Introduction:

In the last twenty years graph theory(GT) has attracted a considerable part of scientific thought. For example, it has found applications in many branches of mathematics, e.g., group theory, matrix theory, probability, topology, combinatorics and operation research. GT has been applied also in statistical mechanics, electrical circuit designing and computer engineering. Chemical applications of GT so far developed form a vast literature, a significant part of which constitutes : (i) structure-property correlations through various kinds of atom-connectivity indices,(ii)enumeration of possible reaction paths, isomerisation etc.,(iii) organisation and classification of large polycyclic benzenoids and hetero atom analogues into isomers and isoskeletal analogues according to a formula periodic table developed graph-theoretically (based on the idea of partially ordered sets) and (iv) study of the adjacency matrices of molecular graphs particularly for understanding properties of conjugated molecules. The last category of applications depends on the fact that the HUckel hamiltonian matrix of the molecule becomes the same as the adjacency matrix of its carbon-carbon σ-bond skeleton (the graphical representation) of the molecule. In general, any system involving a binary relation is representable in the form of a graph and the latter may be regarded as a mathematical tool for handling the system. There is an abundance of mathematical problems where application of the language and techniques of GT provide easily understandable solution.

The whole work reported in this dissertation can be divided into two broad sections depending on the motif of using a graph.

Section-A. This consists of chapters 2-6 and is devoted to reporting output of works where a graph is used as a mathematical tool for handling eigenvalue problem of real symmetric matrices. It has been shown that GT techniques can yield many complicated results of matrix theory, provide easy and pictorial understanding of many highly complicated mathematical methods and offer simplified methods of calculation in each case.

Chapter-1 contains a few important definitions, and is excluded from sections A & B. Chapter-2 of section-A is a review of graph theoretical methods of construction of characteristic polynomials. In chapter-3 two new graph theoretical methods are described for construction of eigenvectors.

Chapter-4 contains a new recursion formula for construction of characteristic polynomial of the adjacency matrix (**A**) of the graph and cofactor of any element of det(x**I**-**A**) where **I** is the unit matrix of the size of **A**. In chapter-5 the theory has been utilised for stepwise factorisation of symmetric graphs. This chapter shows the efficiency of graph theory to compete with group theory in bringing out eigenvalues and eigenvectors without using any character table etc. In chapter-6 a method has been developed to convert every undirected graph into a linear chain. In matrix theory this runs parallel to Householder's method of reduction of a symmetric matrix to tridiagonal form.

Section-B consists of chapters 7 & 8. In chapter-7, the graph theoretical methods developed in section-A have been utilised to explain the trends in charge-transfer bands of some molecular complexes . Here a graph which is the same as the σ-bond topology of carbon atoms and conjugated heteroatoms of an organic molecule is used as the pictorial representation of the HUckel hamiltonian matrix of the conjugated compound. From such trends in charge-transfer bands the HUckel parameters of some heteroatoms and inductive effect parameters of CH_3-, C_2H_5- and t-butyl groups have been calculated. In chapter-8 it has been shown how Budan-Fourier theorem can be utilised to obtain energy level patterns of heteroconjugated and cross-conjugated systems from the sign-change patterns of their characteristic polynomials obtained graph theoretically. Thus from a pair of molecules having the same σ-bond skeleton we can predict which one will be a π-donor and which one an acceptor.

Object of each of the investigations reported in the thesis is mentioned at the begining of the corresponding chapter.