PREFACE

This thesis summarizes the results of the X-ray Crystallographic studies on some biologically important small molecules carried out by the author as part-time and full-time research scholar in the School of Physics, Bharathidasan University, Tiruchirapalli, under the guidance of Professor V. Parthasarathi during the period 2001 to 2006.

Single crystal X-ray diffraction studies provide the knowledge on stereochemistry and molecular geometry of the molecules. A careful crystal structure analysis can provide a wealth of information, concerning bond lengths, bond angles, non-covalent interactions and details of molecular conformation. It also provides with great accuracy, the relative atomic positions needed for advanced theoretical work. The X-ray crystallography is a tool to determine both configurational and conformational features which decides the activity of the molecules like drugs, steroids etc.

The thesis consists of five parts. Part I includes two chapters. Chapter I gives an introduction to the principles of X-ray crystal structure analysis by diffraction from single crystals and Chapter II deals with a brief account of the significance of the compounds and the synthetic procedures for these compounds taken up for the present structural investigations.

Part II consists of Chapters III to VIII. In Chapter III and IV, the structures, conformations and C-H..O interactions of five D-homoestra-1,3,5(10)-triienes are presented. In Chapter V, a comparative study of these five structures with other related molecules are discussed. The structural reports of two androst-5-ene derivatives are presented in Chapter VI and those of the androstane in Chapter VIII. A comparative analysis of the two androst-5-ene structures with other androst-5-ene structures available in the literature is illustrated in Chapter VII.
Chapters IX, X and XI are included in Part III. Chapters IX and X describe the structure analyses of six indolizine derivatives while Chapter XI compares the bond lengths and bond angles of the indolizine ring system of these six molecules with other closely related structures.

Part IV consists of Chapters XII and XIII. The crystal and molecular structures of three 1-nitroso-piperidine derivatives are discussed in Chapter XII. The conformations of the piperidine rings and orientation of the substituents to the piperidine ring of these three structures are compared with the related piperidine derivatives studied by other authors in Chapter XIII.

Part V has three chapters, XIV, XV and XVI, discusses the conformational features of three different molecules namely, derivatives of a cyclohexanone, an indozal and a propenoate.

Each chapter on crystal structure includes structure solution, structure refinement and the discussion on the molecular geometry and conformation. Details of crystal data and structure solutions and refinement are tabulated at relevant places. The bond lengths and bond angles involving non-hydrogen atoms are schematically presented in diagrams. The torsion angles of non-hydrogen atoms are listed in Tables at the appropriate places. The crystallographic numbering scheme is followed to represent each atom in a molecule. The references cited in the text are given collectively in alphabetical order at the end of the thesis.

The anisotropic displacement parameters and the structure factor tables \((h, k, l, F_0^2, F_c^2)\) are given in the compact disk (CD) enclosed in a pouch at the inner side of the back cover of the thesis.
Based on the studies reported on this thesis, the following papers have been published. The reprints as pdf files are provided in the CD.

(1). 16-(4-Cyanobenzylidene)-3β-pyrrolidinoandrostan-5-en-17β-ol monohydrate

(2). 16-(4-Cyanobenzylidene)-17-oxoandrostan-5-en-3β-ol.

(3). 3-(4-Chlorobenzoyl)-7-(N,N-dimethylamino)-1-phenylindolizine and 3-(2,4-dichlorobenzoyl)-7-(N,N-dimethylamino)-1-phenylindolizine

(4). Dimethyl 3-benzoyl-7-(N,N-dimethylamino)indolizine-1,2-dicarboxylate

(5). Dimethyl 7-(N,N-dimethylamino)-3-(4-methylbenzoyl)indolizine-1,2-dicarboxylate.

(6). Dimethyl 3-(4-bromobenzoyl)-7-(N,N-dimethylamino)indolizine-1,2-dicarboxylate.

(7). 17-Butyl-16,17a-dioxo-17-aza-D-homoestra-1,3,5(10)-trien-3-yl acetate.

(8). 17-Allyl-16,17a-dioxo-17-aza-D-homoestra-1,3,5(10)-trien-3-yl acetate
(9). (8 R,9 S,13 S,14 S)-17-Butyl-16,17a-dioxo-17-aza-D-homoestra-1,3,5(10)-triene-3-ol.

(10). (8 R,9 S,13 S,14 S)-17-Butyl-3-methoxy-17-aza-D-homoestra-1,3,5(10)-triene-16,17a-dione.

(11). r-2, c-6-Bis(2-chlorophenyl)- t-3, t-5-dimethyl-1-nitrosopiperidin-4-one oxime

(12). r-2, c-6-Bis(4-chlorophenyl)- t-3, t-5-dimethyl-1-nitrosopiperidin-4-one oxime.

(13). t-3-Methyl-1-nitroso- r-2, c-6-diphenylpiperidin-4-one oxime monohydrate.

(14). 3, t-6-Dihydroxy- t-5-methoxycarbonyl- c-6-methyl- r-4-phenyl-4,5,6,7-tetrahydro-1H-indazole.

(15). c-5-Hydroxy- r-2, c-4-bis(isopropoxycarbonyl)- t-5-methyl- t-3-phenylcyclohexanone

(16). 17-Allyl-16,17a-dioxo-17-aza-D-homoestra-1,3,5(10)-trien-3-ol.
(17). Dimethyl 7-(N,N-dimethylamino)-3-(2-Methoxybenzoyl)indolizine-1,2-dicarboxylate

(18). Ethyl (E)-2-benzoyl-3-phenylpropenoate.