Chapter 1

Introduction

The origin of graph theory can be traced back to a Swiss Mathematician named Leonhard Euler solving the Königsberg seven bridges problem in the 18th century. Euler's solution for the seven bridges problem was a new type of geometry called "Geometry of Position," later renamed Graph Theory. In 1736, Euler was the first Mathematician who published the first article on graph theory due to his efforts to solve the Königsberg problem. Nearly a century ago, Cayley was interested in an analytical form derived from differential calculus to examine a particular class of graphs known as trees. He linked his results on trees with contemporary studies of chemical composition. Since then, graph theory has received wide attention and has been studied and applied to various fields such as Computer science, Chemical sciences, Operational research, and Social network analysis, to name a few. Among the various applications, our focus in this thesis is on the applications of graph theory in theoretical chemistry.

In the study of theoretical chemistry, the extensive focus of researchers has been to establish relationships between a substance's chemical and physical properties and the structure of the corresponding molecules. It is, therefore, not an exaggeration to say that theoretical chemistry has benefited a lot during the past 50 years from applying graph-theoretic [1, 2] and information-theoretic techniques [3, 4] to characterize molecular structures. The modeling of a chemical structure and its physical property led to the evolution of a new branch of mathematical chemistry called "Chemical Graph Theory(CGT)". Broadly, CGT uses graph theory and statistics to identify structural features involved in structure-property activity relationships. Further, the topological characterization of chemical structures allows the classification of molecules and modeling unknown structure with desired properties. Partitioning a molecular property and recombining its fragmental values by additive models remains one of the main tasks here.

Structural descriptors play an essential role in investigating molecular structures in various fields such as mathematical/computational chemistry, pharmaceutical science, materials science, and engineering, to name a few. The descriptors have often been used to characterize molecular networks since they quantify structural features. Indeed, QSAR and QSPR are well-known application areas where molecular structure descriptors have been proven beneficial. In particular, predicting biological and pharmacological properties using descriptors has been a problem of great interest

and importance. To this end, numerous descriptors are identified and considered viable; however, no single graph invariant can completely characterize the underlying graph topology.

In this thesis, we focus on analyzing the extremal properties of degree-based descriptors on various graph classes and focus on developing novel descriptors using graph matrices. Before that, we begin with some basic definitions and concepts required for further reading this thesis.

1.1   Graph-Theoretical Concepts

A graph is denoted by $G = G(V(G), E(G))$, consisting of a finite, non-empty set $V(G)$ of vertices, together with a set $E(G)$ of unordered pairs of vertices called edges. If $V(G)$ has finite number of elements, then G is called a finite graph; otherwise, it is called an infinite graph. If $V(G)$ has a single element, then G is called a trivial graph; otherwise, nontrivial graph.

For $e \in E(G)$, if $e = uv$, where $u, v \in V(G)$; we say that u and v are adjacent vertices, and e is said to be incident with u and v, or we say that e joins the vertex u and v. If two or more edges join the same pair of vertices then these edges are called multiple edges. An edge with identical ends $e = uu$ is called a loop. A graph is called a simple graph if it has no multiple edges or loops. Let n denote the number of vertices and m denote the number of edges. A walk is an alternating sequence of vertices and edges $< v_0, e_0, v_1, e_1, \ldots, e_{k-1}, v_k >$ such that $e_i = v_{i-1}v_i, \ \forall i = 1 \ to \ k$, and the number k is the length of the walk. If all the vertices and edges of a walk are distinct, we call it a path. A graph is connected if any two vertices are connected by a path. For $k \geq 3$, a walk $< v_0, e_0, v_1, e_1, \ldots, e_{k-1}, v_k >$ in which no vertices and edges are repeated is called a cycle if $v_0 = v_k$, it is denoted by C_k and k is called the length of the cycle. A tree is a connected graph that has no cycles. If G is a tree graph then $m = n - 1$, where n and m represents the number of vertices and number of edges respectively.

The degree of a vertex $u \in V(G)$ denoted by $d(u)$ or $d_G(u)$, is the number of edges incident to u. A vertex of degree one is called a pendant vertex and the edge incident to the pendant vertex is called the pendant edge. An isolated vertex is a vertex of degree zero. The maximum and minimum degree of a graph G are defined as

$$\triangle(G) \ or \ \triangle = max\{d(u) : \ u \in V(G)\}$$
$$\delta(G) \ or \ \delta = min\{d(u) : \ u \in V(G)\}.$$

The neighborhood set of a vertex $v \in V(G)$ is a set $N_G(v) = \{u \in V(G) : uv \in E(G)\}$, which consists of all vertices which are adjacent to v, *i.e.*, $|N_G(v)| = d(v)$.

The cyclomatic number of a connected graph is defined as $cy(G) = |E(G)| - |V(G)| + 1$. When G is a tree, we have $|E(G)| = |V(G)| - 1$. Since we know that trees have no cycles, we get $cy(G) = 0$. When $|V(G)| = |E(G)|$, G has cyclomatic number 1 and is called as unicyclic graph. When $|E(G)| = |V(G)| + 1$, G has cyclomatic number 2 and is referred to as bicyclic graph. When $|E(G)| = |V(G)| + 2$, G has cyclomatic number 3 and G is referred to as tricyclic graph.

Alternatively, a graph that has a unique cycle is called a unicyclic graph. If the graph has two cycles, then it is known as a bicyclic graph. If a graph has three cycles, then it is known as a tricyclic graph.

A graph G is regular, if every vertex has the same degree and particularly a graph is called k regular if every vertex has degree equal to k.

A path $< v_1 v_2, \ldots, v_{k-1} v_k >$ is called pendant path if $d(v_1) = 1$, $d(v_i) = 2$ for $i = 2, 3, ..., k-1$ and $d(v_k) \geq 3$.

A matching M of a graph $G = G(V(G), E(G))$ is a subset of $E(G)$ such that no two edges are adjacent in G. A vertex $u \in V(G)$ is called $M-$saturated if it is incident to an edge of M. If all the vertices of a graph G are $M-$saturated, then the matching M is called perfect matching. The other notations and definitions are taken from the book [5] and are introduced at the place of first use.

1.1.1 Molecular Graphs

We next introduce *molecular graphs*, on which our primary focus is. When applying graph theory to molecules, we have the vertices corresponding to atoms and the edges to chemical bonds - usually covalent bonds. The resulting graph depicts how atoms are bonded and which path or paths connect one atom with another in the molecule is called a molecular graph. For a topological representation of a hydrocarbon molecule, see Figure 1.1(a).

In a molecular graph, an edge between two nodes symbolizes the existence of a chemical bond between the atoms represented by those nodes, no matter what the valence of the chemical bond is. Sometimes it is necessary to consider the valence of the chemical bonds to deal with molecules with the same number of atoms and topology but different kinds of chemical bonds - simple, twofold,

triple, or quadruple covalent bonds. The result is called a molecular pseudograph or multigraph. We will not consider pseudographs here, so there will be no multiple edges between connected nodes. Usually, hydrogen atoms are not depicted in molecular graphs, in which case we speak of hydrogen-depleted (hydrogen-suppressed) molecular graphs; see Figure 1.1(b). Henceforth, all molecular graphs are meant to be hydrogen-suppressed, although not explicitly stated.

(a) Topological representation of a hydrocarbon

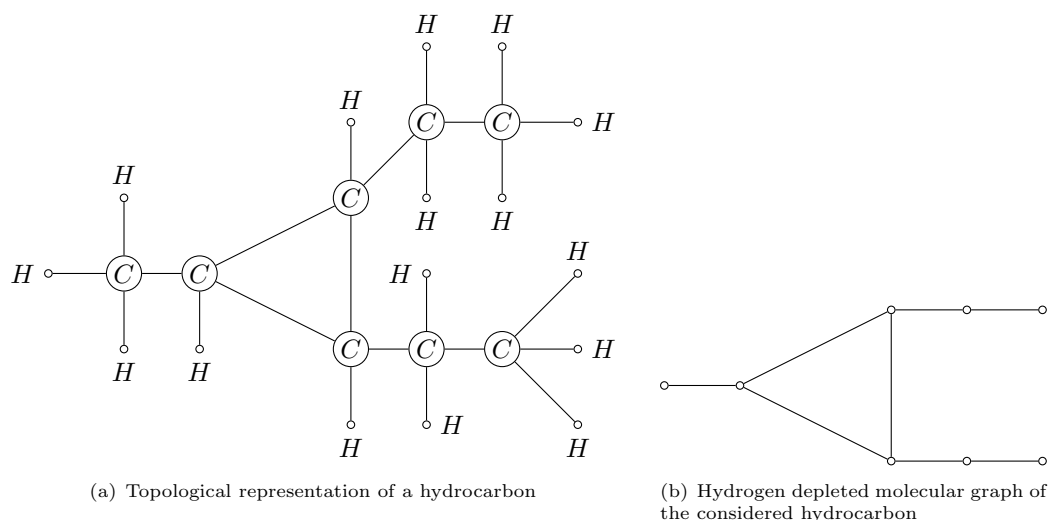(b) Hydrogen depleted molecular graph of the considered hydrocarbon

FIGURE 1.1: A hydrocarbon and its hydrogen depleted molecular graph representation.

The structural information contained in a molecular graph can now be codified by means of different mathematical objects, like matrices, numerical indices, polynomials, spectra, groups, and operators. Our interests lie in the numerical indices called the topological indices.

1.2 Topological Indices

This section introduces types of molecular descriptors called topological indices (TI). An invariant is a graph property that depends only on the topological structure of the graphs and not on the representation of graphs, such as particular drawing/labeling. Graph invariants representing topological and algebraic properties (such as vertex degrees, edge degrees, paths, distances between vertices, cycles, spanning trees, and orbits of the automorphism group, to name a few) have been used to define topological indices. Graph invariants and hence, topological indices are essential in predicting a chemical compound's physicochemical, biomedical, environmental, and toxicological properties directly from its molecular structure. In the literature, many topological indices have been proposed such that each describes structural complexity based on a particular property, thus

indicating indices cannot be uniquely defined. Therefore it is not surprising that diverse ideas and contrasting methodologies have been a backbone in developing novel descriptors to compare and characterize systems. Numerous indices are available in the literature; for example, see [6, 7].

Topological descriptors are broadly classified based on the graph property it represents. Distance-based, degree-based, and distance and degree-based are a few classes of topological indices.

Next, we present some of the most commonly cited distance-based and degree-based topological indices along with a brief literature survey and their applications in chemical graph theory.

1.2.1   Distance-Based Topological Indices

Distance-based topological indices are calculated based on the distance between any two vertices in a graph. One of the oldest topological indices was introduced in 1947 by the chemist Harold Wiener [8] when he was analyzing the chemical properties of paraffins (alkanes). This index is known as the Wiener index and is one of the most studied topological indices both from a theoretical and experimental perspective; [9–15].

The Wiener index $W(G)$, for a graph G, is defined as

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v) = \sum_{\{u,v\} \subseteq V(G)} d(u,v), \tag{1.1}$$

where $d(u,v)$ represent the shortest-path distance between the vertices u and v. There are various algorithms [16–18] for the evaluation of this index is available in the literature. In particular, this index has been calculated for trees [9, 19, 20], cyclic graphs [21], line graphs and nanotubes to name a few. In 1998, Gutman and Klavžar [22] established a relation between Wiener indices of phenylenes and benzoid compounds. For more details on Wiener index, see the articles [23, 24].

In 1993, the hyper Wiener index was introduced by Randić for acyclic graphs [25] and was extended to general graphs by Klein *et al.* in [26]. For a graph G, the hyper Wiener index $WW(G)$ is defined as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d^2(u,v) \tag{1.2}$$

This index shows a good correlation between various physico-chemical and biological properties [27–29] of a chemical compounds. The relation between Wiener and hyper Wiener index is given in articles [30–32].

The modification of Wiener index, known as generalized Wiener index [7], is defined as

$$W_k(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u,v)]^k \tag{1.3}$$

If we take $k = -1$, then it is known as "reciprocal Wiener index" and if $k = -2$, then it is known as the "Harary index". Sometimes the reciprocal Wiener index is also referred as the Harary index.

1.2.2 Degree-Based Topological Indices

This section presents the degree-based indices used in the rest of the chapters, especially in Chapters 5 to 7, for our comparative analysis. A topological descriptor whose computation is based only on the degree of a vertex is known as vertex-degree-based (VDB) indices. A large number of such descriptors have been proposed, and the computation of these indices for various chemical networks is an active area of research in both chemical and mathematical literature [8, 33–48].

Randić index [49] is one of the most widely studied and used degree-based index. The Randić index [49] for a graph G, is defined as-

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}. \tag{1.4}$$

It has been observed that Randić index has a good correlation with several physicochemical properties of alkanes such as boiling point, chromatographic retention times, enthalpies of formation, etc. For mathematical properties and chemical application of this index we refer to a series of articles [50–55].

A generalized version of Randić index [50], for a graph G, is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha, \tag{1.5}$$

where $\alpha \in \mathbb{R}$, and for $\alpha = -1/2$, we obtain Randić index.

Another variation of the Randić index was first introduced by Siemion Fajtlowicz [56] known as Harmonic index. For a graph G, it is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}. \tag{1.6}$$

Favaron *et al.*, [57] has given the relation between Harmonic index and eigenvalues of a graph.

The Zagreb indices [58] are one of the most important and well-studied topological indices in the literature. It first appeared in 1972, during the study of π−energy of conjugate molecules. For a graph G, the first and second Zagreb indices [58, 59] are defined as-

$$ZM_1(G) = \sum_{u \in V(G)} d^2(u) = \sum_{uv \in E(G)} (d(u) + d(v)) \tag{1.7}$$

$$ZM_2(G) = \sum_{uv \in E(G)} d(u)d(v). \tag{1.8}$$

Following this work, there was a plethora of literature published on Zagreb indices [40, 60–62].

Further, many modified forms and variants of Zagreb indices were also introduced. One of the modified Zagreb index $^m M_2(G)$ introduced by J. Hao [63], in 2009, is defined by

$$^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)} \tag{1.9}$$

In 2014, Furtula and Gutman [40] studied the difference between first and second Zagreb index. They found that this difference is closely related to the vertex degree based invariant

$$RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1), \tag{1.10}$$

known as the reduced second Zagreb index.

G. Shirdel *et al.* [64] introduced a new version of Zagreb index named hyper-Zagreb index. For a graph G, the hyper Zagreb index is defined as

$$HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2. \tag{1.11}$$

Some new results on the hyper-Zagreb index is found in article [65].

Another index proven useful in the study of heat formation of heptanes and octanes is Augmented Zagreb index [66], which is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2} \right)^3.$$ (1.12)

Motivated by the concept of line graph $L(G)$ of a graph G where the edges in G represents the vertices of line graph $L(G)$, Miličević *et al.* [67] introduced a pair of topological indices in terms of edge degree instead of vertex degree in Zagreb index. For a graph G, first and second reformulated Zagreb indices are defined as-

$$EM_1(G) = \sum_{e \in E(G)} d^2(e),$$ (1.13)

$$EM_2(G) = \sum_{e \sim f} d(e)d(f),$$ (1.14)

where $e \sim f$ means the edge e and f are adjacent in graph G, i.e., the edge e and f have a common vertex. Further, if $e = uv$, then note that $d(e) = d(u) + d(v) - 2$.

The inverse sum index introduced by Vukičević and Gašperov [68], in 2010, is shown to be a significant predictor of the total surface area of octane isomers. For a graph G, the inverse sum index $ISI(G)$ is defined as-

$$ISI(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d(u)} + \frac{1}{d(v)}} = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}.$$ (1.15)

In 2010, Vukičević and Gašperov [68] considered the large class of molecular descriptors, which consist of 148 discrete Adriatic descriptors for improving the various quantitative structure-property activity relationship $(QSPR/QSAR)$. They found and established that only a few of these descriptors were useful and distinct. Among these descriptors, the symmetric division degree index was determined to be a useful discrete Adriatic index. The symmetric division degree (SDD), index [68] is defined as

$$SDD(G) \sum_{uv \in E(G)} \{ \frac{d(u)}{d(v)} + \frac{d(v)}{d(u)} \}.$$ (1.16)

For more work related to SDD index, we refer to [69–76].

In 2015, Furtula and Gutman [77] introduced a topological index known as Forgotten topological index. For a graph G, it is defined as

$$F(G) = \sum_{u \in V(G)} d^3(u) = \sum_{uv \in E(G)} (d^2(u) + d^2(v)). \tag{1.17}$$

Albertson index [78] of a graph G is defined as

$$Alb(G) = \sum_{uv \in E(G)} |d(u) - d(v)|. \tag{1.18}$$

Gutman *at al.* [79], in 2017, introduced a topological index known as sigma index, defined by

$$\sigma(G) = \sum_{uv \in E(G)} (d(u) - d(v))^2 \tag{1.19}$$

1.3 Applications of Topological Indices

The study of topological descriptors has a wide range of applications in many different areas, such as thermo-chemistry, Hückel theory, spectral analysis, aromatic sextet theory, computer-assisted drug discovery, and deriving multi-linear regression models. We now discuss the two most important application of molecular graphs and their topological characterization.

Chemoinformatics

Chemoinformatics is a trending branch of research that combines chemistry, mathematics, and information science. The research in this field is concerned with the quantitative structure-activity (QSAR) and structure-property/toxicity ($QSPR/QSTR$) relationships, as the properties of molecules are derivable from their chemical structures. The main objective of QSAR/ QSPR/ QSTR is to quantify the molecular structures so as to build a correlation model between the chemical structures and their corresponding physicochemical properties [80–83].

This study has made it possible to predict a specific activity of a chemical compound even before its synthesis. Because molecular descriptors make it possible to quantify a chemical structure with a numerical value, they are crucial in this study for examining the characterization of chemical compounds without conducting any actual tests. Over the years, researchers have focused on

the relationship between graph -theoretic topological indices and physicochemical properties of underlying chemical structures [41, 84–91].

Pharmaceutical Industries

The application of molecular topology to the pharmacological research was only a matter of time, the pioneering work being done in the mid-1980s, and the first papers appearing at the beginning of the 1990s. The main incentive for developing new molecular descriptors was triggered especially by the pharmaceutical industry in its continuous need for improving drug design methods as these descriptors can be correlated with physicochemical properties of chemical compounds [92, 93]. Over a year, more than half a million new substances are synthesized or characterized to treat various syndromes. In contrast, only a few are and can be tested biologically, thereby increasing the cost of any new medicine. Therefore, any method helping investigators to know which structures are worthy of being synthesized and tested and which are not, results in enormous savings. Indeed, a significant role for the topological indices can be to provide a helpful starting point in computer-assisted drug discovery and predictive toxicological studies. This is one of the significant roles of the topological indices as it can provide a helpful starting point in computer-assisted drug discovery and predictive toxicological studies [94, 95].

Whatever the field, the interest in molecular topology is clear: Predicting with confidence some specific activity of a molecule saves time and money. Although the applications of molecular topology are manifold, the focus on pharmacological studies is soaring because of their novelty value and social impact.

1.4 Objective of the Thesis

The objective of this thesis is three-fold: We consider the mathematical, computational, and application-oriented analysis of vertex-degree-based indices. With this in mind, we study the following problems:

(i) Characterizing the extremal values of vertex-degree-based indices for certain classes of graphs.

(ii) Facilitating easy ways to compute vertex-degree-based indices by establishing relations with certain polynomials.

(iii) Constructing novel topological indices that can correlate well with the physicochemical properties of chemicals.

(iv) Comparing existing and proposed indices to establish the potentiality and predict expected values of these properties.

Next, we give a brief literature survey of the state-of-art in each of these problems.

1.5 Literature Review

For a topological index, in place of computation of exact value, characterizing its extremal values and finding the extremal graphs are interesting and considered important. Suppose an index correlates well with a certain physicochemical property of chemical compounds. With the help of bounds, we can quickly determine the range for related molecular properties. When analyzing the existing descriptors, many well-known graph families and vertex-degree-based topological indices exist in the literature for which the estimation of a range for index values remains open. Recently finding the extremal values or bounds for the topological indices of graphs and the related problems of characterizing the extremal graphs have attracted the attention of many researchers. Many results are available in the literature, see articles [46, 59, 61, 96–98].

In particular, for the bounds of reformulated Zagreb indices we refer to [99–104]. Recently, in [105, 106], the authors gave bounds for SDD index using the Zagreb indices and other edge/vertex degree based indices. For more related work on SDD index, we refer the reader to [69–73, 75, 76, 105–107].

In another direction, traditionally, the computation of topological indices involved only their definitions. Such computations are known to be time-consuming. Several techniques are introduced to reduce topological indices' computation time. Among them, the polynomial representation of indices has received wide attention in the literature. For instance, Hosoya polynomial, also known as Wiener polynomial [12, 108], is used to compute various indices such as Wiener index [8], Hosoya index [109] and Hyper Wiener index [26], etc. For example, the derivative of the Hosoya polynomial, when evaluated at 1, gives the Weiner index. Hyper Weiner index and Tratch-Zefirov index can be obtained similarly [110].

In 2015, Deutsch and Klavžar [111] introduced a polynomial known as *M-polynomial*. For a graph G, it is defined as

$$M(G; x, y) = \sum_{i \leq j} m_{ij} x^i y^j, \tag{1.20}$$

where m_{ij} denotes the number of edges $uv \in E(G)$ such that $\{d(u), d(v)\} = \{i, j\}$, where $d(u), d(v)$ denote degree of the vertex u and v in the graph G.

Note that the *M-polynomial* is a general polynomial because, with the help of this polynomial, one can determine many degree-based indices. At least nine such indices have been computed. For more details on *M-polynomial*, we refer to [112–118].

In the third direction, when one introduces a new topological descriptor/index in CGT, one needs to justify its potential ability and effectiveness to be a viable descriptor. Thousands of topological indices exist in chemical graph theory, such as distance-based indices, vertex-degree-based, and eigenvalue-based indices, to name a few. Only a few topological indices have been recognized as promising and worthy of practical applications in analyzing chemical structures. Hence, one can justify its well-definedness by using the discriminating power or the sensitivity to different compounds within a dataset. Further, by comparing it with existing indices and their behavior to various properties, one can test the potential ability and effectiveness.

For instance, recently, Furtula, Das, and Gutman [107] had done a comparative analysis of the SDD index with other popular VDB indices such as the Zagreb index, geometric-arithmetic index, atom-bond connectivity index, and inverse sum index, using the data of octane isomer. They concluded that the SDD index has the right to be considered as a viable and applicable molecular descriptor.

Similarly, Furtula and Gutman [77], pointed out the importance of $F(G)$. It can be used to obtain high accuracy of the prediction of logarithm of the octanol-water partition coefficient. The mathematical properties of $F(G)$ are given in the following articles [119, 120].

1.6 Outline of the Thesis

A molecular graph having a perfect matching plays a crucial role in the analysis of the resonance energy and stability of the molecules. In this thesis, we investigate the bounds of topological indices, especially for reformulated second Zagreb index and symmetric division deg index, of graphs with

the cyclomatic number at most three. Also, we construct some new topological indices and compare these indices with well-studied VDB indices. The thesis is mainly divided into seven chapters.

Firstly, we determine the bounds of the second reformulated Zagreb index for special graph classes: trees, unicyclic graphs, bicyclic graphs, and tricyclic graphs. **Chapter 2** focuses on finding the bounds of the second reformulated Zagreb index. In particular, we give the bounds for special graph classes, such as the trees, unicyclic graphs, bicyclic graphs, and tricyclic graphs. To study the bounds for these graphs, we propose to use certain transformations that help us obtain the required results. Further, we also find the extremal graphs which attain these bounds.

Next, we determine the sequence of lower bounds of SDD index for trees, unicyclic graphs, and bicyclic graphs that have a perfect matching. We also compute an upper bound of the SDD index for trees, unicyclic graphs, and bicyclic graphs with a maximum degree of four, which admits a perfect matching. **Chapter 3** details the study on the range of the SDD index for molecular graphs, that is, the upper bound and lower bound for the SDD index. We also give tight bounds by presenting the extremal graphs that attain the first four lower bounds of SDD index for trees and unicyclic graphs with maximum degree 4 that admits perfect matching. Also, we identify those graphs that attain the upper bounds of these trees and unicyclic graphs.

In Chapter 4, we present the first five lower bounds of the SDD index for all bicyclic graphs that have a perfect matching and the graphs that attain the bounds. Further, we compute an upper bound of the SDD index for bicyclic graphs with a maximum degree of four, which admits a perfect matching.

From the application perspective, our next work focuses on the predictive power of the SDD index. Here we analyze the SDD index against the physicochemical properties such as the melting point (MP), octanol-water partition coefficient ($logP$), log Henry constant ($logH$), log water solubility ($logSw$), and relative enthalpy of formation (dHf) of polychlorobiphenyl (PCB) congeners. Further, we compare the SDD index with the other well-studied VDB indices, such as ZM_1, ZM_2, R, AZI, H, and ISI. **Chapter 5** summarizes our findings and presents the statistical analysis for the PCB congener data.

From the computational perspective, we use the concept of *M-polynomial* and show how to compute the degree-based indices such as Forgotten index, Reduced Second Zagreb index, Sigma index, Hyper-Zagreb index, and Albertson index directly. In addition, we present as an application how to quickly and effectively compute these degree-based topological indices using *M-polynomial* for

carbon nanotube structures, $HC_5C_7[p,q]$, $SC_5C_7[p,q]$ and $VC_5C_7[p.q]$. **Chapter 6** details the computation technique using *M-polynomial* and its applications to nanotubes.

Finally, we achieve our objective of proposing novel descriptors in **Chapter 7**, where we construct 8 novel topological indices, denoted by AL_1, AL_2, AL_3, AL_4, AL_5, AL_6, AL_7 and AL_8. We give a method to compute these indices from a neighborhood matrix of graphs. To establish our aim, we study the proposed indices' discriminating ability and perform correlation and regression analysis using the widely available datasets on the physicochemical properties of the octane isomers and PCB congeners. Further, we also make a comparative study with a few existing VDB indices to establish the potentiality and use them to predict expected values of the properties for PCB congeners.

The thesis also contains two appendices **Appendix A and B,** containing the experimental values of the physicochemical properties of octane isomers and PCB congeners used in our computation and the predicted values for some specific properties based on this research work. Also, we give the computed data of AL indices of the octane isomers and PCB congeners that enable our predictability analysis.

$$**********$$