8)$ | $(7,9)$ | $(8,9)$ | $(9,9)$ |
|---|---|---|---|---|---|---|
| Number of edges | $4m$ | $4m$ | $2m$ | $2m$ | $4m$ | $15mn - 18m$ |

Table 3.2: Edge partition of graph of $NPHX[m,n]$ nanotubes based on degree sum of vertices lying at unit distance from end vertices of each edge.

**Theorem 3.1.5.** *Let the graph of $NPHX[m,n]$ nanotube, then its Randić index is*

$$\chi(NPHX[m,n]) = \left(5n - \frac{10 + 4\sqrt{6}}{3}\right)m.$$

*Proof.* By using the partition given in table 3.1 and apply the formula of the Randić index we can compute this index for $NPHX[m,n]$ nanotube. Since

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

This implies that
$\chi(NPHX[m,n]) = (8m)\frac{1}{\sqrt{2\times 3}} + (15mn - 10m)\frac{1}{\sqrt{3\times 3}}$.
After a bit calculation, we get

$$\chi(NPHX[m,n]) = \left(5n - \frac{10 + 4\sqrt{6}}{3}\right)m. \quad \square$$

Now we compute two important topological indices $ABC_4$ and $GA_5$ for $2D$-lattice of $NPHX[m,n]$ nanotube. There are six types of edges in $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. In table 3.2, such a partition is given.

In the following theorem, $ABC_4$ index of $NPHX[m,n]$ nanotube is computed.

**Theorem 3.1.6.** *Consider the graph of $NPHX[m,n]$ nanotubes, then its $ABC_4$ index is*

$$ABC_4(NPHX[m,n]) = \left(\frac{20}{3}n + \frac{2\sqrt{462}}{21} + \frac{\sqrt{14}}{4} + \frac{2\sqrt{2}}{3} + \frac{\sqrt{30}}{3} - 6\right)m.$$

*Proof.* We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table

3.2 explains such a partition for $NPHX[m,n]$ nanotube. Now by using the partition given in table 3.2 we can apply the formula of $ABC_4$ index to compute this index for $NPHX[m,n]$ nanotube.
Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that
$ABC_4(NPHX[m,n]) = (4m)\sqrt{\frac{6+7-2}{6\times 7}} + (4m)\sqrt{\frac{6+8-2}{6\times 8}} + (2m)\sqrt{\frac{8+8-2}{8\times 8}} + (2m)\sqrt{\frac{7+9-2}{7\times 9}} + (4m)\sqrt{\frac{8+9-2}{8\times 9}} + (15mn - 18m)\sqrt{\frac{9+9-2}{9\times 9}}$.
After an easy simplification, we get

$$ABC_4(NPHX[m,n]) = \left(\frac{20}{3}n + \frac{2\sqrt{462}}{21} + \frac{\sqrt{14}}{4} + \frac{2\sqrt{2}}{3} + \frac{\sqrt{30}}{3} - 6\right)m. \quad \square$$

Now we compute $GA_5$ index of $NPHX[m,n]$ nanotube.

**Theorem 3.1.7.** *Let the graph of $NPHX[m,n]$ nanotube, then its $GA_5$ index is*

$$GA_5(NPHX[m,n]) = \left(15n + \frac{8\sqrt{42}}{13} + \frac{16\sqrt{3}}{7} + \frac{3\sqrt{7}}{4} + \frac{48\sqrt{2}}{17} - 16\right)m.$$

*Proof.* The edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge is given in table 3.2. Now we apply the formula of $GA_5$ index to compute this index for $NPHX[m,n]$ nanotube.
Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

This gives that
$GA_5(NPHX[m,n]) = (4m)\frac{2\sqrt{6\times 7}}{6+7} + (4m)\frac{2\sqrt{6\times 8}}{6+8} + (2m)\frac{2\sqrt{8\times 8}}{8+8} + (2m)\frac{2\sqrt{7\times 9}}{7+9} + (4m)\frac{2\sqrt{8\times 9}}{8+9} + (15mn - 18m)\frac{2\sqrt{9\times 9}}{9+9}$.
After an easy simplification, we get

$$GA_5(NPHX[m,n]) = \left(15n + \frac{8\sqrt{42}}{13} + \frac{16\sqrt{3}}{7} + \frac{3\sqrt{7}}{4} + \frac{48\sqrt{2}}{17} - 16\right)m. \quad \square$$

Now we compute counting polynomials namely Omega, Sadhana and PI for this finite family of nanotubes.

| Types of qoc | Types of edges | No of co-distant edges | No of qoc |
|---|---|---|---|
| $C_1$ | $e_1$ | $3m$ | $n$ |
| $C_2$ | $e_2$ | $2n$ | $m$ |
| $C_3$ | $e_3$ | $2m$ | $n-1$ |
| $C_k$, where $k = 1, 2, \ldots, j$ | $e_k$ where $k = 4, 5$ | $2i$ where $i = 1, 2, ..., \lfloor \frac{n}{2} \rfloor - 1$ | 2 |
| | | $4m$ | $n - 2m + 1$ |

Table 3.3: Number of co-distant edges of H-Naphtalenic nanotube $NPHX[m, n]$ when $m \leq \lfloor \frac{n}{2} \rfloor$.

**Theorem 3.1.8.** *The Omega polynomial of H-Naphtalenic nanotube $NPHX[m, n]$, $\forall\ m, n \in \mathbb{N}$ is equal to:*

$$\Omega(NPHX[m,n],x) = \begin{cases} \eta + 4\sum\limits_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} x^{2i} + 2(n-2m+1)x^{4m}, & m \leq \lfloor \frac{n}{2} \rfloor, \\ \eta + 4\sum\limits_{i=1}^{n-1} x^{2i} + 2(2m-n+1)x^{2n}, & m > \lfloor \frac{n}{2} \rfloor, \end{cases}$$

*where $\eta = nx^{3m} + mx^{2n} + (n-1)x^{2m}$.*

*Proof.* Let $G$ be the graph of H-Naphtalenic nanotube $NPHX[m, n]$, $\forall\ m, n \in \mathbb{N}$ with vertex set and edge set cardinalities are $10mn$ and $15mn - 2m$ respectively. Table 3.3 shows the number of co-distant edges in $G$ for $m \leq \lfloor \frac{n}{2} \rfloor$, table 3.4 shows the number of co-distant edges in $G$ for $m > \lfloor \frac{n}{2} \rfloor$. The qoc in this nanotube is depicted in 3.2 where horizontal and vertical quasi-orthogonal cuts (qoc) are depicted in figure $a$ and oblique qoc's are depicted in figure $b$. The oblique qoc's for $e_4$ and $e_5$ are same.
By using table 3.3 and 3.4, the proof is straightforward. Now we apply formula and do some easy calculation to get our result.

$$\Omega(G, x) = \sum_k m(G, k) \times x^k.$$

For $m \leq \lfloor \frac{n}{2} \rfloor$,

| Types of qoc | Types of edges | No of co-distant edges | No of qoc |
|---|---|---|---|
| $C_1$ | $e_1$ | $3m$ | $n$ |
| $C_2$ | $e_2$ | $2n$ | $m$ |
| $C_3$ | $e_3$ | $2m$ | $n-1$ |
| $C_k$, where $k = 1, 2, ..., j$ | $e_k$ where $k = 4, 5$ | $2i$ where $i = 1, 2, ..., n-1$ | 2 |
| | | $2n$ | $2m - n + 1$ |

Table 3.4: Number of co-distant edges of H-Naphtalenic nanotube $NPHX[m, n]$ when $m > \lfloor \frac{n}{2} \rfloor$.

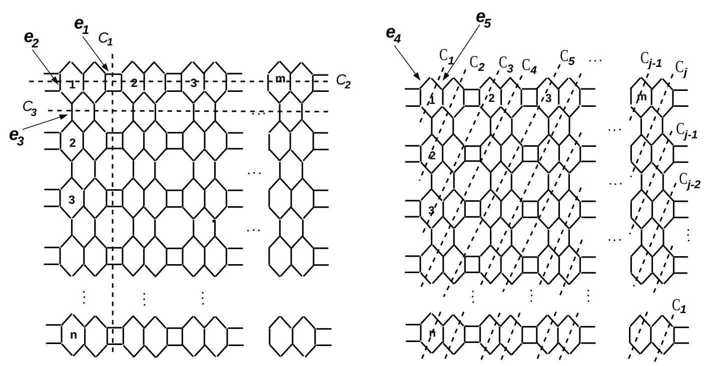

Fig a.

Fig b.

Figure 3.2: Fig a: The horizontal and vertical qoc's, where Fig b: The oblique qoc's.

$$\begin{aligned} \Omega(G, x) &= nx^{3m} + mx^{2n} + (n-1)x^{2m} + \\ & \quad 2\left\{2 \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} x^{2i} + (n - 2m + 1)x^{4m}\right\}. \end{aligned}$$

$$\begin{aligned} \Longrightarrow \Omega(G, x) &= nx^{3m} + mx^{2n} + (n-1)x^{2m} + 2(n - 2m + 1)x^{4m} + \\ & \quad 4x^2 + 4x^4 + ... + 4x^{2\lfloor \frac{n}{2} \rfloor - 2}. \end{aligned}$$

For $m > \lfloor \frac{n}{2} \rfloor$,

$$\Omega(G,x) = nx^{3m} + mx^{2n} + (n-1)x^{2m} + 2\left\{2\sum_{i=1}^{n-1} x^{2i} + (2m-n+1)x^{2n}\right\}.$$

$$\Longrightarrow \Omega(G,x) = nx^{3m} + mx^{2n} + (n-1)x^{2m} + 2(2m-n+1)x^{2n} + 4x^2 + 4x^4 + ... + 4x^{2n-2}. \quad \square$$

In the following theorem, the Sadhana polynomial of H-Naphtalenic nanotube $NPHX[m,n]$ is computed.

**Theorem 3.1.9.** *The Sadhana polynomial of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$ is as follows:*

$$Sd(NPHX[m,n],x) = \begin{cases} \eta + 4\sum\limits_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} x^{15mn-2m-2i} + \\ 2(n-2m+1)x^{15mn-6m}, & m \leq \lfloor \frac{n}{2} \rfloor, \\ \eta + 4\sum\limits_{i=1}^{n-1} x^{15mn-2m-2i} + \\ 2(2m-n+1)x^{15mn-2m-2n}, & m > \lfloor \frac{n}{2} \rfloor, \end{cases}$$

*where* $\eta = nx^{15mn-5m} + mx^{15mn-2m-2n} + (n-1)x^{15mn-4m}$.

*Proof.* Let $G$ be the graph of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$ with vertex set and edge set cardinalities are $10mn$ and $15mn-2m$ respectively. By using table 3.3 and 3.4 the proof is easy. Now we apply formula and do some computation to get our result.

$$Sd(G,x) = \sum_k m(G,k) \times x^{e-k}.$$

For $m \leq \lfloor \frac{n}{2} \rfloor$,

$$Sd(G,x) = nx^{15mn-5m} + mx^{15mn-2m-2n} + (n-1)x^{15mn-4m} + 2\left\{2\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} x^{15mn-2m-2i} + (n-2m+1)x^{15mn-6m}\right\}.$$

$$\Longrightarrow Sd(G,x) = nx^{15mn-5m} + mx^{15mn-2m-2n} + (n-1)x^{15mn-4m} + 2(n-2m+1)x^{15mn-6m} + 4x^{15mn-2m-2} + 4x^{15mn-2m-4} + ... + 4x^{15mn-2m-2\lfloor \frac{n}{2} \rfloor -2}.$$

For $m > \lfloor \frac{n}{2} \rfloor$,

$$Sd(G,x) = nx^{15mn-5m} + mx^{15mn-2m-2n} + (n-1)x^{15mn-4m} + 2\Big\{2\sum_{i=1}^{n-1} x^{15mn-2m-2i} + (2m-n+1)x^{15mn-2m-2n}\Big\}.$$

$$\Longrightarrow Sd(G,x) = nx^{15mn-5m} + mx^{15mn-2m-2n} + (n-1)x^{15mn-4m} + 2(2m-n+1)x^{15mn-2m-2n} + 4x^{15mn-2m-2} + 4x^{15mn-2m-4} + ... + 4x^{15mn-2m-2n+2}. \quad \square$$

Now we compute PI polynomial of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$. Following theorem shows the PI polynomial for this finite family of nanotubes.

**Theorem 3.1.10.** *Consider the graph of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$. Then its PI polynomial is as follows:*

$$PI(NPHX[m,n],x) = \begin{cases} \eta + \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor -1} 8ix^{15mn-2m-2i} + \\ 8m(n-2m+1)x^{15mn-6m}, & m \leq \lfloor \frac{n}{2} \rfloor, \\ \eta + \sum_{i=1}^{n-1} 8ix^{15mn-2m-2i} + \\ 4n(2m-n+1)x^{15mn-2m-2n}, & m > \lfloor \frac{n}{2} \rfloor, \end{cases}$$

*where $\eta = 3mnx^{15mn-5m} + 2mnx^{15mn-2m-2n} + 2m(n-1)x^{15mn-4m}$.*

*Proof.* Let $G$ be the graph of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$. The proof of this result is just calculation based. We easily prove it by using table 3.3 and 3.4. We know that

$$PI(G,x) = \sum_{k} m(G,k) \times k \times x^{e-k}.$$

For $m \leq \lfloor \frac{n}{2} \rfloor$,

$$\begin{aligned} PI(G,x) &= 3mnx^{15mn-5m} + 2mnx^{15mn-2m-2n} + 2m(n-1)x^{15mn-4m} + \\ & 2\Big\{ \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} 4ix^{15mn-2m-2i} + 4m(n-2m+1)x^{15mn-6m} \Big\}. \end{aligned}$$

$$\begin{aligned} \Longrightarrow PI(G,x) &= 3mnx^{15mn-5m} + 2mnx^{15mn-2m-2n} + 2m(n-1)x^{15mn-4m} + \\ & 8m(n-2m+1)x^{15mn-6m} + 8x^{15mn-2m-2} + \\ & 16x^{15mn-2m-4} + ... + 8(\lfloor \frac{n}{2} \rfloor - 1)x^{15mn-2n-2(\lfloor \frac{n}{2} \rfloor)-2}. \end{aligned}$$

For $m > \lfloor \frac{n}{2} \rfloor$,

$$\begin{aligned} PI(G,x) &= 3mnx^{15mn-5m} + 2mnx^{15mn-2m-2n} + 2m(n-1)x^{15mn-4m} + \\ & 2\Big\{ \sum_{i=1}^{n-1} 4ix^{15mn-2m-2i} + 2n(2m-n+1)x^{15mn-2m-2n} \Big\}. \end{aligned}$$

$$\begin{aligned} \Longrightarrow PI(G,x) &= 3mnx^{15mn-5m} + 2mnx^{15mn-2m-2n} + 2m(n-1)x^{15mn-4m} + \\ & 4n(2m-n+1)x^{15mn-2m-2n} + 8x^{15mn-2m-2} + \\ & 16x^{15mn-2m-4} + ... + 8(n-1)x^{15mn-2m-2n+2}. \quad \square \end{aligned}$$

## 3.2 Results for $VC_5C_7[p,q]$, $(p,q>1)$, nanotubes

In this section, we compute the certain topological indices for $VC_5C_7[p,q]$ nanotubes. This nanotube is a $C_5C_7$ net and constructed by alternating $C_5$ and $C_7$ following the trivalent decoration as shown in Figure 3.4. This type of tiling can either cover a cylinder or a torus also. The graph of $VC_5C_7[p,q]$, in which $p$ is the number of pentagons in one row and $q$ is the number of periods in whole lattice. A period consist of four rows as in Figure 3.3 in which $m$-th period is shown. There are $16p$ vertices in one period and $3p$ vertices which are joined at the end of the graph of these nanotubes, so vertex cardinality is $|V(VC_5C_7[p,q])| = 16pq + 3p$. In a same

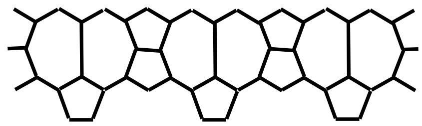


Figure 3.3: $m$-th period of $VC_5C_7$ nanotube.

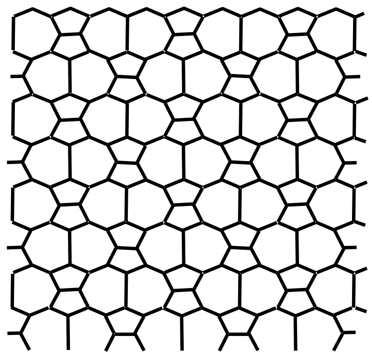

Figure 3.4: The graph of $VC_5C_7[p,q]$ nanotube with $p=3$ and $q=4$.

manner, there are $24p$ edges in one period and $3p$ extra edges which are joined to the end of the graph in these nanotubes, so we have $|E(VC_5C_7[p,q])| = 24pq - 3p$. Now we find edge partition of graph of $VC_5C_7[p,q]$ nanotubes based on degrees of end vertices of each edge. Table 3.5 shows such a partition for $VC_5C_7[p,q]$ nanotubes. In the following theorem, a closed formula of $ABC$ for $VC_5C_7[p,q]$ nanotubes is computed.

**Theorem 3.2.1.** *Consider the graph of $VC_5C_7[p,q]$ nanotubes, then its $ABC$ index is equal to*

$$ABC(VC_5C_7[p,q]) = \left(16q + \frac{11\sqrt{2}}{2} - \frac{28}{3}\right)p.$$

*Proof.* Consider the graph of $VC_5C_7[p,q]$ nanotubes. By using the edge partition

| $(d_u, d_v)$ where $uv \in E(G)$ | $(2,2)$ | $(2,3)$ | $(3,3)$ |
|---|---|---|---|
| Number of edges | $p$ | $10p$ | $24pq - 14p$ |

Table 3.5: Edge partition of $VC_5C_7[p,q]$ nanotubes based on degrees of end vertices of each edge.

based on the degrees of end vertices of each edge of graph of $VC_5C_7[p,q]$ nanotubes given in table 3.5, we compute the $ABC$ index. Since

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

This gives that
$ABC(VC_5C_7[p,q]) = (p)\sqrt{\frac{2+2-2}{2\times 2}} + (10p)\sqrt{\frac{2+3-2}{2\times 3}} + (24pq - 14p)\sqrt{\frac{3+3-2}{3\times 3}}$.
After some calculation, we get

$$ABC(VC_5C_7[p,q]) = \left(16q + \frac{11\sqrt{2}}{2} - \frac{28}{3}\right)p. \quad \square$$

The geometric-arithmetic index for $VC_5C_7[p,q]$ nanotubes is computed in the following theorem.

**Theorem 3.2.2.** *Consider the graph of $VC_5C_7[p,q]$ nanotube, then its $GA$ index is*

$$GA(VC_5C_7[p,q]) = \left(24q + 4\sqrt{6} - 13\right)p.$$

*Proof.* Consider the graph of $VC_5C_7[p,q]$. Table 3.5 shows the partition of edge set of graph of $VC_5C_7[p,q]$ based on the degrees of end vertices of each edge. Since

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

This implies that
$GA(VC_5C_7[p,q]) = (p)\frac{2\sqrt{2\times 2}}{2+2} + (10p)\frac{2\sqrt{2\times 3}}{2+3} + (24pq - 14p)\frac{2\sqrt{3\times 3}}{3+3}$.
After simplification, we get

$$GA(VC_5C_7[p,q]) = \left(24q + 4\sqrt{6} - 13\right)p. \quad \square$$

Now we compute Randić and zagreb indices for these nanotubes. Since there are three types of edges in graph of $VC_5C_7[p,q]$ nanotubes. Table 1.1 shows such types of edges in the lattice given in Figure 3.4. By using partition of edge set of graph of $VC_5C_7[p,q]$ nanotubes, we compute Randić and zagreb indices for these nanotubes. In following theorems, we compute Randić index for these nanotubes.

**Theorem 3.2.3.** *Let the graph of $VC_5C_7[p,q]$ nanotubes, then its Randić index of is*

$$\chi(VC_5C_7[p,q]) = \left(8q + \frac{5\sqrt{6}}{3} - \frac{25}{6}\right)p.$$

*Proof.* By we use the partition given in table 3.5 and apply in the formula of the Randić index. Since

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

This implies that

$\chi(VC_5C_7[p,q]) = (p)\frac{1}{\sqrt{2\times 2}} + (10p)\frac{1}{\sqrt{2\times 3}} + (24pq - 14p)\frac{1}{\sqrt{3\times 3}}$.

After a bit calculation, we get

$$\chi(VC_5C_7[p,q]) = \left(8q + \frac{5\sqrt{6}}{3} - \frac{25}{6}\right)p. \quad \square$$

In following theorem, we compute zagreb index of $VC_5C_7[p,q]$ nanotubes.

**Theorem 3.2.4.** *Consider the graph of $VC_5C_7[p,q]$ nanotubes, the first zagreb index of $VC_5C_7[p,q]$ nanotubes is*

$$M_1(VC_5C_7[p,q]) = \big(144q - 30\big)p.$$

*Proof.* We use the description of variety of edges in graph of $VC_5C_7[p,q]$ nanotubes given in table 3.5 to compute this index. Since

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v).$$

This implies that $M_1(VC_5C_7[p,q]) = (p)(2+2) + (10p)(2+3) + (24pq - 14p)(3+3)$. This gives that

$$M_1(VC_5C_7[p,q]) = \big(144q - 30\big)p. \quad \square$$

Now we compute two important topological indices $ABC_4$ and $GA_5$ for two dimensional lattice of $VC_5C_7[p,q]$ nanotubes. In order to compute these indices, we need an edge partition of graph of $VC_5C_7[p,q]$ nanotubes based on the degree sum of vertices lying at unit distance from end vertices of each edge. In table 3.6 such a partition of graph of $VC_5C_7[p,q]$ nanotubes are shown. In the following theorem, $ABC_4$ index of $VC_5C_7[p,q]$ nanotubes is computed.

| $(S_u, S_v)$ where $uv \in E(G)$ | Number of edges |
|---|---|
| $(5,5)$ | $p$ |
| $(5,8)$ | $2p$ |
| $(6,8)$ | $2p$ |
| $(8,8)$ | $2p$ |
| $(6,7)$ | $6p$ |
| $(7,9)$ | $3p$ |
| $(8,9)$ | $4p$ |
| $(9,9)$ | $24pq - 23p$ |

Table 3.6: Edge partition of graph of $VC_5C_7[p,q]$ nanotubes based on degree sum of vertices lying at unit distance from end vertices of each edge.

**Theorem 3.2.5.** *Consider the graph of $VC_5C_7[p,q]$ nanotubes, then its $ABC_4$ index is*

$$ABC_4(VC_5C_7[p,q]) = \left(\frac{32}{3}q + \frac{2\sqrt{2}}{5} + \frac{\sqrt{110}}{10} + \frac{\sqrt{14}}{4} + \frac{\sqrt{462}}{7} + \frac{3\sqrt{2}+\sqrt{30}}{3} - \frac{83}{9}\right)p.$$

*Proof.* We use the edge partition of graph of $VC_5C_7[p,q]$ nanotubes based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 3.6 explains such a partition for $VC_5C_7[p,q]$ nanotubes.

Now by using the partition given in Table 2 we can apply the formula of $ABC_4$ index to compute this index for $VC_5C_7[p,q]$ nanotubes. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that $ABC_4(VC_5C_7[p,q]) = (p)\sqrt{\frac{5+5-2}{5\times5}} + (2p)\sqrt{\frac{5+8-2}{5\times8}} + (2p)\sqrt{\frac{6+8-2}{6\times8}} + (2p)\sqrt{\frac{8+8-2}{8\times8}} + (6p)\sqrt{\frac{6+7-2}{6\times7}} + (3p)\sqrt{\frac{7+9-2}{7\times9}} + (4p)\sqrt{\frac{8+9-2}{8\times9}} + (24pq-23p)\sqrt{\frac{9+9-2}{9\times9}}$.

After an easy simplification, we get

$$ABC_4(VC_5C_7[p,q]) = \left(\frac{32}{3}q + \frac{2\sqrt{2}}{5} + \frac{\sqrt{110}}{10} + \frac{\sqrt{14}}{4} + \frac{\sqrt{462}}{7} + \frac{3\sqrt{2}+\sqrt{30}}{3} - \frac{83}{9}\right)p. \quad \square$$

Now we compute $GA_5$ index of $VC_5C_7[p,q]$ nanotubes.

**Theorem 3.2.6.** *Let the graph of $VC_5C_7[p,q]$ nanotubes, then its $GA_5$ index is*

$$GA_5(VC_5C_7[p,q]) = \left(24q + \frac{8\sqrt{10}}{13} + \frac{8\sqrt{3}}{7} + \frac{12\sqrt{42}}{13} + \frac{9\sqrt{7}}{8} + \frac{48\sqrt{2}}{17} - 20\right)p.$$

*Proof.* The edge partition of graph of $VC_5C_7[p,q]$ nanotubes based on the degree sum of vertices lying at unit distance from end vertices of each edge is given in table 3.6. Now we apply the formula of $GA_5$ index to compute this index for $VC_5C_7[p,q]$ nanotubes. Since

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v}.$$

This gives that
$GA_5(VC_5C_7[p,q]) = (p)\frac{2\sqrt{5\times5}}{5+5} + (2p)\frac{2\sqrt{5\times8}}{5+8} + (2p)\frac{2\sqrt{6\times8}}{6+8} + (2p)\frac{2\sqrt{8\times8}}{8+8} + (6p)\frac{2\sqrt{6\times7}}{6+7} + (3p)\frac{2\sqrt{7\times9}}{7+9} + (4p)\frac{2\sqrt{8\times9}}{8+9} + (24pq-23p)\frac{2\sqrt{9\times9}}{9+9}$.
After an easy simplification, we get

$$GA_5(VC_5C_7[p,q]) = \left(24q + \frac{8\sqrt{10}}{13} + \frac{8\sqrt{3}}{7} + \frac{12\sqrt{42}}{13} + \frac{9\sqrt{7}}{8} + \frac{48\sqrt{2}}{17} - 20\right)p. \quad \square$$

## 3.3 Results for $CNC_k[n], k \geq 3, n \geq 1$ nanocones

Now we determine the fourth $ABC$ and fifth $GA$ indices of $CNC_k[n], k \geq 3, n \geq 1$ nanocones. A $CNC_k[n]$ nanocones consists of a cycle $C_k$ as its core and encompassing the layers of hexagons on its conical surface. If there are $n$ layers of hexagons on the conical surface around $C_k$, then we represent the graph of that nanocones as $CNC_k[n]$ in which number $n$ denotes the number of layers of hexagons and number in the subscript shows the sides of polygon which acts as the core of nanocones. A general representation of $CNC_k[n]$ nanocones is shown in Figure 3.5, in which parameters $k$ and $n$ are shown. For further study of nanocones, See [3, 56, 46, 2].

In the following theorem, we present exact formula to calculate $ABC_4$ index of $CNC_k[n], k \geq 3, n \geq 1$ nanocones.

| $(S_u,S_v)$ | $(5,5)$ | $(5,7)$ | $(6,7)$ | $(7,9)$ | $(9,9)$ |
|---|---|---|---|---|---|
| Number of edges | $k$ | $2k$ | $2k(n-1)$ | $kn$ | $\frac{3}{2}kn^2-\frac{1}{2}kn$ |

Table 3.7: The edge partition of $CNC_k[n]$ based on the degree sum of neighbors of end vertices of each edge.

**Theorem 3.3.1.** *Consider the graph of $CNC_k[n], k \geq 3, n \geq 1$ nanocones, then its $ABC_4$ index is equal to*

$$\begin{aligned} ABC_4(CNC_k[n]) &= \frac{2\sqrt{2}}{5}\big(k\big) + \frac{\sqrt{14}}{7}\big(2k\big) + \frac{\sqrt{462}}{42}\big(2k(n-1)\big) \\ & \frac{\sqrt{2}}{3}\big(kn\big) + \frac{4}{9}\bigg(\frac{3}{2}(kn^2) - \frac{1}{2}(kn)\bigg). \end{aligned}$$

*Proof.* Consider the graph of $CNC_k[n], k \geq 3, n \geq 1$ nanocones. We have $|V(CNC_k[n])| = k(n+1)^2$ and $|E(CNC_k[n])| = \frac{3}{2}(kn^2) + \frac{5}{2}(kn) + k$. In order to compute the fourth $ABC$ index of $CNC_k[n]$ nanocones, we find the general partition of $CNC_k[n]$ nanocones in two parameters $k$ and $n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 3.7 shows such partition.
Now by using the edge partition given in Table 3.7, we compute the $ABC_4$ index of $CNC_k[n]$ nanocones.
Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

$ABC_4(CNC_k[n]) = (k)\sqrt{\frac{5+5-2}{5\times5}} + (2k)\sqrt{\frac{5+7-2}{5\times7}} + 2k(n-1)\sqrt{\frac{6+7-2}{6\times7}} + (kn)\sqrt{\frac{7+9-2}{7\times9}} + (\frac{3}{2}kn^2 - \frac{1}{2}kn)\sqrt{\frac{9+9-2}{9\times9}}$.
After an easy simplification, we get

$$\begin{aligned} ABC_4(CNC_k[n]) &= \frac{2\sqrt{2}}{5}\big(k\big) + \frac{\sqrt{14}}{7}\big(2k\big) + \frac{\sqrt{462}}{42}\big(2k(n-1)\big) \\ & \frac{\sqrt{2}}{3}\big(kn\big) + \frac{4}{9}\bigg(\frac{3}{2}(kn^2) - \frac{1}{2}(kn)\bigg). \quad \square \end{aligned}$$

Following theorem presents the $GA_5$ index of $CNC_k[n]$ nanocones.

| $(d_u,d_v)$ | $(2,2)$ | $(2,3)$ | $(3,3)$ |
|---|---|---|---|
| Number of edges | $k$ | $2kn$ | $\frac{3}{2}kn^2+\frac{1}{2}kn$ |

Table 3.8: The edge partition of $CNC_k[n]$ based on the degrees of end vertices of each edge.

**Theorem 3.3.2.** *Consider the graph of $CNC_k[n], k \geq 3, n \geq 1$ nanocones, then its $GA_5$ index is equal to*

$$GA_5(CNC_k[n]) = k+\frac{\sqrt{35}}{6}\big(2k\big)+\frac{2\sqrt{42}}{13}\big(2k(n-1)\big)+\frac{3\sqrt{7}}{8}\big(kn\big)+\bigg(\frac{3}{2}(kn^2)-\frac{1}{2}(kn)\bigg).$$

*Proof.* Consider $G$ be the graph of $CNC_k[n], k \geq 3, n \geq 1$ nanocones. We have $|V(CNC_k[n])| = k(n+1)^2$, and $|E(CNC_k[n])| = \frac{3}{2}(kn^2)+\frac{5}{2}(kn)+k$. By using the edge partition given in table 3.7, we compute the $ABC_4$ index of $CNC_k[n]$ nanocones.

Since

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v}.$$

$GA_5(G) = (k)\frac{2\sqrt{5\times5}}{5+5}+(2k)\frac{2\sqrt{5\times7}}{5+7}+2k(n-1)\frac{2\sqrt{6\times7}}{6+7}+(kn)\frac{2\sqrt{7\times9}}{7+9}+(\frac{3}{2}kn^2-\frac{1}{2}kn)\frac{2\sqrt{9\times9}}{9+9}$.
After an easy simplification, we get

$$GA_5(CNC_k[n]) = k+\frac{\sqrt{35}}{6}\big(2k\big)+\frac{2\sqrt{42}}{13}\big(2k(n-1)\big)+\frac{3\sqrt{7}}{8}\big(kn\big)+\bigg(\frac{3}{2}(kn^2)-\frac{1}{2}(kn)\bigg). \qquad \square$$

Now we compute the edge partition of $CNC_k[n]$ nanocones with respect to degree of end vertices of edges. Following table shows such partition of $CNC_k[n]$ nanocones. In the following theorem, $ABC$ index of $CNC_k[n]$ nanocones is presented.

**Theorem 3.3.3.** *Consider the graph of $CNC_k[n], k \geq 3, n \geq 1$ nanocones, then its $ABC$ index is equal to*

$$ABC(CNC_k[n]) = \frac{\sqrt{2}}{2}\big(k(1+2n)\big)+\frac{2}{3}\bigg(\frac{3}{2}kn^2+\frac{1}{2}kn\bigg).$$

*Proof.* By using the edge partition based on the degrees of end vertices of each edge of $CNC_k[n]$ nanocones given in table 3.8 we compute the $ABC$ index of $CNC_k[n]$

nanocones.

Since

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

$ABC(CNC_k[n]) = (k)\sqrt{\frac{2+2-2}{2\times 2}} + (2kn)\sqrt{\frac{2+3-2}{2\times 3}} + (\frac{3}{2}kn^2 + \frac{1}{2}kn)\sqrt{\frac{3+3-2}{3\times 3}}.$

After an easy simplification, we get

$$ABC(CNC_k[n]) = \frac{\sqrt{2}}{2}\big(k(1+2n)\big) + \frac{2}{3}\left(\frac{3}{2}kn^2 + \frac{1}{2}kn\right). \quad \square$$

The $GA$ index of $CNC_k[n]$ nanocones is computed in the following theorem.

**Theorem 3.3.4.** *Consider the graph of $CNC_k[n], k \geq 3, n \geq 1$ nanocones, then its $GA$ index is equal to*

$$GA(CNC_k[n]) = k + \frac{2\sqrt{6}}{5}\big(2kn\big) + \frac{k}{2}\big(3n^2 + n\big).$$

*Proof.* By using the edge partition based on the degrees of end vertices of each edge of $CNC_k[n]$ nanocones given in table 3.8 we compute the $GA$ index of $CNC_k[n]$ nanocones.

Since

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

$GA(CNC_k[n]) = (k)\frac{2\sqrt{2\times 2}}{2+2} + (2kn)\frac{2\sqrt{2\times 3}}{2+3} + (\frac{3}{2}kn^2 + \frac{1}{2}kn)\frac{2\sqrt{3\times 3}}{3+3}.$

After simplification, we get

$$GA(CNC_k[n]) = k + \frac{2\sqrt{6}}{5}\big(2kn\big) + \frac{k}{2}\big(3n^2 + n\big). \quad \square$$

## 3.4 A characterization of $k$-regular graphs for $GA_5$ index

Now we describe an important result about $GA_5$ index for regular graphs. In the next theorem, we give a characterization of $k$-regular graphs with respect to their $GA_5$ index. We have an important result about $GA_5$ index for $k$-regular graphs.

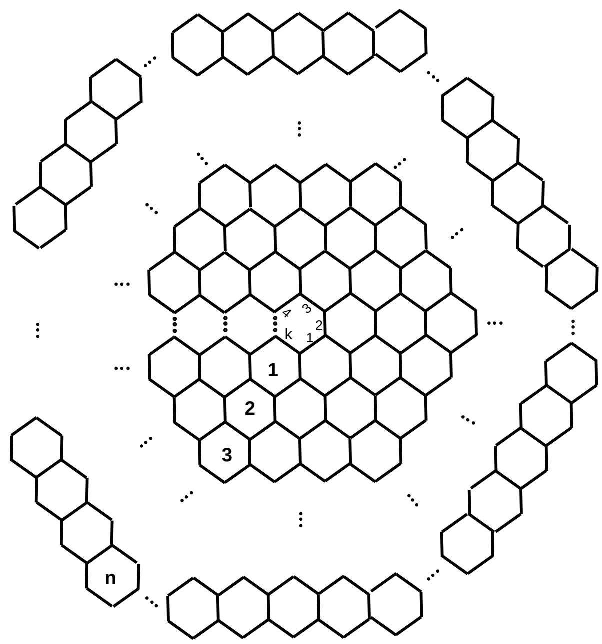


Figure 3.5: A general representation of graph of $CNC_k[n]$ nanocones.

**Lemma 3.4.1.** [32] *Let $G$ be a graph with vertex set $V$ and edge set $E$ and $e = uv \in E$, then*

$$GA_5(G) = |E|\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{(\delta_G(u) + \delta_G(v))}. \tag{3.4.1}$$

**Theorem 3.4.2.** *For every non-trivial connected graph $G$, we have $GA_5(G) = |E(G)|$ if and only if $G$ is $k$-regular.*

*Proof.* Let $G$ be a $k$-regular graph. We define a factor $\eta$ for every edge $e = uv \in E(G)$, as follows:

$$\eta = \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u) + \delta_G(v)}.$$

Since $G$ is $k$-regular then for every edge $e = uv \in E(G)$, $\delta_G(v) = \delta_G(u) = k^2$. So one can easily verify that $\eta = 1$ for every edge of $G$. From above lemma, we get $GA_5(G) = \eta|E(G)|$. So using these facts, we get $GA_5(G) = |E(G)|$.
Conversely, let $GA_5(G) = |E(G)|$ which implies that

$$\eta_1 + \eta_2 + \eta_2 + \eta_3 + ... + \eta_{|E(G)|} = |E(G)|$$

for every edge of $G$, implying that $\eta_i = 1$ for $1 \leq i \leq |E(G)|$. This clearly shows that $G$ is a $k$-regular graph. □

As an immediate application of Theorem 3.0.28, the $GA_5$ index for all nanotori is presented in next corollary.

**Corollary 3.4.3.** *The $GA_5$ index of all nanotori is equal to their edge set cardinality.*

# Chapter 4

# Topological indices of networks

In this chapter, we study the topological indices of certain networks like silicate, hexagonal, oxide and honeycomb networks.

These results are of very important because they discuss the deep topology of underlying networks. Rajan et al. [53] studied certain degree based topological indices namely Randić, Zagreb, $ABC$ and $GA$ indices of silicate, hexagonal, honeycomb and oxide networks. We extend their work to $ABC_4$ and $GA_5$ indices. We define a new class of silicate networks named as chain silicate networks and study their topological indices.

## 4.1 Results for silicate networks

Silicates are building blocks of the common rock-forming minerals and the largest, very interesting and most complicated minerals by far. The tetrahedron($SiO_4$) is basic unit of silicates. Silicates are obtained by fusing metal oxides or metal carbonates with sand. Almost all silicates contain ($SiO_4$) tetrahedra. A silicate sheet is a ring of tetrahedrons which are linked by shared oxygen vertices to other rings in a two dimensional plane that produces a sheet-like structure. Cyclic silicates are structures which give cycles of different length after being linked by shared oxygen vertices. Some sheet and cyclic silicates are shown in Figure 4.3. There are also other types of silicates which are shown in Figure 4.2. From chemical point of view, the corner vertices of tetrahedron ($SiO_4$) are actually the oxygen atoms

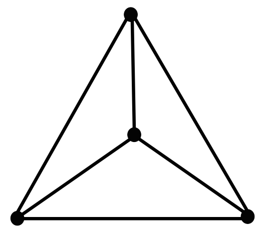

Figure 4.1: A $(SiO_4)$ tetrahedron in which corner vertices are oxygen vertices and central vertex is silicon vertex.

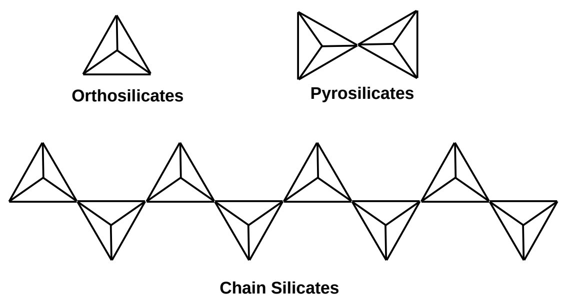


Figure 4.2: Ortho, Pyro and chain silicates.

and central vertex represents silicon atom. Usually, we call these corner atoms as oxygen vertices, central atom as silicon vertex and bonds between them as edges from graphical point of view. A $(SiO_4)$ tetrahedron is shown in Figure 4.1. A silicate network of dimension $n$ symbolizes as $(SL_n)$, where $n$ is the number of hexagons between the center and boundary of $SL_n$. A silicate network of dimension three is shown in Figure 4.4. The number of vertices in $SL_n$ are $15n^2 + 3n$ and number of edges are $36n^2$. Table 4.1 shows the partition of edge set of $(SL_n)$ based on the degree sum of vertices lying at unit distance from end vertices of each edge, and by using this partition we compute the $ABC_4$ and $GA_5$ indices of silicate networks. In the following theorem, the exact formula of $ABC_4$ index for silicate networks is computed.

**Theorem 4.1.1.** *Consider the silicate networks $SL_n$, then its $ABC_4$ index is equal*

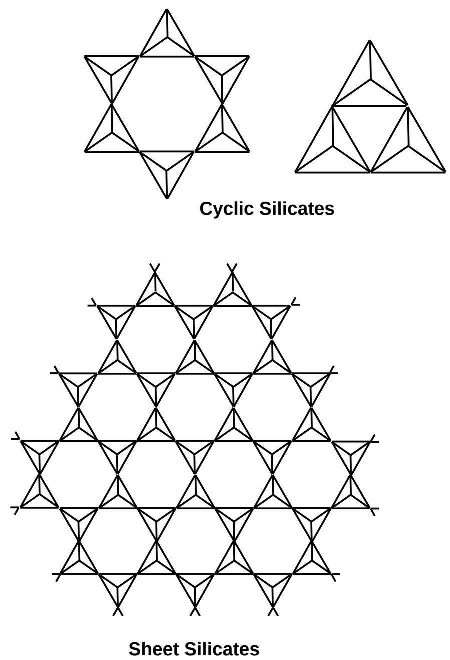


Figure 4.3: Cyclic and sheet silicates.

*to*

$$\begin{aligned} ABC_4(SL_n) &= \left(\frac{\sqrt{690}+3\sqrt{58}}{5}\right)n^2 + \left(\frac{4\sqrt{7}}{15} + \frac{16\sqrt{2}}{3} + \frac{2\sqrt{258}}{9} + \frac{8\sqrt{13}}{9} + \right. \\ & \left. \frac{2\sqrt{22}}{3} - \frac{\sqrt{690}}{3} - \frac{6\sqrt{58}}{5}\right)n + \frac{2\sqrt{370}}{5} + \frac{3\sqrt{58}}{5} + \frac{2\sqrt{690}}{15} + \frac{7\sqrt{2}}{3} - \\ & \frac{16\sqrt{2}}{3} - \frac{2\sqrt{258}}{9} - \frac{4\sqrt{13}}{3} - \frac{2\sqrt{22}}{3}. \end{aligned}$$

*Proof.* Let $G$ be the graph of silicate networks $SL_n$. We have $|V(SL_n)| = 15n^2 + 3n$ and $|E(SL_n)| = 36n^2$. We find the edge partition of silicate networks $SL_n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.1 explains such partition for $SL_n$.

Now by using the partition given in table 4.1 we can apply the formula of $ABC_4$ index to compute this index for $G$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that

| $(S_u, S_v)$ where $uv \in E(G)$ | Number of edges |
|---|---|
| $(15, 15)$ | $6n$ |
| $(15, 24)$ | $24$ |
| $(15, 27)$ | $24(n-1)$ |
| $(18, 27)$ | $12(n-1)$ |
| $(18, 30)$ | $18n^2 - 30n + 12$ |
| $(24, 27)$ | $12$ |
| $(27, 27)$ | $6(2n-3)$ |
| $(27, 30)$ | $12(n-1)$ |
| $(30, 30)$ | $18n^2 - 36n + 18$ |

Table 4.1: Edge partition of silicate networks based on degree sum of neighbors of end vertices of each edge.

$$ABC_4(G) = (6n)\sqrt{\tfrac{15+15-2}{15\times 15}} + (24)\sqrt{\tfrac{15+24-2}{15\times 24}} + 24(n-1)\sqrt{\tfrac{15+24-2}{15\times 24}} + 12(n-1)\sqrt{\tfrac{18+27-2}{18\times 27}} + (18n^2 - 30n + 12)\sqrt{\tfrac{18+30-2}{18\times 30}} + (12)\sqrt{\tfrac{24+27-2}{24\times 27}} + 6(2n-3)\sqrt{\tfrac{27+27-2}{27\times 27}} + 12(n-1)\sqrt{\tfrac{27+30-2}{27\times 30}} + (18n^2 - 36n + 18)\sqrt{\tfrac{30+30-2}{30\times 30}}.$$

After an easy simplification, we get

$$\begin{aligned} ABC_4(SL_n) &= \left(\frac{\sqrt{690} + 3\sqrt{58}}{5}\right)n^2 + \left(\frac{4\sqrt{7}}{15} + \frac{16\sqrt{2}}{3} + \frac{2\sqrt{258}}{9} + \frac{8\sqrt{13}}{9} + \right. \\ & \left. \frac{2\sqrt{22}}{3} - \frac{\sqrt{690}}{3} - \frac{6\sqrt{58}}{5}\right)n + \frac{2\sqrt{370}}{5} + \frac{3\sqrt{58}}{5} + \frac{2\sqrt{690}}{15} + \frac{7\sqrt{2}}{3} - \\ & \frac{16\sqrt{2}}{3} - \frac{2\sqrt{258}}{9} - \frac{4\sqrt{13}}{3} - \frac{2\sqrt{22}}{3}. \quad \square \end{aligned}$$

Following theorem computes the $GA_5$ index of silicate networks $SL_n$.

**Theorem 4.1.2.** *Consider the silicate networks $SL_n$, then its $GA_5$ index is equal to*

$$\begin{aligned} GA_5(SL_n) &= \left(\frac{36 + 9\sqrt{15}}{2}\right)n^2 + \left(\frac{72\sqrt{5}}{7} + \frac{24\sqrt{6}}{5} + \frac{72\sqrt{10}}{19} - \frac{15\sqrt{15}}{2} - 18\right)n \\ & \frac{96\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} + 3\sqrt{15} - \frac{72\sqrt{5}}{7} - \frac{24\sqrt{6}}{5} - \frac{72\sqrt{10}}{19}. \end{aligned}$$

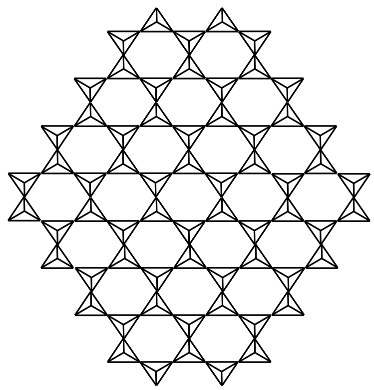

Figure 4.4: A silicate network $SL_n$ with $n = 3$.

*Proof.* Let $G$ be the graph of silicate networks $SL_n$. The edge partition of silicate networks $SL_n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge is given in table 4.1. Now we apply the formula of $GA_5$ index to compute this index for $G$. Since

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

This gives that
$GA_5(G) = (6n)\frac{2\sqrt{15\times15}}{15+15} + (24)\frac{2\sqrt{15\times24}}{15+24} + 24(n-1)\frac{2\sqrt{15\times27}}{15+27} + 12(n-1)\frac{2\sqrt{18\times27}}{18+27} + (18n^2 - 30n + 12)\frac{2\sqrt{18\times30}}{18+30} + (12)\frac{2\sqrt{24\times27}}{24+27} + 6(2n-3)\frac{2\sqrt{27\times27}}{27+27} + 12(n-1)\frac{2\sqrt{27\times30}}{27+30} + (18n^2 - 36n + 18)\frac{2\sqrt{30\times30}}{30+30}$.
After an easy simplification, we get

$$\begin{aligned} GA_5(SL_n) &= \left(\frac{36+9\sqrt{15}}{2}\right)n^2 + \left(\frac{72\sqrt{5}}{7} + \frac{24\sqrt{6}}{5} + \frac{72\sqrt{10}}{19} - \frac{15\sqrt{15}}{2} - 18\right)n \\ & \frac{96\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} + 3\sqrt{15} - \frac{72\sqrt{5}}{7} - \frac{24\sqrt{6}}{5} - \frac{72\sqrt{10}}{19}. \quad \square \end{aligned}$$

Now, we define a new family of silicate networks named as chain silicate networks and then compute its certain degree based topological indices.

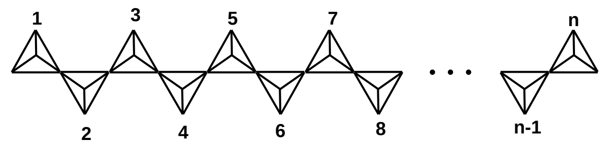


Figure 4.5: Chain silicate networks of dimension $n$.

| $(d_u, d_v)$ where $uv \in E(G)$ | $(3,3)$ | $(3,6)$ | $(6,6)$ |
|---|---|---|---|
| Number of edges | $n+4$ | $2(2n-1)$ | $n-2$ |

Table 4.2: Edge partition of $CS_n$ based on degrees of end vertices of each edge.

## 4.2 Chain silicate networks

When tetrahedra are arranged linearly, chain silicate are obtained. We define chain silicate networks of dimension $n$ as follows: A chain silicate network of dimension $n$ symbolizes as $(CS_n)$ is obtained by arranging $n$ tetrahedra linearly. The number of vertices in $(CS_n)$ with $n > 1$ are $3n+1$ and number of edges are $6n$. A chain silicate network of dimension $n$ is shown in Figure 4.5. Now we find the partition of edge set of $(CS_n)$ based on the degrees of end vertices of each edge, and by using this partition we compute certain topological indices which are based on this partition. Table 4.2 shows such a partition.

Now in the following theorem, we computed the $ABC$ index of chain silicate networks $CS_n$.

**Theorem 4.2.1.** *Consider the chain silicate networks $(CS_n), n > 1$, then its ABC index is equal to*

$$ABC(CS_n) = \left(\frac{2}{3} + \frac{2\sqrt{14}}{3} + \frac{\sqrt{10}}{6}\right)n + \left(\frac{8}{3} - \frac{\sqrt{14}}{3} - \frac{\sqrt{10}}{3}\right).$$

*Proof.* Let $G$ be the graph of chain silicate networks $(CS_n)$. The number of vertices in $CS_n$ are $3n+1$ and number of edges are $6n$. Now by using the edge partition based on the degrees of end vertices of each edge of chain silicate networks $(CS_n)$ given in table 4.2 we compute the $ABC$ index of chain silicate networks $(CS_n)$. Since

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

This implies that
$ABC(CS_n) = (n+4)\sqrt{\frac{3+3-2}{3\times 3}} + 2(2n-1)\sqrt{\frac{3+6-2}{3\times 6}} + (n-2)\sqrt{\frac{6+6-2}{6\times 6}}$.
After an easy simplification, we get

$$ABC(CS_n) = \left(\frac{2}{3} + \frac{2\sqrt{14}}{3} + \frac{\sqrt{10}}{6}\right)n + \left(\frac{8}{3} - \frac{\sqrt{14}}{3} - \frac{\sqrt{10}}{3}\right). \quad \square$$

Following theorem gives $GA$ index of chain silicate networks $CS_n$.

**Theorem 4.2.2.** *Consider the chain silicate networks* $(CS_n), n > 1$, *then its* $GA$ *index is equal to*

$$GA(CS_n) = \left(\frac{6 + 8\sqrt{2}}{3}\right)n + \left(\frac{6 - 4\sqrt{2}}{3}\right).$$

*Proof.* By using the edge partition based on the degrees of end vertices of each edge of chain silicate networks $(CS_n)$ given in table 4.2, we compute the $GA$ index of chain silicate networks $(CS_n)$. Since

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

This gives that
$GA(CS_n) = (n+4)\frac{2\sqrt{3\times 3}}{3+3} + 2(2n-1)\frac{2\sqrt{3\times 6}}{3+6} + (n-2)\frac{2\sqrt{6\times 6}}{6+6}$.
After simplification, we get

$$GA(CS_n) = \left(\frac{6 + 8\sqrt{2}}{3}\right)n + \left(\frac{6 - 4\sqrt{2}}{3}\right). \quad \square$$

There are seven types of edges in $CS_n$ based on degree sum of vertices of neighbors of end vertices for each edge. In table 4.2, such partition of $CS_n$ with $n > 3$ is presented. Now by using above table, we compute $ABC_4$ and $GA_5$ index of chain silicate networks $CS_n$. Following theorem presents the $ABC_4$ index of chain silicate networks $CS_n$.

| $(S_u, S_v)$ where $uv \in E(G)$ | Number of edges |
|---|---|
| $(12, 12)$ | 6 |
| $(12, 21)$ | 6 |
| $(15, 15)$ | $n-2$ |
| $(15, 21)$ | 4 |
| $(15, 24)$ | $4(n-3)$ |
| $(21, 24)$ | 2 |
| $(24, 24)$ | $n-4$ |

Table 4.3: Edge partition of $CS_n$ based on degree sum of neighbors of end vertices of each edge.

**Theorem 4.2.3.** *Consider the chain silicate networks $(CS_n)$, then its $ABC_4$ index is equal to*

$$ABC_4(CS_n) = \begin{cases} \frac{3\sqrt{22}+2\sqrt{42}}{6}, & n=2; \\ \frac{\sqrt{22}}{2} + \frac{2\sqrt{7}}{15} + \frac{\sqrt{217}}{7} + \frac{2\sqrt{10}}{21} + \frac{4}{3}\sqrt{\frac{34}{35}}, & n=3; \\ \left(\frac{2\sqrt{7}}{15} + \frac{\sqrt{370}}{15} + \frac{\sqrt{46}}{24}\right)n + \frac{\sqrt{22}}{2} + \frac{\sqrt{217}}{7} + \frac{\sqrt{602}}{42} + & \\ \frac{4}{3}\sqrt{\frac{34}{35}} - \frac{\sqrt{46}}{6} - \frac{4\sqrt{7}}{15} - \frac{\sqrt{370}}{5}, & n>3. \end{cases}$$

*Proof.* There are three cases to discuss while proving this result. Firstly, we prove this result for $n = 2$. Let $G$ be the graph of $CS_2$, there are two type of edges in $CS_2$ based on the degree sum of vertices lying at unit distance from end vertices of each edge as follows: first type is, for $e = uv \in E(G)$ such that $S_u = S_v = 12$ and other type is, for $e = uv \in E(G)$ such that $S_u = 12$ and $S_u = 18$. There are six edges in each partite set of $CS_2$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that

$$ABC_4(CS_2) = (6)\sqrt{\frac{12+12-2}{12 \times 12}} + (6)\sqrt{\frac{12+18-2}{12 \times 18}}$$

| $(S_u, S_v)$ where $uv \in E(G)$ | $(12,12)$ | $(15,15)$ | $(12,21)$ | $(21,21)$ | $(15,21)$ |
|---|---|---|---|---|---|
| Number of edges | 6 | 1 | 6 | 1 | 4 |

Table 4.4: Edge partition of $CS_3$ based on degree sum of neighbors of end vertices of each edge.

.

After a bit calculation we get,

$$ABC_4(CS_2) = \frac{3\sqrt{22} + 2\sqrt{42}}{6}.$$

Now we prove this result for $n = 3$. For this, we need edge partition of $CS_3$ as we have in first case. Following table shows such partition of $CS_3$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This gives that

$ABC_4(CS_3) = (6)\sqrt{\frac{12+12-2}{12\times12}} + (1)\sqrt{\frac{15+15-2}{15\times15}} + (6)\sqrt{\frac{12+21-2}{12\times21}} + (1)\sqrt{\frac{21+21-2}{21\times21}} + (4)\sqrt{\frac{15+21-2}{15\times21}}.$

After an easy calculation,

$$ABC_4(CS_3) = \frac{\sqrt{22}}{2} + \frac{2\sqrt{7}}{15} + \frac{\sqrt{217}}{7} + \frac{2\sqrt{10}}{21} + \frac{4}{3}\sqrt{\frac{34}{35}}.$$

Now we have third case to prove this result for $n > 3$. We find the edge partition of chain silicate networks $CS_n$ for $n > 3$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.4 explains such partition for $CS_n$. Since

Now by using the partition given in table 4.3 we can apply the formula of $ABC_4$ index to compute this index for $G$.

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

This implies that

$ABC_4(G) = (6)\sqrt{\frac{12+12-2}{12\times12}} + (6)\sqrt{\frac{12+21-2}{12\times21}} + (n-2)\sqrt{\frac{15+15-2}{15\times15}} + (4)\sqrt{\frac{15+21-2}{15\times21}} + 4(n-$

$3)\sqrt{\frac{15+24-2}{15\times 24}} + (2)\sqrt{\frac{21+24-2}{21\times 24}} + (n-4)\sqrt{\frac{24+24-2}{24\times 24}}$.
After an easy simplification, we get
$ABC_4(CS_n) = \big(\frac{2\sqrt{7}}{15} + \frac{\sqrt{370}}{15} + \frac{\sqrt{46}}{24}\big)n + \frac{\sqrt{22}}{2} + \frac{\sqrt{217}}{7} + \frac{\sqrt{602}}{42} + \frac{4}{3}\sqrt{\frac{34}{35}} - \frac{\sqrt{46}}{6} - \frac{4\sqrt{7}}{15} - \frac{\sqrt{370}}{5}$. □

Now we present $GA_5$ index of chain silicate networks $(CS_n)$.

**Theorem 4.2.4.** *Consider the chain silicate networks $(CS_n)$, then its $GA_5$ index is equal to*

$$GA_4(CS_n) = \begin{cases} \frac{30+12\sqrt{6}}{5}, & n = 2; \\ 8 + \frac{24\sqrt{7}}{11} + \frac{2\sqrt{35}}{3}, & n = 3; \\ \big(\frac{26+16\sqrt{10}}{13}\big)n + \frac{24\sqrt{7}}{11} + \frac{2\sqrt{35}}{3} + \frac{8\sqrt{14}}{15} - \frac{48\sqrt{10}}{13}, & n > 3. \end{cases}$$

*Proof.* There are three cases to discuss while proving this result. Firstly, we prove this result for $n = 2$. Let $G$ be the graph of $CS_2$ ,there are two type of edges in $CS_2$ based on the degree sum of vertices lying at unit distance from end vertices of each edge as follows: first type is, for $e = uv \in E(G)$ such that $S_u = S_v = 12$ and other type is, for $e = uv \in E(G)$ such that $S_u = 12$ and $S_u = 18$. There are six edges in each partite set of $CS_2$.
Now we apply the formula of $GA_5$ index to compute this index for $CS_2$. Since

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

$$GA_5(CS_2) = (6)\frac{2\sqrt{12\times 12}}{12+12} + (6)\frac{2\sqrt{12\times 18}}{12+18}.$$

After an easy calculation, we get

$$GA_5(CS_2) = \frac{30+12\sqrt{6}}{5}.$$

To prove this result for $n = 3$ we use the same partition given in table 4.4. $GA_5(CS_3) = (6)\frac{2\sqrt{12\times12}}{12+12} + (1)\frac{2\sqrt{15\times15}}{15+15} + (6)\frac{2\sqrt{12\times21}}{12+21} + (1)\frac{2\sqrt{21\times21}}{21+21} + (4)\frac{2\sqrt{15\times21}}{15+21}$.
After an easy simplification, we get

$$GA_5(CS_3) = 8 + \frac{24\sqrt{7}}{11} + \frac{2\sqrt{35}}{3}.$$

Now we discuss the third case for $n > 3$. Table 3. shows required partition for chain silicate networks $CS_n, n > 3$. Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

This implies that
$GA_5(CS_n) = (6)\frac{2\sqrt{12\times12}}{12+12} + (6)\frac{2\sqrt{12\times21}}{12+21} + (n-2)\frac{2\sqrt{15\times15}}{15+15} + (4)\frac{2\sqrt{15\times21}}{15+21} + 4(n-3)\frac{2\sqrt{15\times25}}{15+24} + (n-4)\frac{2\sqrt{24\times24}}{24+24}$. After an easy calculation, we get

$$GA_5(CS_n) = (\frac{26 + 16\sqrt{10}}{13})n + \frac{24\sqrt{7}}{11} + \frac{2\sqrt{35}}{3} + \frac{8\sqrt{14}}{15} - \frac{48\sqrt{10}}{13}. \quad \square$$

In the following section, we study hexagonal networks and compute the $ABC_4$ and $GA_5$ indices for these networks.

## 4.3 Results for hexagonal networks

It is well known fact, that there exist three regular plane tilings with composition of same kind of regular polygons such as triangular, hexagonal and square. In the construction of hexagonal networks, triangular tiling is being used. A hexagonal network of dimension $n$ is usually denoted as $HX_n$, where $n$ is the number of vertices on each side of hexagon. The number of vertices in hexagonal networks $HX_n$ with $n > 1$ are $3n^2 - 3n + 1$ and number of edges are $9n^2 - 15n + 6$. A hexagonal network $HX_n$ with $n = 6$ is depicted in Figure 4.6. In any hexagonal network there are twelve types of edges based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.5 shows such edge partition of hexagonal networks $HX_n$ for $n > 4$. Now we calculate $ABC_4$ and $GA_5$ indices of chain silicate networks $HX_n$. Following theorem computed the $ABC_4$ index of hexagonal networks.

**Theorem 4.3.1.** *Consider the hexagonal networks $HX_n, n > 1$, then its $ABC_4$*

| $(S_u, S_v)$ where $uv \in E(G)$ | Number of edges |
|---|---|
| $(14, 19)$ | 12 |
| $(19, 20)$ | 12 |
| $(20, 20)$ | $6(n-5)$ |
| $(19, 29)$ | 12 |
| $(19, 32)$ | 12 |
| $(20, 32)$ | $12(n-4)$ |
| $(14, 29)$ | 6 |
| $(29, 32)$ | 12 |
| $(29, 36)$ | 6 |
| $(32, 36)$ | $12(n-3)$ |
| $(32, 32)$ | $6(n-4)$ |
| $(36, 36)$ | $9n^2 - 51n + 72$ |

Table 4.5: Edge partition of $HX_n$ based on degree sum of vertices lying at unit distance from end vertices of each edge.

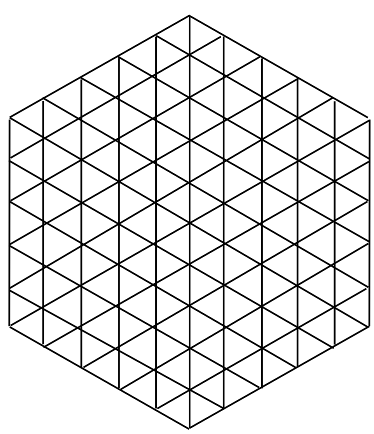

Figure 4.6: Hexagonal network $HX_n$ with $n = 6$.

*index is equal to*

$$ABC_4(HX_n) = \begin{cases} \frac{\sqrt{130}+9\sqrt{2}}{5}, & n=2; \\ \frac{2\sqrt{210}}{7} + \frac{3\sqrt{41}}{203} + \frac{6\sqrt{290}}{29} + \frac{6\sqrt{203}}{29}, & n=3; \\ 12\sqrt{\frac{31}{266}} + 6\sqrt{\frac{41}{406}} + 12\sqrt{\frac{46}{551}} + 3\sqrt{\frac{59}{58}} + & \\ \frac{21}{\sqrt{38}} + \frac{3\sqrt{203}}{29} + \frac{\sqrt{33}}{2} + \frac{\sqrt{70}}{3} + \frac{36}{19}, & n=4; \\ \frac{\sqrt{70}}{4}n^2 + \left(\frac{3\sqrt{38}}{10} + \frac{3\sqrt{5}}{2} + \frac{\sqrt{33}}{2} + \frac{3\sqrt{62}}{16} - \frac{17\sqrt{70}}{21}\right)n + & \\ 12\sqrt{\frac{31}{266}} + 12\sqrt{\frac{37}{380}} + 12\sqrt{\frac{49}{608}} + 12\sqrt{\frac{59}{928}} + & \\ 6\sqrt{\frac{41}{406}} + 12\sqrt{\frac{46}{551}} + \frac{3\sqrt{203}}{29} - \frac{3\sqrt{38}}{2} - \frac{3\sqrt{33}}{2} - & \\ \frac{3\sqrt{62}}{4} + 2\sqrt{70} - 6\sqrt{5}, & n>4. \end{cases}$$

*Proof.* Consider the graph of hexagonal networks $HX_n$. We have $|V(HX_n)| = 3n^2 - 3n + 1$ and $|E(HX_n)| = 9n^2 - 15n + 6$. Now there are four cases to discuss while proving this result. Firstly, we prove this result for $n = 2$. let $G$ be the graph of $HX_2$, there are two type of edges in $HX_2$ based on the degree sum of vertices lying at unit distance from end vertices of each edge as follows: first type is, for $e = uv \in E(G)$ such that $S_u = S_v = 10$ and other type is, for $e = uv \in E(G)$ such that $S_u = 10$ and $S_u = 18$. There are six edges in each partite set of $HX_2$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that

$$ABC_4(HX_2) = (6)\sqrt{\frac{10+10-2}{10 \times 10}} + (6)\sqrt{\frac{10+18-2}{10 \times 18}}.$$

After a bit calculation we get,

$$ABC_4(HX_2) = \frac{\sqrt{130} + 9\sqrt{2}}{5}.$$

Now we prove this result for $n = 3$. For this, we need edge partition of $HX_3$ as we have in first case. Following Table shows such a partition of $HX_3$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

| $(S_u, S_v)$ where $uv \in E(G)$ | $(14, 18)$ | $(14, 29)$ | $(18, 29)$ | $(29, 36)$ |
|---|---|---|---|---|
| Number of edges | 12 | 6 | 12 | 12 |

Table 4.6: Edge partition of $HX_3$ based on degree sum of neighbors of end vertices of each edge.

| $(S_u, S_v)$ where $uv \in E(G)$ | Number of edges |
|---|---|
| $(14, 19)$ | 12 |
| $(19, 19)$ | 6 |
| $(14, 29)$ | 6 |
| $(19, 29)$ | 12 |
| $(19, 32)$ | 12 |
| $(29, 32)$ | 12 |
| $(29, 36)$ | 6 |
| $(32, 36)$ | 12 |
| $(36, 36)$ | 12 |

Table 4.7: Edge partition of hexagonal network $HX_4$ based on degree sum of neighbors of end vertices of each edge.

This gives that
$ABC_4(HX_3) = (12)\sqrt{\frac{14+18-2}{14\times18}} + (6)\sqrt{\frac{14+29-2}{14\times29}} + (12)\sqrt{\frac{18+29-2}{18\times29}} + (12)\sqrt{\frac{29+36-2}{29\times36}}$.
After an easy calculation,

$$ABC_4(HX_3) = \frac{2\sqrt{210}}{7} + \frac{3\sqrt{41}}{203} + \frac{6\sqrt{290}}{29} + \frac{6\sqrt{203}}{29}.$$

Now we discuss the third case to prove this result for $n = 4$. To prove this result for $HX_4$, we need edge partition of $HX_4$ based on the degree sum of neighbors of end vertices of each edge. Following Table shows such a partition for hexagonal network $HX_4$. Now we apply the formula of $ABC_4$ index to compute this index for hexagonal index $HX_4$. Since

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that
$ABC_4(HX_4) = (12)\sqrt{\frac{14+19-2}{14\times19}}+(6)\sqrt{\frac{19+19-2}{19\times19}}+(6)\sqrt{\frac{14+29-2}{14\times29}}+(12)\sqrt{\frac{19+29-2}{19\times29}}+(12)\sqrt{\frac{19+32-2}{19\times32}}+$
$(12)\sqrt{\frac{29+32-2}{29\times32}} + (6)\sqrt{\frac{29+36-2}{29\times36}} + (12)\sqrt{\frac{32+36-2}{32\times36}} + (12)\sqrt{\frac{36+36-2}{36\times36}}$.
After an easy simplification, we get

$$ABC_4(HX_4) = \frac{21}{\sqrt{38}} + \frac{3\sqrt{203}}{29} + \frac{\sqrt{33}}{2} + \frac{\sqrt{70}}{3} + \frac{36}{19}.$$

Now we have fourth case to prove this result for $n > 4$. Let $G$ be the graph of hexagonal networks $HX_n$ with $n > 4$.
We find the edge partition of chain silicate networks $HX_n$ for $n > 4$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.5 explains such partition for $HX_n, n > 4$.
Now by using the partition given in table 4.5 we can apply the formula of $ABC_4$ index to compute this index for $G$.
Since

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that
$ABC_4(G) = (12)\sqrt{\frac{14+19-2}{14\times19}} + (12)\sqrt{\frac{19+20-2}{19\times20}} + 6(n-5)\sqrt{\frac{20+20-2}{20\times20}} +$
$(12)\sqrt{\frac{19+29-2}{19\times29}} + (12)\sqrt{\frac{19+32-2}{19\times32}} + 12(n-4)\sqrt{\frac{20+32-2}{20\times32}} + (6)\sqrt{\frac{14+29-2}{14\times29}} +$
$(12)\sqrt{\frac{29+32-2}{29\times32}} + (6)\sqrt{\frac{29+36-2}{29\times36}} + 12(n-3)\sqrt{\frac{32+36-2}{32\times36}} +$
$6(n-4)\sqrt{\frac{32+32-2}{32\times32}} + (9n^2-51n+72)\sqrt{\frac{36+36-2}{36\times36}}$.
After an easy simplification, we get
$ABC_4(G) = \frac{\sqrt{70}}{4}n^2 + \left(\frac{3\sqrt{38}}{10} + \frac{3\sqrt{5}}{2} + \frac{\sqrt{33}}{2} + \frac{3\sqrt{62}}{16} - \frac{17\sqrt{70}}{21}\right)n + 12\sqrt{\frac{31}{266}} + 12\sqrt{\frac{37}{380}} +$
$12\sqrt{\frac{49}{608}} + 12\sqrt{\frac{59}{928}} + 6\sqrt{\frac{41}{406}} + 12\sqrt{\frac{46}{551}} + \frac{3\sqrt{203}}{29} - \frac{3\sqrt{38}}{2} - \frac{3\sqrt{33}}{2} - \frac{3\sqrt{62}}{4} + 2\sqrt{70} - 6\sqrt{5}$. □

We compute $GA_5$ index of hexagonal networks $HX_n$. In the following theorem, $GA_5$ index of hexagonal networks $HX_n$ is being computed.

**Theorem 4.3.2.** *Consider the hexagonal networks $HX_n, n > 1$, then its $GA_5$ index is equal to*

$$GA_5(HX_n) = \begin{cases} \frac{42+18\sqrt{5}}{7}, & n = 2; \\ \frac{9\sqrt{7}}{2} + \frac{12\sqrt{406}}{43} + \frac{72\sqrt{58}}{47} + \frac{144\sqrt{29}}{65}, & n = 3; \\ \frac{8\sqrt{266}}{11} + \frac{12\sqrt{406}}{43} + \frac{\sqrt{551}}{2} + \frac{32\sqrt{38}}{17} + \frac{96\sqrt{58}}{61} + \\ \frac{72\sqrt{29}}{65} + \frac{144\sqrt{2}}{17} + 18, & n = 4; \\ 9n^2 + \left(\frac{48\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} - 39\right)n + \frac{24\sqrt{406}}{43} + \frac{16\sqrt{95}}{13} + \frac{\sqrt{551}}{2} + \\ \frac{32\sqrt{38}}{17} + \frac{4\sqrt{266}}{11} + \frac{96\sqrt{58}}{61} + \frac{72\sqrt{29}}{65} - \frac{192\sqrt{10}}{13} - \frac{432\sqrt{2}}{17} + 18 & n > 4. \end{cases}$$

*Proof.* Firstly, we prove this result for $n = 2$. let $G$ be the graph of $HX_2$, there are two type of edges in $HX_2$ based on the degree sum of vertices lying at unit distance from end vertices of each edge as follows: first type is, for $e = uv \in E(G)$ such that $S_u = S_v = 10$ and other type is, for $e = uv \in E(G)$ such that $S_u = 10$ and $S_u = 18$. There are six edges in each partite set of $HX_2$. Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

$$GA_5(HX_2) = (6)\frac{2\sqrt{10 \times 10}}{10 + 10} + (6)\frac{2\sqrt{10 \times 18}}{10 + 18}.$$

After a bit calculation, we get

$$GA_5(HX_2) = \frac{42 + 18\sqrt{5}}{7}.$$

Now we prove this result for $n = 3$. For this, we need edge partition of $HX_3$ as we have in first case. Table 4.6 shows such partition of $HX_3$. Now we compute the fifth $GA$ index of $HX_3$. Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

$$GA_5(HX_3) = (12)\frac{2\sqrt{14 \times 18}}{14 + 18} + (6)\frac{2\sqrt{14 \times 29}}{14 + 29} + (12)\frac{2\sqrt{18 \times 29}}{18 + 29} + (12)\frac{2\sqrt{29 \times 36}}{29 + 36}.$$

After an easy calculation, we get

$$GA_5(HX_3) = \frac{9\sqrt{7}}{2} + \frac{12\sqrt{406}}{43} + \frac{72\sqrt{58}}{47} + \frac{144\sqrt{29}}{65}$$

Now we discuss the third case to prove this result for $n = 4$. To prove this result for $HX_4$, we need edge partition of $HX_4$ based on the degree sum of neighbors of end vertices of each edge. Table 4.7 shows such partition for hexagonal network $HX_4$. Now we compute the result for $n = 4$. Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

This implies that
$GA_5(HX_4) = (12)\frac{2\sqrt{14\times19}}{14+19} + (6)\frac{2\sqrt{19\times19}}{19+19} + (6)\frac{2\sqrt{14\times29}}{14+29} + (12)\frac{2\sqrt{19\times29}}{19+29} + (12)\frac{2\sqrt{19\times32}}{19+32} + (12)\frac{2\sqrt{29\times32}}{29+32} + (6)\frac{2\sqrt{29\times36}}{29+36} + (12)\frac{2\sqrt{32\times36}}{32+36} + (12)\frac{2\sqrt{36\times36}}{36+36}$.
After an easy calculation, we get

$$GA_5(HX_4) = \frac{8\sqrt{266}}{11} + \frac{12\sqrt{406}}{43} + \frac{\sqrt{551}}{2} + \frac{32\sqrt{38}}{17} + \frac{96\sqrt{58}}{61} + \frac{72\sqrt{29}}{65} + \frac{144\sqrt{2}}{17} + 18.$$

Now we have fourth case to prove this result for $n > 4$. Let $G$ be the graph of hexagonal networks $HX_n$ with $n > 4$. We find the edge partition of chain silicate networks $HX_n$ for $n > 4$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.5 explains such partition for $HX_n, n > 4$. Now by using the partition given in table 4.5 we can apply the formula of $ABC_4$ index to compute this index for $G$. Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

This gives that
$GA_5(HX_n) = (12)\frac{2\sqrt{14\times19}}{14+19} + (12)\frac{2\sqrt{19\times20}}{19+20} + 6(n-5)\frac{2\sqrt{20\times20}}{20+20} + (12)\frac{2\sqrt{19\times29}}{19+29} + (12)\frac{2\sqrt{19\times32}}{19+32} + 12(n-4)\frac{2\sqrt{20\times32}}{20+32} + (6)\frac{2\sqrt{14\times29}}{14+29} + (12)\frac{2\sqrt{29\times32}}{29+32} + (6)\frac{2\sqrt{29\times36}}{29+36} + 12(n-3)\frac{2\sqrt{32\times36}}{32+36} + 6(n-4)\frac{2\sqrt{32\times32}}{32+32} + (9n^2 - 51n + 72)\frac{2\sqrt{36\times36}}{36+36}$.
After an easy simplification, we get
$GA_5(HX_n) = 9n^2 + \left(\frac{48\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} - 39\right)n + \frac{24\sqrt{406}}{43} + \frac{16\sqrt{95}}{13} + \frac{\sqrt{551}}{2} + \frac{32\sqrt{38}}{17} + \frac{4\sqrt{266}}{11} + \frac{96\sqrt{58}}{61} + \frac{72\sqrt{29}}{65} - \frac{192\sqrt{10}}{13} - \frac{432\sqrt{2}}{17} + 18.$ □

| $(d_u, d_v)$ where $uv \in E(G)$ | $(2,4)$ | $(4,4)$ |
|---|---|---|
| Number of edges | $12n$ | $18n^2 - 12n$ |

Table 4.8: Edge partition of $OX_n$ based on degrees of end vertices of each edge.

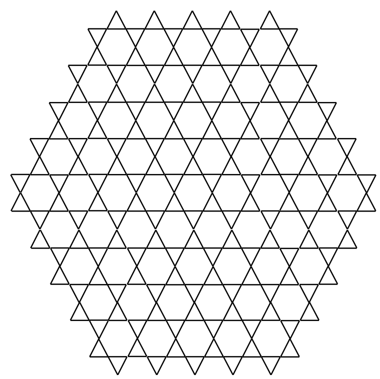

Figure 4.7: An oxide network $OX_5$.

## 4.4 Oxide networks

Oxide networks play a vital role in the study of silicate networks . If we delete silicon vertices from a silicate network, we get an oxide networks. (See Figure 4.7). An $n$-dimensional oxide network is denoted as $OX_n$. The number of vertices in $9n^2+3n$ and number of edges are $18n^2$. There are two types of edges based on the degrees of end vertices of each edge in oxide networks $OX_n$. Table 4.8 shows such types of edges for oxide networks $OX_n$.

Now we compute certain degree based topological indices of oxide networks $OX_n$. In the following theorem, we present $ABC$ index of oxide networks.

**Theorem 4.4.1.** *Consider the oxide networks $(OX_n), n > 1$, then its $ABC$ index is equal to*

$$ABC(OX_n) = \frac{9\sqrt{6}}{2}n^2 + 3n(2\sqrt{2} - \sqrt{6}).$$

*Proof.* By using the edge partition based on the degrees of end vertices of each edge of oxide networks $(OX_n)$ given in table 4.8 we compute the $ABC$ index of oxide networks $(OX_n)$. Since

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

This gives that
$ABC(OX_n) = (12n)\sqrt{\frac{2+4-2}{2\times 4}} + (18n^2 - 12n)\sqrt{\frac{4+4-2}{4\times 4}}$.
After an easy simplification, we get

$$ABC(OX_n) = \frac{9\sqrt{6}}{2}n^2 + 3n(2\sqrt{2} - \sqrt{6}). \quad \square$$

Following theorem gives exact formula $GA$ index of oxide networks $OX_n$.

**Theorem 4.4.2.** *Consider the oxide networks* $(OX_n), n > 1$, *then its* $GA$ *index is equal to*

$$GA(OX_n) = 18n^2 + 4n(2\sqrt{2} - 3).$$

*Proof.* By using the edge partition based on the degrees of end vertices of each edge of oxide networks $(OX_n)$ given in table 4.8 we compute the $GA$ index of oxide networks $(OX_n)$. Since

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

This implies that
$GA(OX_n) = (12n)\frac{2\sqrt{2\times 4}}{2+4} + (18n^2 - 12n)\frac{2\sqrt{4\times 4}}{4+4}$.
After simplification, we get

$$GA(OX_n) = 18n^2 + 4n(2\sqrt{2} - 3).$$

$\square$

There are six types of edges based on degree sum of vertices lying at unit distance from end vertices of each edge in oxide networks $OX_n$. We use this partition of edges of $OX_n$ to calculate $ABC_4$ and $GA_5$ indices for oxide networks. Table 4.9 shows such types of edges of oxide networks $OX_n$. Now we compute $ABC_4$ and $GA_5$ indices of oxide networks $OX_n$. Following theorem gives formula $ABC_4$ index of oxide networks $OX_n$.

| $(S_u, S_v)$ where $uv \in E(G)$ | Number of edges |
|---|---|
| $(8, 12)$ | $12$ |
| $(12, 14)$ | $12$ |
| $(8, 14)$ | $12(n-1)$ |
| $(14, 14)$ | $6(2n-3)$ |
| $(14, 16)$ | $12(n-1)$ |
| $(16, 16)$ | $18n^2 - 36n + 18$ |

Table 4.9: Edge partition of $OX_n$ based on degree sum of vertices lying at unit distance from end vertices of each edge.

**Theorem 4.4.3.** *Consider the oxide networks $(OX_n), n > 1$, then its $ABC_4$ index is equal to*

$$\begin{aligned} ABC_4(OX_n) &= \frac{9\sqrt{30}}{8}n^2 + \left(\frac{6\sqrt{35}}{7} + \frac{6\sqrt{26}}{7} - \frac{9\sqrt{30}}{4} + 3\sqrt{2}\right)n + \\ &\quad \frac{12\sqrt{7}}{7} + \frac{9\sqrt{30}}{8} - \frac{6\sqrt{35}}{7} - \frac{9\sqrt{26}}{7} + 3\sqrt{3} - 3\sqrt{2}. \end{aligned}$$

*Proof.* We find the edge partition of oxide networks $OX_n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.9 explains such partition for $OX_n$.

Now by using the partition given in table 4.9 we can apply the formula of $ABC_4$ index to compute this index for $G$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that

$ABC_4(G) = (12)\sqrt{\frac{8+12-2}{8\times12}} + (12)\sqrt{\frac{12+14-2}{12\times14}} + 12(n-1)\sqrt{\frac{8+14-2}{8\times14}} + 6(2n-3)\sqrt{\frac{14+14-2}{14\times14}} + 12(n-1)\sqrt{\frac{14+16-2}{14\times16}} + (18n^2 - 36n + 18)\sqrt{\frac{16+16-2}{16\times16}}$.

After an easy simplification, we get

$$
\begin{aligned}
ABC_4(OX_n) &= \frac{9\sqrt{30}}{8}n^2 + \left(\frac{6\sqrt{35}}{7} + \frac{6\sqrt{26}}{7} - \frac{9\sqrt{30}}{4} + 3\sqrt{2}\right)n + \\
& \quad \frac{12\sqrt{7}}{7} + \frac{9\sqrt{30}}{8} - \frac{6\sqrt{35}}{7} - \frac{9\sqrt{26}}{7} + 3\sqrt{3} - 3\sqrt{2}. \quad \square
\end{aligned}
$$

In the following theorem, $GA_5$ index of oxide networks $OX_n$ is computed.

**Theorem 4.4.4.** *Consider the oxide networks* $(OX_n), n > 1$, *then its* $GA_5$ *index is equal to*

$$
GA_5(OX_n) = 18n^2 - \left(\frac{48\sqrt{7}}{11} + \frac{16\sqrt{14}}{15} - 24\right)n + \frac{24\sqrt{6}}{5} + \frac{24\sqrt{42}}{13} - \frac{16\sqrt{14}}{15} - \frac{48\sqrt{7}}{11}.
$$

*Proof.* The edge partition of oxide networks $OX_n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge is given in table 4.9. Now we apply the formula of $GA_5$ index to compute this index for $G$. Since

$$
GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.
$$

This gives that
$GA_5(G) = (12)\frac{2\sqrt{8\times12}}{8+12} + (12)\frac{2\sqrt{12\times14}}{12+14} + 12(n-1)\frac{2\sqrt{8\times14}}{8+14} +$
$6(2n-3)\frac{2\sqrt{14\times14}}{14+14} + 12(n-1)\frac{2\sqrt{14\times16}}{14+16} + (18n^2 - 36n + 18)\frac{2\sqrt{16\times16}}{16+16}$.
After an easy simplification, we get

$$
GA_5(OX_n) = 18n^2 - \left(\frac{48\sqrt{7}}{11} + \frac{16\sqrt{14}}{15} - 24\right)n + \frac{24\sqrt{6}}{5} + \frac{24\sqrt{42}}{13} - \frac{16\sqrt{14}}{15} - \frac{48\sqrt{7}}{11}. \quad \square
$$

## 4.5 Honeycomb networks

Honeycomb networks are widely used in computer graphics, cellular phone base stations, image processing and as a representation of benzoid hydrocarbons in chemistry. If we recursively use hexagonal tiling in a particular pattern, honeycomb networks are formed. An $n$-dimensional honeycomb network is denoted as $HC_n$, where $n$ is the number of hexagons between central and boundary hexagon. Honeycomb network $HC_n$ is constructed from $HC_{n-1}$ by adding a layer of hexagons

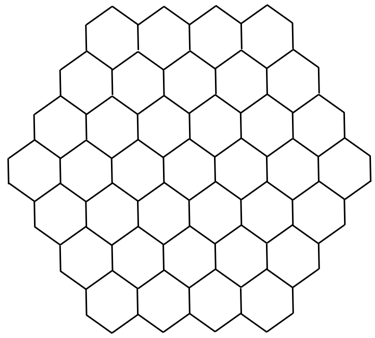

Figure 4.8: A 4-dimensional honeycomb network.

| $(S_u, S_v)$ where $uv \in E(G)$ | $(5,5)$ | $(5,7)$ | $(7,9)$ | $(9,9)$ |
|---|---|---|---|---|
| Number of edges | 6 | $12(n-1)$ | $6(n-1)$ | $9n^2-21n+12$ |

Table 4.10: Edge partition of $HC_n$ based on degree sum of neighbors of end vertices of each edge.

around boundary of $HC_{n-1}$. (See Figure 4.8). The number of vertices in honeycomb network $HC_n$ are $6n^2$ and number of edges are $9n^2-3n$. There are four types of edges in $HC_n$ based on degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.10 shows such types of edges. By using this partition of edges of $HC_n$, we compute $ABC_4$ and $GA_5$ indices of $HC_n$. Now we compute $ABC_4$ index of honeycomb network $HC_n$ for $n > 1$. In the following theorem, we computed $ABC_4$ index of honeycomb network $HC_n$.

**Theorem 4.5.1.** *Consider the honeycomb networks $(HC_n), n > 1$, then its $ABC_4$ index is equal to*

$$ABC_4(HC_n) = 4n^2 + \left(\frac{12\sqrt{14}}{7} + 2\sqrt{2} - \frac{28}{3}\right)n + \frac{12\sqrt{2}}{5} - \frac{12\sqrt{14}}{7} - 2\sqrt{2} + \frac{16}{3}.$$

*Proof.* We find the edge partition of honeycomb networks $HC_n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. Table 4.10 explains such partition for $HC_n$.

Now by using the partition given in table 4.10 we can apply the formula of $ABC_4$ index to compute this index for $G$. Since

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

This implies that
$ABC_4(G) = (6)\sqrt{\frac{5+5-2}{5\times5}} + 12(n-1)\sqrt{\frac{5+7-2}{5\times7}} + 6(n-1)\sqrt{\frac{7+9-2}{7\times9}} +$
$(9n^2 - 21n + 12)\sqrt{\frac{9+9-2}{9\times9}}.$
After an easy simplification, we get
$ABC_4(HC_n) = 4n^2 + \big(\frac{12\sqrt{14}}{7} + 2\sqrt{2} - \frac{28}{3}\big)n + \frac{12\sqrt{2}}{5} - \frac{12\sqrt{14}}{7} - 2\sqrt{2} + \frac{16}{3}.$ □

In the following theorem, $GA_5$ index of honeycomb network $HC_n$ is computed.

**Theorem 4.5.2.** *Consider the honeycomb networks* $(HC_n), n > 1$, *then its* $GA_5$ *index is equal to*

$$GA_5(HC_n) = 9n^2 + \big(\frac{9\sqrt{7}}{4} + 2\sqrt{35} - 21\big)n + 18 - \frac{9\sqrt{7}}{4} - 2\sqrt{35}.$$

*Proof.* The edge partition of honeycomb networks $HC_n$ based on the degree sum of vertices lying at unit distance from end vertices of each edge is given in table 4.10. Now we apply the formula of $GA_5$ index to compute this index for $G$. Since

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

This implies that
$GA_5(G) = (6)\frac{2\sqrt{5\times5}}{5+5} + 12(n-1)\frac{2\sqrt{5\times7}}{5+7} + 6(n-1)\frac{2\sqrt{7\times9}}{7+9} + (9n^2 - 21n + 12)\frac{2\sqrt{9\times9}}{9+9}.$
After an easy simplification, we get

$$GA_5(HC_n) = 9n^2 + \big(\frac{9\sqrt{7}}{4} + 2\sqrt{35} - 21\big)n + 18 - \frac{9\sqrt{7}}{4} - 2\sqrt{35}. \quad \square$$

In this chapter, we have given analytically closed results of certain degree based topological indices of networks named as silicate, chain silicate, hexagonal. oxide and honeycomb networks.

# Chapter 5

# Conclusion and open problems

Molecular descriptors are the numeric numbers which represent the whole structure of the graph, having a underlying chemical structure. Among them, topological indices are those which correlate various physico-chemical properties of underlying chemical compounds.

In the study of Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships, physicochemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are used to predict bioactivity of the chemical compounds.

To compute and study topological indices of nanostructures is a respected problem in theoretical nanoscience. In this thesis, we have calculated the exact formulas of Randić, Zagreb, $ABC$, $GA$, $ABC_4$ and $GA_5$ indices for H-naphtalenic and $V_5C_7[p,q]$ nanotubes and $CNC_k[n]$ nanocones. We have given an important characterization of $GA_5$ index for $k$-regular graphs, which is of much importance because all nanotori are $k$-regular. So by using this characterization, we have concluded that $GA_5$ index of all nanotori will be their edge set cardinality. We have also computed the exact expressions for certain counting related polynomials named as Omega, Sadhana and PI polynomials for H-naphtalenic nanotubes, which are used to calculate their corresponding topological indices.

The study of topological indices for networks is of much importance because these numeric number discuss the topology of underlying networks. We have studied certain degree based topological indices of various interconnecting networks named as silicates, hexagonal, oxide and honeycomb. We have defined a new class of silicate networks and then have studied various degree based topological indices for them.

We close the discussion by raising questions that naturally arise from the text.

**Open Problem 1**: *Determine the exact expressions for the* $ABC_k$ *index for the k=2,3,5 of H-naphtalenic and* $VC_5C_7$ *nanotubes.*

**Open Problem 2**: *Determine the exact formula for* $GA_k$ *index for k=2,3,4 for H-naphtalenic and* $VC_5C_7$ *nanotubes.*

**Open Problem 3**: *Determine the exact expressions of Randi'c, Zagreb,* $ABC_k$, $GA_k$ *for Y-junction nanotubes where k=1,2,3,4,5.*

**Open Problem 4**: *Characterize the k-regular graphs for* $ABC_k$ *index for the k=2,3,5 and* $GA_k$ *index for k=2,3,4.*

**Open Problem 5**: *Compute the exact expressions of Randi'c, Zagreb,* $ABC_k$, $GA_k$ *for benzenoid structures and Fibonacene.*

**Open Problem 6**: *Compute the closed formulas of Omega, Sadhana and PI polynomials for nanotubes like* $TUC_4C_8(R)[p,q]$ *and* $TUC_4[p,q]$.

**Open Problem 7**: *Construct new families of networks by using some graph operations and then study their topological indices.*

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