(i)

PREFACE

The thesis embodies the results of the investigations carried out by the author as a part-time research scholar, during the period from August 1984 to August 1990 at the Department of Physics, Bharathidasan University, Tiruchirapalli. It presents a detailed account of the crystal structure analyses of eight substituted thiophene compounds by single crystal X-ray diffraction method.

Chapter I deals with certain ideas on the resonance delocalization observed in a thiophene ring, and the brief experimental procedures which were followed to prepare and crystallize the eight thiophene compounds taken up for the present structural investigations. Chapter II serves as an introduction to the principles underlying structure analysis by X-ray diffraction from single crystals. In Chapters III to IX and in the Appendix, the structural reports of each of the eight substituted thiophene compounds are discussed. Each chapter 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. Lists of observed and calculated structure factors for all the compounds are enclosed at the end of the thesis.
The fractional atomic coordinates of all the non-hydrogen atoms and of those hydrogen atoms which are located by the structure solution methods are listed in the Tables. The rest of the hydrogen atoms are shown in the molecular structure of each compound. The crystallographic numbering scheme is followed to represent each atom in a molecule. The atoms in the thiophene ring are numbered as S(1), C(2), C(3), C(4) and C(5) starting from the hetero atom S as shown below:

![Thiophene Ring Diagram]

IUPAC nomenclature is followed for numbering the atoms in the cases of fused rings.

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.

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 eight substituted thiophene compounds. It also includes a brief account of the preliminary antimicrobial study of these compounds. A brief summary of the results of the investigations is given at the end.

The results of the investigations have been published/communicated in the following papers:


4) Structure of Ethyl 2-amino-4(m-nitrophenyl)thiophene-3-carboxylate benzene solvate (to be communicated).

5) Structure of Ethyl 2-amino-4,5,6,7-tetrahydrocyclohexa(b)thiophene-3-carboxylate (to be communicated).
vi) Structure of Ethyl 2-(o-hydroxybenzylideneamino)-4,5,6,7-tetrahydrocyclohexa(b)thiophene-3-carboxylate. (under preparation)

vii) Structure of Ethyl 2-amino 4(H) 5,6,7,8-tetrahydrocyclohepta(b)thiophene-3-carboxylate (under preparation).