Chapter 1

Introduction
1.1 Introduction

In recent years, graph theory has evolved as an important mathematical tool in a wide field of subjects, ranging from operational research and chemistry to genetics, and from electrical engineering to architecture and geography to sociology and linguistics. At the same time it has also established as a worthwhile mathematical discipline in its own right. Graph theory is a significant tool, which helps the information seekers to connect the dots and arrive at a conclusion that is, it helps to know how well the contents under observation are connected to each other.

Graph theory started in the year 1736 at the first time when Euler solved the famously known Konigsberg bridge problem [36], the very first problem in graph theory. Hence this concept emerged to be a different discipline to view the real world problems. This problem lead to the concept of Eulerian graph.

There may be very few or no fields in real life which remains untouched and not considered on the background of graph theory. A wide range of applications pertaining to the diverse fields of sciences can be found.

In computer science, graphs are used to represent networks of communication, data organization, computational devices, the flow of computation, etc. For instance, the link structure of a website can be
represented by a directed graph, in which the vertices represent web
pages and directed edges represent links from one page to another and
determining the frequencies in the GSM models of mobile networks.
Predicting the timings of flights and flow of virus in the relative cloud
of networks.

In **condensed matter physics** [78], the three-dimensional struc-
ture of complicated simulated atomic structures can be studied quan-
titatively by gathering statistics on graph-theoretic properties related
to the topology of the atoms.

In **statistical physics** [78], graphs can represent local connections
between interacting parts of a system, as well as the dynamics of a
physical process on such systems. Graphs are also used to represent
the micro-scale channels of porous media, in which the vertices repre-
sent the pores and the edges represent the smaller channels connecting
the pores. Likewise, graph theory is useful in **biology** [78] and con-
servation efforts where a vertex can represent regions where certain
species exist (or habitats) and the edges represent migration paths,
or movement between the regions, coding sequencing of DNA and
analysing the spread of disease for a given instance.

In **sociometry** [53] we investigate a positional aspect of the status
of a person in an organization or a group, and again graph theory
intends to be applicable for determining the relations and discuss its
limitations.
1.2 Preamble of Chemical Graph Theory

Chemical graph theory serves as a branch of mathematical chemistry focused on hypothesis of Chemical graphs. Graphs would models from chemical compounds for which atoms are represented as nodes and their bonds by edges of a graph. The fundamental thought for chemical graphs theory is that physico-chemical properties for molecules could be concentrated on by utilizing the data encoded over comparing their chemical graphs. This data will be held in the nearness pattern, which is, in turn reliant on those valences of singular atoms and subsequently natural neighbourhood. There would be large portions of factors that might help understanding the components and their action toward which those neighbouring elements predicts the different physico-chemical properties of a molecule.

Instead of trying to explore the exact QSAR, chemical graph theory focus on a more feasible characterization. And this phenomena is attained on consideration of various QSPRs of molecular graphs namely known as topological indices or molecular descriptors and recognizing the strong correlation of various properties of the chemical compounds under consideration. By this one can clearly understand that chemical graph theory plays a vital part in mathematical base of the large area of QSAR and QSPR research.

A graph parameter or topological invariant is any property that
never depends on the vertex labelling and is only concerned with abstract structure. In the present era a finite number of topological invariants have been recognized up to date in QSAR/ QSPR studies.

1.2.1 Topological Indices

A large number of quantities namely diameter, radius, minimal and maximal degrees and the eigenvalues of a graph to describe the structure of graphs have been determined. In molecular chemistry, where graphs are taken as simple mathematical models for complex molecular structures, it has proven useful to define several so-called topological indices. Formally, a topological index is mainly a function running from the set of graphs to the real numbers. Further quantifies the structural properties on a real scale. The notion of a “topological index” came to be known for the first time when Japanese chemist Hosoya, investigated the relation between the physicochemical properties of a molecule and the number of its independent edge subsets (matchings) [55]. And hence Hosoya was able to prove a relation between the number of matchings (which is called the “Hosoya index in his honor now) of a molecular graph and the boiling point or the heat of vaporization.

The study of chemical graph theory began in 1947 at the first time by American Chemist Harold Wiener. He proposed the idea of molecular-graph-based structure descriptors importantly known as Wiener index
for determining the boiling point of paraffin \cite{105}. The study of Wiener index is one of the current areas of research in mathematical chemistry, with the help of which we can obtain good correlations between Wiener index (of molecular graphs) and the physico-chemical properties of the underlying organic compounds. Hence provides a rough measure of the compactness of the molecule under consideration.

The **Wiener index** is defined as the sum of the distances between every pair of vertices of a connected graph $G$ and denoted as $W(G)$. Thus,

$$W(G) = \sum_{\{u, v\} \subseteq V(G)} d(u, v)$$

where $d(u, v)$ is the distance between the vertices $u$ and $v$ and $V(G)$ is the vertex set.

For more about the Wiener index one can refer \cite{26, 31, 50, 76, 84, 85, 103}. Several other topological indices based on the degrees of vertices are introduced in the literature. The interest in topological indices is mainly related to their use in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) \cite{43}. The most studied degree based topological index is the Zagreb index.

\textit{Introduction}
The first and second Zagreb indices of a graph $G$ are defined as [49]

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

where, $d(u)$ is the degree of a vertex $u$ in $G$ and $E(G)$ is an edge set of $G$.

The mathematical properties and chemical applications of Zagreb indices were studied in [43, 49, 50, 76].

Another degree based topological index is defined as

$$F(G) = \sum_{u \in V(G)} [d(u)]^3,$$

commonly known as forgotten index, which was encountered by Furtula and Gutman [38]. Recently there has been some interest about $F(G)$ [38, 50].

Further we moved into understanding the different path of defining the zagreb index, known to be the first and second Zagreb co-indices of a graph $G$ and defined as [32]

$$\overline{M}_1(G) = \sum_{uv \not\in E(G)} [d(u) + d(v)] \quad \text{and} \quad \overline{M}_2(G) = \sum_{uv \not\in E(G)} [d(u)d(v)].$$

More results on Zagreb coindices can be found in [7, 6].

The eccentric connectivity indices of a connected graph $G$ are defined as [8, 101]

$$\xi_1(G) = \sum_{uv \in E(G)} [e(u) + e(v)] \quad \text{and} \quad \xi_2(G) = \sum_{uv \in E(G)} e(u)e(v),$$
where, $e(u)$ is the eccentricity of vertex $u$ in $G$.

Details on mathematical and chemical applications of eccentric connectivity indices can be found in [9, 27, 33, 41, 57, 58, 67, 73, 97, 111].

The **Harmonic Index** of a graph $G$ is defined as [37]

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$ 

Recent results on the harmonic index can be found in [21, 29, 56, 69, 109, 110].

For any positive integer $n$, $Z_2^n = Z_2 \times Z_2 \times \cdots \times Z_2$ ($n$ factors) is a group under the operation $\oplus$ with modulo 2 defined by

$$(x_1, x_2, \ldots, x_n) \oplus (y_1, y_2, \ldots, y_n) = (x_1 + y_1, x_2 + y_2, \ldots, x_n + y_n).$$

Element of $Z_2^n$ is an $n$-tuple $(x_1, x_2, \ldots, x_n)$ written as $x = x_1x_2\ldots x_n$ where every $x_i$ is either 0 or 1 and is called a string or word. The number of 1’s in $x = x_1x_2\ldots x_n$ is called the weight of $x$ and is denoted by $wt(x)$.

Let $x = x_1x_2\ldots x_n$ and $y = y_1y_2\ldots y_n$ be the elements of $Z_2^n$. Then

the sum $x \oplus y$ is computed by adding the corresponding components of $x$ and $y$ under addition modulo 2. That is, $x_i + y_i = 0$ if $x_i = y_i$ and $x_i + y_i = 1$ if $x_i \neq y_i$, $i = 1, 2, \ldots, n$.

The **Hamming distance** $H_d(x, y)$ between the strings $x = x_1x_2\ldots x_n$ and $y = y_1y_2\ldots y_n$ is the number of $i$’s such that $x_i \neq y_i$, $1 \leq i \leq n$ [39, 80]. Thus $H_d(x, y) = \text{Number of positions in which } x \text{ and } y \text{ differ}$.
\[ = \text{wt}(x \oplus y). \]

**Hamming index** is the sum of Hamming distances between all pairs of strings (or rows) generated by the incidence matrix of a graph \( G \) and is denoted by \( H_B(G) \). Thus,

\[
H_B(G) = \sum_{1 \leq i < j \leq n} H_d(s(v_i), s(v_j)).
\]

### 1.2.2 Spectral Graph Theory

Another important field of interest in graph theory is Spectra of Graphs. L. M. Lihtenbaum (1956) [47] and L. Collatz and U. Sinogowitz (1957) [13] at the first time lead a milestone in to the field through their fundamental paper. Earlier from the work of E. Hückel (1931) [40], theoretical chemists were interested in studying the stability of certain non-saturated hydrocarbons as well as other chemically relevant facts through graph spectra.

Many matrices have been defined in this field of Spectral graph theory. The most prominent matrices used are adjacency matrix [23], incidence matrix, Laplacian matrix [72], signless Laplacian matrix [24], distance matrix [3], Seidel matrix [17], complemenatry distance matrix [61].

Let \( G \) be a graph with vertex set \( V(G) = \{v_1, v_2, \ldots, v_n\} \) and edge set \( E(G) \). The adjacency matrix of a graph \( G \) is \( n \times n \) matrix defined as \( A(G) = [a_{ij}] \), where \( a_{ij} = 1 \), if the vertex \( v_i \) is adjacent to vertex \( v_j \).
in $G$ and $a_{ij} = 0$, otherwise. The characteristic polynomial of a graph $G$ is defined as $\phi(G : \lambda) = \det(\lambda I - A(G))$, where $I$ is an identity matrix. The eigenvalues of $A(G)$ are called the eigenvalues of $G$ and their collection is called the spectra of $G$ [23]. From the spectrum one can obtain the number of vertices, edges, loops, triangles, spanning trees. Bounds for the chromatic number in terms of eigenvalues are obtained in [13, 23].

The energy of a graph $G$ is defined as [42]

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|,$$

where $\lambda_i, i = 1, 2, \ldots, n$ is an eigenvalue of $G$.

In 1978, Ivan Gutman [42] conjectured that among all graphs with $n$ vertices the complete graph has maximal energy. Walikar, Ramane and Hampiholi [102] gave many counter examples for this conjecture in 1999 leading to the concept of hyperenergetic graphs. The first systematic construction of hyperenergetic graph was given by Walikar, Ramane and Hampiholi [102]. Gutman [47] showed that there are hyperenergetic graphs with $n$ vertices for every $n \geq 9$. Gutman et al. [46] showed that no Hückel graph (a graph with maximum degree 3) is hyperenergetic.

Two graphs $G_1$ and $G_2$ are said to be equienergetic if $\mathcal{E}(G_1) = \mathcal{E}(G_2)$. R. Balakrishnan [10] proved that there exists non-cospectral, equienergetic graphs of order $4n$, $n \geq 3$. H. S. Ramane et al. [85, 88]
proved that if $G$ is regular graph of order $n$ and of degree $r \geq 3$ then
$$\mathcal{E}(L^2(G)) = (nr - 4)(2r - 3) - 2$$
and
$$\mathcal{E}(L^2(G)) = 2nr(r - 2),$$
where $L^2(G)$ is the second line graph of $G$ and $\overline{G}$ is the complement of $G$.
Thus they constructed large families of noncospectral, equienergetic graphs of order $nr(r - 1)/2$. Pairs of equienergetic chemical trees were first time designed by Brankov, Stevanovic and Gutman \[16\].
Ramane and Walikar \[87\] gave a stronger result by constructing pairs of noncospectral equienergetic graphs on $n$ vertices for all $n \geq 9$. Distance equienergetic graphs are obtained in \[84\].

### 1.3 Fundamental Definitions and Terminologies

For definitions and terminologies of graphs and spectra of graphs we refer the books \[12, 13, 23, 52, 66, 68, 104\].

A graph $G$ consists of a finite nonempty set $V(G) = \{v_1, v_2, \ldots, v_n\}$ of $n$ vertices together with a prescribed set $E(G)$ of $m$ unordered pairs of distinct vertices of $V(G)$. Each pair of vertices in $E(G)$ is an edge of $G$. We consider only simple, undirected graphs without loops. Two vertices are said to be **adjacent** if there is an edge joining them. Then the edge between the vertices $u$ and $v$ is denoted by $uv$. An edge and its end vertex are **incident** with each other. Two edges are adjacent, if they are incident with common vertex.

The **degree** of a vertex is the number of edges incident to it. If all
the vertices have same degree equal to \( r \), then \( G \) is called a \textbf{regular graph} of degree \( r \) or \textbf{\( r \)-regular graph}.

Two graphs \( G \) and \( H \) are said to be \textbf{isomorphic} if there is one-to-one correspondence between their vertex sets which preserves the adjacency, and it is written as \( G \cong H \) or \( G = H \).

A \textbf{subgraph} of \( G \) is a graph having vertex set as a subset of vertex set of \( G \) and edge set as a subset of edge set of \( G \). A \textbf{spanning subgraph} is a subgraph containing all the vertices of \( G \). For any set \( S \) of vertices of \( G \), the \textbf{induced subgraph} \( < S > \) is the maximal subgraph of \( G \) with vertex set \( S \).

A \textbf{walk} of a graph \( G \) is an alternating sequence of vertices and edges, beginning and ending with vertices, in which each edge is incident with the two vertices immediately preceding and following it. It is \textbf{closed} if end vertices are same and is \textbf{open}, otherwise. A walk is a \textbf{trail} if all the edges are distinct and it is a \textbf{path} if all the vertices are distinct. A path with \( n \) vertices is denoted by \( P_n \). A closed walk is called the \textbf{cycle} provided all its \( n \) vertices are distinct and \( n \geq 3 \). A cycle with \( n \) vertices is denoted by \( C_n \).

A graph is \textbf{connected} if every pair of vertices is joined by a path. The \textbf{length of a path} is the number of edges in it. The \textbf{distance} \( d(u, v) \) between two vertices \( u \) and \( v \) of \( G \) is the length of shortest path joining \( u \) and \( v \) if any, otherwise \( d(u, v) = \infty \). A shortest \( u - v \)
path is often called a \textbf{geodesic}. The \textbf{diameter} of a connected graph $G$ denoted by $D = diam(G)$, is the length of any longest geodesic.

The eccentricity $e(v)$ of a vertex $u$ is the maximum distance between $u$ and any other vertex of $G$.

The \textbf{status} \cite{53} of a vertex $u \in V(G)$ is defined as the sum of its distance from every other vertex in $V(G)$ and is denoted by $\sigma(u)$. That is,

$$\sigma(u) = \sum_{v \in V(G)} d(u, v).$$

The \textbf{complement} $\overline{G}$ of a graph $G$ is a graph with vertex set $V(G)$ and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in $G$. A \textbf{self complementary graph} is isomorphic with its complement.

The \textbf{complete graph} $K_n$ is a graph with $n$ vertices in which every pair of vertices is adjacent. Thus $K_n$ has $\binom{n}{2}$ edges and it is regular graph of degree $n - 1$.

A \textbf{bipartite graph} is a graph whose vertex set can be partitioned into two subsets $V_1$ and $V_2$ such that no two vertices in either sets are adjacent. If every vertex of $V_1$ is adjacent to each vertex of $V_2$ then $G$ is a \textbf{complete bipartite graph} and is denoted by $K_{p,q}$, where $|V_1| = p$ and $|V_2| = q$. A \textbf{star} on $n$ vertices is a complete bipartite graph $K_{1,n-1}$.

A \textbf{cut vertex} of a graph is a vertex whose removal increases the number of components. A \textbf{nonseparable graph} is connected, non-
trivial and has no cut vertices. A block of a graph is maximal non-separable subgraph.

The line graph of $G$, denoted by $L(G)$ is the graph whose vertices has one-to-one correspondance with the edges of $G$ and two vertices of $L(G)$ are adjacent whenever the corresponding edges of $G$ are adjacent. If $G$ is an $r$-regular graph then $L(G)$ is $(2r - 2)$-regular graph.

If $G_1$ and $G_2$ are graphs with disjoint vertex sets $V_1$ and $V_2$ and edge sets $E_1$ and $E_2$ then their union $G = G_1 \cup G_2$ has vertex set $V(G) = V_1 \cup V_2$ and edge set $E(G) = E_1 \cup E_2$. The join of $G_1$ and $G_2$, denoted by $G_1 \nabla G_2$, is obtained from $G_1$ and $G_2$ by joining each vertex of $G_1$ to all vertices of $G_2$.

The adjacency matrix of $G$ is the square matrix $A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if $v_i$ is adjacent to $v_j$ and $a_{ij} = 0$ otherwise. The eigenvalues of $A(G)$ will be referred to as the adjacency eigenvalues of $G$ and labeled as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. These form the adjacency spectrum of $G$ [23, 24]. Two graphs are said to be cospectral if they have same spectra.

The ordinary graph energy $\mathcal{E}(G)$ of a graph $G$ is defined as the sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$ [42]. Two graphs $G_1$ and $G_2$ are said to be equienergetic if $\mathcal{E}(G_1) = \mathcal{E}(G_2)$. Trivially cospectral graphs are equienergetic. The theory of ordinary graph energy is extensively elaborated in the book
The **complementary distance** between the vertices $v_i$ and $v_j$ is defined as $c_{ij} = 1 + D - d(v_i, v_j)$, where $D$ is the diameter of $G$. The **complementary distance (CD) matrix** [61] of a graph $G$ is an $n \times n$ real symmetric matrix $CD(G) = [c_{ij}]$, where $c_{ij} = 1 + D - d(v_i, v_j)$, if $i \neq j$ and $c_{ij} = 0$, otherwise.

The **complementary distance energy** of a connected graph $G$ is defined as the sum of the absolute values of the eigenvalues of the complementary distance matrix $CD(G)$.

The **reciprocal complementary distance** between the vertices $v_i$ and $v_j$, denoted by $rc_{ij}$ is defined as $rc_{ij} = \frac{1}{1 + D - d_G(v_i, v_j)}$, where $D$ is the diameter of $G$ and $d_G(v_i, v_j)$ is the distance between $v_i$ and $v_j$ in $G$.

The **reciprocal complementary distance matrix** [61, 63] of a graph $G$ is an $n \times n$ real symmetric matrix $RCD(G) = [rc_{ij}]$, where

$$rc_{ij} = \begin{cases} 
\frac{1}{1 + D - d_G(v_i, v_j)}, & \text{if } i \neq j \\
0, & \text{otherwise}.
\end{cases}$$

The eigenvalues of $RCD(G)$ labeled as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ are said to be the **$RCD$-eigenvalues** of $G$ and their collection is called **$RCD$-spectra** of $G$. Two non-isomorphic graphs are said to be **$RCD$-cospectral** if they have same $RCD$-spectra.
1.4 Outline of the Present Work

The present thesis is divided into 8 chapters.

Chapter 1: This chapter deals with introduction of the thesis topic, bringing into consideration some historical background, milestones lead by different researchers specially concentrating on chemical graph theory and hence recalling some fundamental definitions and terminologies.

Chapter 2: In this chapter we introduce a new distance based parameter, defined as “Harmonic Status Index”, bounds for the harmonic status index of general graphs and standard class of graphs are obtained. This parameter is also studied for some standard class of graphs obtained from complete graph. At the end correlation between harmonic status index and boiling pont of paraffins is obtained in support to the above terminology.

Chapter 3: In this chapter we study the extension part of the second chapter where in we define more generalized and compact parameter known to be harmonic status coincidences. Moreover we have obtained the bounds for some general class of graph and derived class of graph specifically line graph.
Chapter 4: In this chapter we bring forward another distance based topological indices called as first status connectivity index and second status connectivity index of graphs and computed these indices for some standard class of graphs and derived class of graphs like line graphs. Also the bounds for these indices are reported. Further a regression analysis of the boiling points of benzenoid hydrocarbons with the distance based indices have been carried out and compared the linear models, leading to a new path of understanding the boiling points of given compounds.

Chapter 5: This chapter comes forward as an extension part of chapter 4 where, we have defined the first and second status co-indices of a graph $G$. Relations between status connectivity indices and status coindices are established. Their relations with the graph automorphism have been studied. Finally these indices are computed for intersection graph, hypercube, Kneser graph and achiral polyhex nanotorus.

Chapter 6: In this chapter we introduce a new distance invariant called status Hosoya polynomial. Computation of these to the class of graphs have been done. Application have been highlighted by producing their computation to nano structures.

Chapter 7: This chapter begins with the second part of thesis dealing with another important branch of chemical graph theory famously known as spectra of graphs. Motivated from the data of complemen-
tary distance energy we introduce to the redears Reciprocal complementary distance energy. RCD energy for line graphs of regular graphs have been obtained. RCD equienergetic graphs have been studied.

Chapter 8: This chapter is another part adding to the usage of graph theory by the means of digital coddling. Motivated from the work of hamming distance, in this chapter we give the general formulas to calculate the hamming index with respect to incidence matrix for thorn graphs of some standard class of graphs.