Abstract

Many chemical substances consists of molecules. One of the primary goals of chemistry is to build relations between the chemical and physical properties of substance and the structure of the corresponding molecules. Many results along these lines have been obtained. Majority of such chemical rules are qualitative in nature. For example, if a molecule have -COOH group then that molecule exhibits an acidic behavior.

A century-long tendency in chemistry is to go a step further and to find quantitative relations of same kind. But, molecular structure is a non-numerical notion. The measured physical and chemical properties of substances are quantities. So, to build a relation between molecular structure and any physico-chemical property, one must transform the information contained in the molecular structure into a number. A topological index is a quantity that is somehow calculated from the molecular graph and for which we believe that it reflects relevant structural features of the underlying molecule.

Chapter 1 of this dissertation deals with some basic definitions and notions from chemical graph theory.

In chapter 2, we discuss that the spur graph gives the maximum zeroth-order general Randić index for $\alpha > 1$ and general sum-connectivity index, $\alpha \geq 1$ for trees with given independence number.

We generalize the Du et. al. results for sum-connectivity index in chapter 3. We find the maximum value for the general sum-connectivity index of $n-$vertex trees and $n-$vertex unicyclic graphs and characterize the extremal graphs. We also discuss the $n-$vertex unicyclic graphs with second maximum general sum-connectivity index.

In chapter 4, we extend the Goubko's result for any connected graph with cyclomatic number and characterize the minimal first Zagreb index for graphs with fixed number of vertices, pendant vertices and cyclomatic number.

In chapter 5, we find some exact formulae for the first reformulated index of some graph operations i.e. cartesian product, composition, join, link of graphs etc. and

apply these results to graphs of general interest. In last chapter, we derive the exact formulas for distance based topological indices for double graphs and apply these results to special kinds of graphs.