This thesis presents the results of the crystallographic investigations on some heterocyclic compounds carried out by the author as a part-time and full-time research scholar in the Department of Physics, Bharathidasan University, under the guidance of Professor V. Parthasarathi during the period 1991 to 1996.

A careful crystal structure analysis can provide a wealth of information concerning bond lengths and angles, intermolecular interactions, details of conformation, molecular packing and hydrogen bonding. In addition it provides with great accuracy the relative atomic positions needed for advanced theoretical work.

Chapter I serves as an introduction to the principles underlying structure analysis by X-ray diffraction from single crystals. Chapter II deals with a brief account of the significance of the compounds and the preparation procedures of the compounds taken up for the present structural investigations.

In chapters III to IX, the structural reports of seven decahydroquinoline derivatives are discussed. Chapter X presents a comparative study of the structural parameters and the effects of the various substituent groups on the geometries and the molecular conformations of the seven substituted decahydro-quinoline compounds.

In chapters XI to XIII, the structural reports of three isoxazoline derivatives are discussed. Chapter XIV presents a comparative study of these three isoxazoline derivatives.
In chapters XV to XVII, the structural reports of three diazepine derivatives are discussed. Chapter XVIII presents a comparative study on the conformational aspect of diazepine derivatives studied by the author.

Chapter XIX reports the crystal structure solution of a phenanthrene derivative.

Each chapter on crystal structure includes details of intensity data collection, structure solution and refinement and a discussion on the molecular geometry and conformation. Details of crystal data and of structure solution and refinement are tabulated at relevant places. The other tables are collected and presented at the end of each chapter. The crystallographic numbering scheme is followed to represent each atom in a molecule.

The bond lengths and bond angles involving non-hydrogen atoms are schematically presented in diagrams and the corresponding values are listed in Tables as well. For a comparison of the bond lengths, the "Tables of bond lengths determined by X-ray and neutron diffraction" compiled by Allen et al (1987) are used as the standard.

Lists of observed and calculated structure factors for all the compounds are enclosed at the end of the thesis.

Based on the studies reported in this thesis, the following papers have been published/communicated:
2. 5-Phenyl-3-oxa-4-azatricyclo[5.2.1.0^2,6]dec-4-ene:
   Thiruvalluvar, A., Parthasarathi, V., Nagarajan, A. and

3. Redetermination of Bis(N,N-diethyldithiocarbamato)nickel(II):
   Selvaraju, R., Panchanatheswaran, K., Thiruvalluvar, A. and

4. N-Benzoyl-2-phenyldecahydroquinolin-4-one: Thiruvalluvar, A.,
   Sankar Raja Raj, K., Krishna Pillay, M. and

5. 2-(10-Diethylaminomethyl-2,3,6,7-tetramethoxy-9-phenanthryl-
   methyl)-1-pyrroldinecarbonitrile: Kabaleeswaran, V.,
   Rajan, S.S., Thiruvalluvar, A. and Parthasarathi, V.

6. N-Acetyl-3-ethyl-2-phenyldecahydroquinolin-4-one:
   Thiruvalluvar, A., Parthasarathi, V., Natarajan, D., Bhavani,

7. N-Methyl-2-phenyldecahydroquinolin-4-one Oxime:
   Thiruvalluvar, A., Parthasarathi, V., Ganesh, V.K.,
   Acta Cryst. C52, 000 – 000 (in press).

8. N-Nitroso-3,3-diinethyl-2-phenyldecahydroquinolin-4-one:
   Thiruvalluvar, A., Parthasarathi, V., Natarajan, D., Bhavani,
   (in press).

9. 2-Phenyldecahydroquinolin-4-one
   (under preparation).

10. 3-Methyl-2-phenyldecahydroquinolin-4-one
    (under preparation).
11. 2-Phenyldecahydroquinolin-4-one Oxime Hydrochloride (under preparation).
12. 4-(3-Nitrophenyl)-2-oxa-3-azabicyclo[3.3.0]oct-3-ene (under preparation).
13. 5-(4-Chlorophenyl)-3-oxa-4-azatricyclo[5.2.1.0\(^2,6\)]dec-4-ene (under preparation).
14. 2,6-diazabicyclo-3-phenyl-4-methyl[5.4.0\(^1,7\)]undecan-5-one (under preparation).
15. Tetrahydro-2,4,4-trimethyl-N-phenylcarbamoyl-5H-1,5-benzodiazepine (to be communicated).