PREFACE

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 structures with desired properties. Partitioning a molecular property and recombining its fragmental values by additive models remains one of the main tasks here.

The objective of this thesis is three-fold: We consider the mathematical, computational, and application-oriented analysis of vertex-degree-based indices. The main objective of the thesis is that we propose a few novel indices based on distance and degree, study their behavior to analyze if they can serve as a potentially suitable molecular descriptor. If, suppose we can construct at least one topological index that produces a good, or even a reasonable correlation with at least a single molecule property, then, in that case, it will be a significant achievement in structure-property–activity studies. Additionally, while proposing a new topological index, it is vital to assess the capacity of the index to distinguish the molecules within the considered group. Such an assessment is alternatively referred to as the degeneracy analysis or the study of discriminating ability. 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. The outline of the thesis is as follows:

Firstly, we determine the bounds of the second reformulated Zagreb index for special graph classes: 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.

We study the extremal values 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, unicyclic, and bicyclic graphs with maximum degree 4 that admits perfect matching. Also, we identify those graphs that attain the upper bounds of these trees, unicyclic and bicyclic graphs with a maximum degree of four, which admits a perfect matching.

From the application perspective, next we focus 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 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. Based on the highest correlation values, we have also predicted the values for two properties of PCB congeners whose experimental values were not available.

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 $VC_5C_7[p.q]$. Finally, we see that by the application of *M-polynomial* we can reduce drastically the computational effort required to compute most of the degree-based topological indices.

Finally, we achieve our main objective of proposing novel descriptors,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.

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