CHAPTER 1

INTRODUCTION

1.1 BASIC CONCEPTS IN GRAPH THEORY

Graphs serve as mathematical models of many concrete real-world problems. A graph can be used to represent almost any physical situation involving discrete objects and relationships among them. Also many branches of mathematics such as group theory, matrix theory, numerical analysis, probability and topology have their interaction with graph theory. Graph theory was born in 1736 with Euler’s paper in which he solved the celebrated Konigsberg bridge problem. In 1847, G.R. Kirchoff developed the theory of trees for its applications in electrical networks. Cayley discovered trees while trying to enumerate the isomers of saturated hydrocarbons $C_nH_{2n+2}$.

Definition 1.1.1. A graph $G$ is a pair $(V, E)$, where $V$ is a non empty set whose elements are called vertices of $G$ and $E$ is a set of 2-element subsets of $V$, whose elements are called edges of $G$. The sets $V$ and $E$ are the vertex set and edge set of $G$, respectively. We write $V(G)$ and $E(G)$ rather than $V$ and $E$ to emphasize that these are the vertex and edge sets of a particular graph $G$.

If $e = \{u, v\}$ is an edge, it can be written as $e = uv$ and $e$ is said to join the vertices $u$ and $v$; $u$ and $v$ are called adjacent vertices; $u$ and $v$ are said
to be *incident* with \( e \). If two vertices are not joined by an edge, then they are said to be *non-adjacent*. If two distinct edges are incident with a common vertex, then they are said to be adjacent with each other.

**Definition 1.1.2.** The number of elements in the vertex set of a graph is called the *order* of \( G \) and is denoted by \( p \). The number of elements in the edge set of a graph is called the *size* of \( G \) and is denoted by \( q \). A graph with \( p \) vertices and \( q \) edges is called \( (p, q) \) - graph.

**Definition 1.1.3.** Two graphs \( G = (V (G), E (G)) \); and \( H = (V (H), E (H)) \); are identical if \( V (G) = V (H) \) and \( E (G) = E (H) \). \( G \) and \( H \) are *isomorphic* if there exist a bijective function \( \phi : V (G) \rightarrow V (H) \) such that \( uv \) is an edge of \( G \) if and only if \( \phi(u)\phi(v) \) is an edge of \( H \); We write \( G \cong H \).

![Graphs G1 and G2](image)

**Figure 1.1 Isomorphic graphs \( G_1 \) and \( G_2 \)**

**Definition 1.1.4.** A graph \( H \) is called a *subgraph* of a graph \( G \) if \( V (H) \subseteq V (G) \) and \( E (H) \subseteq E (G) \). A *spanning subgraph* of \( G \) is a subgraph \( H \) with
$V(H) = V(G)$. For any subset $S$ of vertices of $G$, the \textit{induced subgraph} $<S>$ is the maximal subgraph of $G$ with vertex set $S$. Therefore two vertices of $S$ are adjacent in $<S>$ if and only if they are adjacent in $G$.

**Definition 1.1.5.** The \textit{degree} of a vertex $v$ denoted by $\deg(v)$ is the number of edges incident with $v$. The minimum degree of a graph $G$ is the minimum degree among the vertices of $G$ and is denoted by $\delta(G)$; the maximum degree of $G$ is the maximum degree among the vertices of $G$ and is denoted by $\Delta(G)$.

**Definition 1.1.6.** Let $G$ be a graph with $n$ vertices $v_1, v_2, v_3, \ldots, v_n$. The $n \times n$ adjacency matrix $A = (a_{ij})$ is defined by

$$a_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ adjacent with vertex } v_j \\ 0 & \text{otherwise} \end{cases}$$

**Definition 1.1.7.** Let $G$ be a graph with $n$ vertices $v_1, v_2, v_3, \ldots, v_n$ and $r$ edges $e_1, e_2, \ldots, e_r$. Then an incidence matrix $n \times r$ matrix is $I = (b_{ij})$ is defined by

$$b_{ij} = \begin{cases} 1 & \text{if the vertex } v_i \text{ is incident with the edge } e_j \\ 0 & \text{otherwise} \end{cases}$$

**Definition 1.1.8.** A walk in $G$ is an alternating sequence $w = v_0e_1v_1e_2v_2 \ldots e_kv_k$ of vertices and edges such that for each $i$, $1 \leq i \leq k$, $e_i = v_{i-1}v_i$. $w$ is said to be a walk from $v_0$ to $v_k$ or $(v_0, v_k)$-walk. $v_0$ is the origin, $v_k$ is the terminus. If all the vertices of a walk are distinct then such a walk is called a path.

**Definition 1.1.9.** If the edges $e_1, e_2, \ldots, e_k$ of a walk are distinct then the walk is called a trial. A trial whose origin and end vertices are same is called a cycle. A graph that has a cycle is called a cyclic graph. A graph that has no cycles is called an acyclic graph.
**Definition 1.1.10.** A *path* is a sequence of distinct vertices \((v_1, v_2, \ldots, v_n)\) such that the consecutive vertices are adjacent.

**Definition 1.1.11.** A graph is said to be *connected* if there is a path between every pair of distinct vertices of the graph.

**Definition 1.1.12.** If the vertices \(u\) and \(v\) are connected in a graph \(G\), then the distance \(d_G(u, v)\) or \(d[u, v]\) is the length of the shortest \(u - v\) path in \(G\). If there is no \(u - v\) path in \(G\) then \(d[u, v] = \infty\).

**Definition 1.1.13.** A *bipartite* graph is the one whose vertex set can be partitioned into two subsets \(X\) and \(Y\) so that each edge has one end in \(X\) and the other end in \(Y\) such a partition \((X, Y)\) is called a bipartition of the graph.

**Definition 1.1.14.** Let \(K_n\) be the *complete graph* with \(n\) vertices, in which each two vertices are adjacent. A complete bipartite graph is a simple bipartite graph such that two vertices are adjacent if and only if they are in different partite sets. A complete multipartite graph is a simple graph \(G\) whose vertices can be partitioned into sets so that \(uv \in E(G)\) if and only if \(u\) and \(v\) belong to different sets of the partition.

**Definition 1.1.15.** For \(k \geq 2\), a graph \(G\) is a *\(k\)-partite graph* or *multipartite graph* if \(V(G)\) can be partitioned into \(k\) non-empty subsets \(V_1, V_2, \ldots, V_k\) such that no edge of \(G\) joins vertices in the same set. The sets \(V_1, V_2, \ldots, V_k\) are called partite sets of \(G\). If \(G\) is a \(k\)-partite graph having partite sets \(V_1, V_2, \ldots, V_k\) such that every vertex of \(V_i\) is joined to every vertex of \(V_j\), where \(1 \leq i, j \leq k\) and \(i \neq j\), then \(G\) is called a complete \(k\)-partite graph or complete multipartite.
Definition 1.1.16. The complement \( \overline{G} \) of a simple graph \( G \) is a simple graph with the same vertex set \( V(G) \), two vertices being adjacent in \( \overline{G} \) if and only if they are not adjacent in \( G \).

Definition 1.1.17. A connected acyclic graph is called a tree. A tree in which one vertex called the root is distinguished from other vertices is called a rooted tree. A binary tree is defined as a tree in which there is exactly one vertex of degree two and each of the remaining vertices is of degree one or three.

The following Theorem is taken from Bondy & Murthy 1976.

**Theorem 1.1.18** For a graph \( G \) with \( p \) vertices and \( q \) edges.

1. \( G \) is tree.
2. Every two vertices are connected by a unique path.
3. \( G \) is connected and \( q = p - 1 \).
4. \( G \) is acyclic and \( q = p - 1 \).

A graph in which each vertex is assigned a unique name or label is called a labeled graph.

The following theorem is taken from Douglas B. West 2001.

**Theorem 1.1.19.** For a set \( S \subseteq \mathbb{N} \) of size \( n \), there are \( n^{n-2} \) trees with vertex set \( S \).

**Definition 1.1.20.** If \( G = (V, E) \) is a graph with at least two vertices, then the vertex deletion subgraph is the subgraph obtained from \( G \) by deleting a vertex \( v \in V \) and also all the edges incident to that vertex. The vertex deletion subgraph of \( G \) is denoted by \( G-\{v\} \).
**Definition 1.1.21.** If $G = (V, E)$ is a graph with at least one edge, then the \emph{edge deletion subgraph} is the subgraph obtained from $G$ by deleting an edge $e \in E$, but not the vertices incident to that edge. The edge deletion subgraph of $G$ is denoted by $G - \{e\}$.

**Definition 1.1.22.** Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be any two graphs. Then their \emph{union} $G_1 \cup G_2$ is the graph whose vertex set is $V_1 \cup V_2$ and edge set is $E_1 \cup E_2$.

**Definition 1.1.23.** Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be any two graphs. Then their \emph{intersection} $G_1 \cap G_2$ is the graph whose vertex set is $V_1 \cap V_2$ and edge set is $E_1 \cap E_2$.

**Definition 1.1.24.** The graph $G_1 \star G_2$ is obtained from $G_1$ and $G_2$ by joining every vertex of $G_1$ to all the vertices of $G_2$.

**Definition 1.1.25.** Let $G_1(V_1, E_1)$ and $G_2(V_2, E_2)$ be two graphs. The \emph{Cartesian product} $G_1 \times G_2$ of two graphs $G_1$ and $G_2$ is defined as $G(V,E)$, whose vertex set $V = V_1 \times V_2$ and the edge set $E$ is defined as follows if $w_1 = (u_1, v_1)$ and $w_2 = (u_2, v_2)$ be two typical vertices of $G$ with $u_1 \in V_1$ and $v_1 \in V_2$ then $w_1w_2 \in E (G)$ iff either (a) $u_1 = u_2$ and $v_1v_2 \in E_2$ (or) (b) $v_1 = v_2$ and $u_1u_2 \in E_1$.

**Definition 1.1.26.** The graph $G^+$ is obtained from any arbitrary graph $G$ by adding a pendant edge to each vertex of $G$.

**Definition 1.1.27.** A caterpillar is the graph derived from a path by attaching any number of pendant vertices to the vertices of the path $P_n$. The $(1, 4)$-
biregular caterpillar graph is obtained from path \( P_n \) by adding exactly two pendant vertex to every interior vertices. It consists of \((3n-4)\) vertices.

**Definition 1.1.28.** (Baskar Babujee & Babitha 2011) If \( G_1(p_1, q_1) \) and \( G_2(p_2, q_2) \) are two connected graphs, \( G_1 \vee G_2 \) is obtained by merging any selected vertex of \( G_2 \) on any selected vertex of \( G_1 \). If we arbitrarily choose the vertices of \( G_1 \) and \( G_2 \) then \( G_1 \vee G_2 \) is a class of graphs consisting of \( p_1 + p_2 - 1 \) vertices and \( q_1 + q_2 \) edges. In general, we can construct \( p_1 p_2 \) possible combinations of graphs from \( G_1 \) and \( G_2 \) up to isomorphism.

![Figure 1.2 Construction of \( G_1 \vee G_2 \)](image)

All the graphs studied in our thesis are finite and simple graphs.

1.2 **ORIGIN AND GROWTH OF CHEMICAL GRAPH THEORY**

In 1947 Wiener introduced two parameters. These parameters were designed for the specific purpose of correlating the boiling points of members of the alkane series of the molecular structure. The first parameter he designated as the polarity number \( P \), which is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds. The second
parameter was described as the path number $W$, which is the sum of the
distances between any two carbon atoms in the molecule in terms of the
carbon-carbon bond. Later path number $W$ was renamed as Wiener number
or Wiener index of a molecule.

Wiener applied these parameters to predict the boiling points of
various members of the alkane series (Schultz 1989). Wiener assumed that the
boiling points of the alkanes satisfied a linear formula

$$t_B = aW + bP + c,$$  \hspace{1cm} (1.1)

where $t_B$ is the boiling point of a given alkane $a, b, c$ are constants, $W$ is the
Wiener number and $P$ is the polarity number.

To carry out his procedure, Wiener needed difference in his
equation rather than absolute values for $t_B$, $W$, $P$ terms.

The difference Equation of (1.1) becomes

$$\Delta t = a\Delta W + b\Delta P$$  \hspace{1cm} (1.2)

where $\Delta t$ represents the difference in boiling points for a normal alkane
molecule and some other alkane molecule containing the same number of
carbon atoms. $\Delta W$ represents corresponding difference in their Wiener
numbers. $\Delta P$ represents corresponding difference in their polarity numbers.

Wiener was able to establish that the constant $a$ could be expressed
as $a = k/n^2$, where $k$ is a new constant and $n$ is the number of alkanes.
Wiener now made a determination of the constants $k$ and $b$ known boiling
point data for 37 different alkane species (ranging from butane through octane).

The correlation equation obtained from least squares fitting procedure of the form

$$\Delta t = \left( \frac{98}{n^2} \right) \Delta W + 5.5 \Delta P$$

(1.3)

The average deviation in the boiling point was found to be $0.47^\circ C$. Wiener then used his Equation (1.3) to calculate the boiling points of 29 nonane and 28 decane species for which reasonable accurate experimental boiling points were accurately known. Wiener was able to demonstrate that his method yielded the boiling points of the 29 nonanes with the average deviation of $1.26^\circ C$ and the boiling points of the 28 decanes with the average deviation of $1.30^\circ C$. Now Wiener was very satisfactory overall result that the deviation of only $0.97^\circ C$ for a total of 94 alkane species that had been correlated (Dennis Rouvray & Bruce King 2002).

In a general sense, molecular descriptors are “terms that characterize a specific aspect of a molecule”. In particular, topological indices have been defined as those “numerical values associated with chemical contribution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity”. They are derived from a graph-theoretical representation of molecules and can be considered as structure – explicit descriptors (Teik-Cheng Kim 2004). A representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. A topological representation of a molecule is called molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are
named vertices and the lines are named edges in graph theory language by Nenad Trinajstic (1936).

**Definitions 1.2.1.**

(i) A molecular graph in which hydrogen atoms are not considered is called Hydrogen-deleted graph.

(ii) The number of bonds incident on \( v \) is called valency of an atom or vertex degree \( \nu \) and is denoted by \( \text{deg}(\nu) \).

(ii) The number of bonds adjacent to \( e_k \) is called edge or bond degree of \( e_k \) and is denoted by \( \text{deg} ( e_k ) \). Two bonds are adjacent if they are incident to the same atom. The following relation is maintained, \( \text{deg} ( e_k ) = \text{deg} ( \nu_i ) + \text{deg} ( \nu_j ) \)(-2), \( \nu_i \) and \( \nu_j \) are incident to \( e_k \).

(iii) Topological distance \( d(\nu_i, \nu_j) \) is the length of the shortest path between vertices \( \nu_i \) and \( \nu_j \).

(iv) Adjacency matrix \( A \) is a square and symmetric matrix of order \( n \) whose elements \( a_{ij} \) are ones or zeros if the corresponding vertices \( \nu_i \) and \( \nu_j \) are adjacent or not.

(v) Distance matrix \( D \) is a square and symmetric matrix of order \( n \) whose elements \( d_{ij} \) correspond to the topological distances between atoms \( \nu_i \) and \( \nu_j \).

(vi) Spectral moments of a matrix are the trace or sum of the main diagonal elements of the different powers of the corresponding matrix.
In addition to the constraints on the degrees of the vertices, two remarks observations should be made in the following observations:

**Observations 1.2.2.**

(i) Since the vertices representing hydrogen are pendant vertices, they go with carbon atoms only one way and hence make no contribution to isomorphism. Therefore we need not show any hydrogen vertices.

(ii) Thus the tree representing $C_kH_{2k+2}$ reduces to one with $k$ vertices, each representing a carbon atom. In this tree no distinction can be made between vertices, and therefore it is unlabeled.

In butane, $C_4H_{10}$ there are only two distinct trees. As every organic chemist knows, there are indeed exactly two different types of butanes: $n$-butane and isobutane.

![Figure 1.3(a) n-butane](image1.png)  
**Figure 1.3(a) n-butane**

![Figure 1.3(b) The path graph $P_4$](image2.png)  
**Figure 1.3(b) The path graph $P_4$**

The molecular graphs or chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds are represented by edges of a graph. In Figure 1.3(a), 1.3(b), 1.4(a) and 1.4(b)
represents $n$-butane by path graph $P_4$ and iso-butane by star graph $k_{1,3}$ respectively.

![Figure 1.4 (a) iso-butane](image1)

![Figure 1.4 (b) The star $K_{1,3}$](image2)

**Definition 1.2.3.** If $A$ is the adjacency matrix of a graph $G$ and $I$ is the unit matrix of order $n$, the characteristic polynomial of the graph $G$ is defined as $Ch(G, x) = |xI - A|$. In other words, the characteristic polynomial of a graph is just the characteristic polynomial of its adjacency matrix.

**Theorem 1.2.4.** If the graphs $G_a$ and $G_b$ are isomorphic, then their characteristic polynomials coincide $Ch(G_a, x) = Ch(G_b, x)$.

![Figure 1.5 (a) Graph $G_a$](image3)

![Figure 1.5 (b) Graph $G_b$](image4)
The characteristic polynomial is given by \( Ch(G, x) = |xI - A| \)

\[
Ch(G_a, x) = Ch(G_b, x) = \begin{vmatrix} x & -1 & 0 & -1 \\ -1 & x & -1 & 0 \\ 0 & -1 & x & -1 \\ -1 & 0 & -1 & x \end{vmatrix} = 0
\]

\[
Ch(G_a, x) = Ch(G_b, x) = x^4 - 4x^2
\]

**Theorem 1.2.5.** The converse of the Theorem 1.2.4 is not true. Thus, if \( G_a \) and \( G_b \) are two graphs having equal characteristic polynomials, \( Ch(G_a, x) = Ch(G_b, x) \), it is not necessarily true that \( G_a \) and \( G_b \) are isomorphic.

**Definition 1.2.6.** If two non isomorphic graphs \( G_a \) and \( G_b \) have equal characteristic polynomials, then the graphs \( G_a \) and \( G_b \) are isospectral.

The chemical graphs of 2, 3 - dimethylheptane and 2- methyl-4- ethylhexane in Figure 1.6 (a) and 1.6 (b) are non isomorphic graphs and they have the same characteristic polynomial \( x^9 - 8x^7 + 19x^5 -14x^3 + 2x \).

![Figure 1.6 (a) Molecular graph of 2, 3 -dimethylheptane](image)

![Figure 1.6 (b) Molecular graph of 2-methyl-4-ethylhexane](image)
A topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariants. Topological indices are used for example in the development of quantitative structure-activity relationships (QSAR) in which the biological activity or other properties of molecules are correlated with their chemical structure. Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices such as distance or adjacency matrices, which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index.

Topological indices are also classified according to their nature in first, second and third generation. In the first generation, topologiccal indices are based on integer graph properties such as topological distances (Diudea et al 2006). The most representative indices of this class are Wiener index $W$, Platt index $F$, reverse Wiener index (Alexandru et al 2000), Hosoya index, modified Wiener indices (Gutman et al 2004) and the centric index of Balaban B and C, 1979. From these topological indices, the only one that has been used in drug discovery research is the Wiener index (Ban et al 2004). Second generation topological indices are real numbers based on integer graph properties. Most of the topological indices used in drug discovery today are of this class. The most successful set of such molecular descriptors are the molecular connectivity indices are introduced by Randic, 1975. In the third generation topological indices are those real numbers based on real number
local properties of the molecular graph. These indices are of recent introduction, have very low degeneracy and offer possibility of a wide selection.

The first of these definitions came almost 25 years later when Hosoya in 1971 recognized that the Wiener index can be obtained from the distance matrix of a molecular graph. After this seminal work of Hosoya, a new type of descriptors arose in the scenario of the characterization of molecular structure by mathematical entities. This work not only opened the door to a further explosion of mathematical and chemical work on the properties and applications of the Wiener index but also to the generation of a large number of new topological indices (Gutman 1994).

1.3 TOPOLOGICAL INDICES BASED ON DISTANCES

The topological indices derived from distance matrix are the Wiener index, the Platt number, the Gordon-Scantlebury index, the Altenburg polynomial, the Balaban index, the Smolenskii function, the Distance polynomial, the information indices and the centric index (Istvan Lukovits 1998).

Some of the definitions of topological indices which we use in our thesis are taken from Bonchev & Rouvray 1991.

**Definition 1.3.1.** Let $G$ be a simple molecular graph with vertex set $V(G)$ with $n$ vertices and edge set $E(G)$ with $m$ edges. The shortest distance between a
pair of vertices \( v_i \) and \( v_j \) of \( G \) is denoted by \( d(v_i,v_j) \). The Wiener index or Wiener number \( W(G) \) of \( G \) is defined as \( W(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i,v_j) \).

Equivalently \( W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) \), where \( d_G(u,v) \) denotes the shortest distance between two vertices \( u \) and \( v \) in \( G \).

**Definition 1.3.2.** Let \( G = (V, E) \) be a graph with \( n \) vertices and \( m \) edges. Let \( V = \{v_1, v_2, \ldots, v_n\} \). The Wiener index or Wiener number \( W(G) \) of a graph \( G \) is defined by \( W(G) = \sum_{i,j} d(v_i,v_j) \).

When \( G \) is a complete graph \( K_n \) the Wiener index is given by the expression \( W(K_n) = \frac{n^2-n}{2} \) and when \( G \) is a path graph, Wiener index can be calculated by the formula \( W(P_n) = \frac{n^3-n}{6} \). The Wiener index for the cycle graph \( C_n \) is \( W(C_n) = \begin{cases} \frac{n(n^2-1)}{8}, & \text{if } n \text{ is odd} \\ \frac{n^3}{8}, & \text{if } n \text{ is even} \end{cases} \). The Wiener index of star graph \( K_{1,n-1} \) is \( W(K_{1,n-1}) = (n-1)^2 \).

For tree \( T \), \( W(K_{1,n-1}) \leq W(T) \leq W(P_n) \). The above two expressions are the lower and upper bounds respectively of the Wiener index for any given connected graph with \( n \) vertices (Gutman et al 1997). In Figure 1.7 (b), the graph \( G \) representing the chemical structure 3-methyl pentane is given.
Figure 1.7 (a) The molecular structure of 3-methyl pentane

\[ d(v_1, v_2) = 1, \quad d(v_1, v_3) = 2, \quad d(v_1, v_4) = 3, \quad d(v_1, v_5) = 4, \quad d(v_1, v_6) = 3 \]
\[ d(v_2, v_1) = 1, \quad d(v_2, v_3) = 1, \quad d(v_2, v_4) = 2, \quad d(v_2, v_5) = 3, \quad d(v_2, v_6) = 2 \]
\[ d(v_3, v_1) = 2, \quad d(v_3, v_2) = 1, \quad d(v_3, v_4) = 1, \quad d(v_3, v_5) = 2, \quad d(v_3, v_6) = 1 \]
\[ d(v_4, v_1) = 3, \quad d(v_4, v_2) = 2, \quad d(v_4, v_3) = 1, \quad d(v_4, v_5) = 1, \quad d(v_4, v_6) = 2 \]
\[ d(v_5, v_1) = 4, \quad d(v_5, v_2) = 3, \quad d(v_5, v_3) = 2, \quad d(v_5, v_4) = 1, \quad d(v_5, v_6) = 3 \]
\[ d(v_6, v_1) = 3, \quad d(v_6, v_2) = 2, \quad d(v_6, v_3) = 1, \quad d(v_6, v_4) = 2, \quad d(v_6, v_5) = 3 \]

Figure 1.7 (b) Molecular graph of 3-methyl pentane
Polarity number is defined as the number of pairs of carbon atoms separated by three carbon atoms. 
\[ P = d(v_1, v_6) + d(v_1, v_4) + d(v_2, v_5) + d(v_5, v_6) \] = 4
and Wiener number 
\[ W(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i, v_j) = 31. \]

1.4 TOPOLOGICAL INDICES BASED ON CONNECTIVITY

The most of the proposed topological indices are related either to a vertex adjacency relationship (atom-atom connectivity) in the graph (molecular structure) \( G \) or to topological distances in \( G \). Therefore, the origin of topological indices can be traced either to the adjacency matrix of a graph or to the distance matrix of a graph (Zhou & Gutman 2004). The topological indices traced through adjacency matrix are the Zagreb index (Gutman & Das 2004), the connectivity index, the maximum eigenvalue index, the comparability index, and the Z index. In addition to the Wiener index, the Hosoya Z index defined by Hosoya, Zagreb group indices \( M_1 \) and \( M_2 \), the Randić \( \chi \) index of molecular connectivity, the Kier and Hall valence connectivity indices \( m, n \), the Balaban J index, the Schultz MTI index, and the bond connectivity index \( \varepsilon \) introduced by Estrada are other examples of topological indices (Devillers & Balaban 1999).


**Definition 1.4.1.** The Zagreb group indices of a graph \( G \) denoted by \( M_1(G) \) is the first Zagreb index and \( M_2(G) \) is the second Zagreb index are defined as

\[ M_1(G) = \sum_{v \in V(G)} \text{deg}(v)^2 \]
\[ M_2(G) = \sum_{(u,v) \in E(G)} \text{deg}(u) \cdot \text{deg}(v) \]
The sum in the first Zagreb index is over all vertices of $G$, while the sum in the second Zagreb index is over all edges of $G$.

![Figure 1.8 (a) Molecular structure of tetracyclic alkaloids](image)

*Figure 1.8 (a) Molecular structure of tetracyclic alkaloids*

![Figure 1.8 (b) The graph $G$ representing the chemical compound tetracyclic alkaloids](image)

*Figure 1.8 (b) The graph $G$ representing the chemical compound tetracyclic alkaloids*

Figure 1.8 (a) above displays the molecular structure of tetracyclic alkaloids and Figure 1.8 (b) represents the molecular graph of tetra cyclic alkaloids as a chemical compound. In this graph, total number of vertices is isomorphic to the graph $G$. We calculate the Wiener index of the graph in Figure 1.8 (b) as

The Wiener index $W(G) = 701$. 
The first Zagreb index $M_1(G) = \sum_{v \in V(G)} \deg^2(v) = 116$. 

The second Zagreb index $M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v) = 145$.

Platt was also interested in devising a scheme for predicting the physical parameters such as molar refractions, molar volumes, boiling points, heats of formation, and heats of vaporization of alkanes. In light of this Platt introduced an index $F(G)$ called Platt number.

**Definition 1.4.2.** Platt number $F(G)$ is equal to the total sum of degrees of edges in a graph. The degree of an edge $e$, $D(e)$ is the number of the adjacent edges. $M$ is the number of edges in $G$.

$$F(G) = \sum_{i=1}^{M} D(e_i)$$

![Molecular graph of 2,4- dimethyl pentane](image)

**Figure 1.9 Molecular graph of 2,4- dimethyl pentane**

The Platt number of the molecular graph in Figure 1.9 is 14.

### 1.5 GENERAL SURVEY ON TOPOLOGICAL INDICES

At the beginning of the twenty first century a large number of topological indices have been defined in literature. However, only a small fraction of these indices have been extensively used in studies of structure–activity relationships. The role of these descriptors for instance in drug discovery have been well established and several successful applications have
been reported. Estrada (2001) introduces a method to generalize some of the
most well known topological indices, called “Classical topological indices”.
This approach permits the generalization of several of these classical indices
as well as their optimization for a better description of the properties under
study. A two-volume monograph by Trinajstic also offers an excellent
computation of $W$ and combinatorial expressions for $W$, for various classes of
trees, few conjectures and open problems were mentioned. Fischermann et al
(2002) calculated the Wiener Index versus maximum degree in trees. Danial
Bonchev et al (2002) derived a formula for Wiener index of thorn trees, stars,
rings and rods. Xiaoying Wu et al (2003) constructed a graph with its Wiener
number less than some integer, among all graphs with $n$ vertices and $k$ cut
vertices. (Senpeng Eu & Bo-yin yang 2005) calculated the explicit formulae
for generalized Wiener indices which hold on hexagonal chains.
(MehdiEliasi & BijanTaeri 2008) introduced the four new operations on
graphs and studied the Wiener indices of the resulting graph. Dankelmann et
al (2009) introduced the edge Wiener index of a graph which is the sum of the
distances between all pairs of edges of $G$ and proved the sharp upper bound
for graphs of order $n$. Ivan Gutman (2009) introduced a simple formula for
computing $TW$. Mehdi Eliasi et al (2012) determined the Wiener index
of graphs which were constructed by some graph operations such as Mycielski’s
construction and generalised hierarchical product of graphs. Ivan Gutman
et al (2014) characterized eulerian graphs with smallest and greatest Wiener
indices. Collections of research papers in the area of chemical graph theory
have been edited by Balaban et al (1975).
1.6 TOPOLOGICAL MODELS FOR PREDICTION OF ANTI-HIV AND ANTI-CANCER ACTIVITY

In chemistry, a graph represents the topology of a molecule in the sense that it depicts the pattern of connectedness of atoms in the molecule, being at the same time, independent of such metric aspects of molecular structure as equilibrium distance between nuclei, bond angles, etc. When a single number represents a graph invariant, it is known as topological index or topological descriptor. These indices are derived from matrices, like distance matrix and adjacency matrix, which represent a molecular graph. Though numerous topological descriptors have been reported in literature, only handful of them has been successfully employed for structure-activity relationship studies. Notable amongst these are Wiener index, Randic connectivity index and eccentric connectivity index.

In the last decade, synthetic chemists have done tremendous research efforts for the development of newer anti-HIV agents. Structure-based designs, spurred by the significant pitfalls of the traditional method and the rapid advances in molecular-structure determination and computational resources, have now been accepted as a rational approach for the generation of new pharmaceuticals. The successful implementation of quantitative structure–property/activity relationship (QSPR/QSAR) certainly decreases the number of compounds synthesized, by making it possible to select most promising compounds. Garg et al (2005) developed quantitative structure-activity relationships for the anti-HIV potencies of several series of compounds, including non-nucleoside RT inhibitors. Harish Dureja & Anil Kumar Madan (2009) predicted anti-HIV activity of dimethylaminopyridin – 2 ones using topochemical descriptors. Singh et al (2009) studied, clinical status of anti-cancer agents derived from marine sources. Nonempirical parameters
of chemical structure derived from graph theoretic formalism are being used more frequently by many researchers in QSAR studies pertaining to molecular design, pharmaceutical drug-design and environmental hazard assessment of chemicals.

1.7 CHAPTER ORGANIZATION

The thesis is organized into five chapters as follows:

Chapter 1 is an introductory chapter in which the basic concepts of graph theory are outlined. Also in light of our work, the definitions, the literature survey of topological indices and some results related and have been listed.

In Chapter 2, Wiener index of graphs isomorphic to molecular structure, derived from standard structures is listed. Wiener index of class of trees, $W(G \oplus P_m)$ and $W(G \ominus C_m)$ are also enumerated.

In Chapter 3, The Wiener index of graphs and complement of graphs are calculated using degree sequence. Also some characterization results are stated and proved.

In Chapter 4, the terminal Wiener index for the binary tree and for some new class of graphs derived from a given connected graph are calculated, some new graphs are defined and Terminal Wiener index are calculated for them. The detour saturated trees $T_s(n)$ and $T_d(n)$, nanostardendrimer $D_s(n)$ are investigated. The terminal Wiener index of caterpillar graph derived from path graph is also found out.

In Chapter 5, quantitative structure activity relationship studies performed anti- HIV activities of quinolone carboxylic acid are analyzed.
The Wiener index, first and second Zagreb indices for the anti-cancer activity of some marine pyridoacridine alkaloids are studied. The values of all the three indices for each of the analogs comprising the dataset are computed and it is compared with the biological activity of the reported anti-cancer activity.