PREFACE

The thesis entitled " INVESTIGATION OF CRYSTAL AND MOLECULAR STRUCTURES OF FEW CHEMICAL COMPOUNDS BY X-RAY DIFFRACTION METHODS " deals with the elucidation of the structure and conformation of molecules exhibiting interesting stereochemical features.

Preliminary investigations of the crystals were carried out by means of oscillation and Weissenberg photographs taken at the X-ray diffraction laboratory of the Department of Physics, Gauhati University, Guwahati.

Three dimensional X-ray diffraction intensity data from single crystal samples were collected in an Enraf-nonius CAD - 4 diffractometer at the Department of Bio-physics, All India Institute of Medical Sciences, New Delhi. The structures have been solved by direct methods and refined by standard least-squares methods. The computer programs used for structure solution are SHELXS-86 (Sheldrick, 1986); SHELXS-97 (Sheldrick, 1997); the refinements were carried out by using SHELXL-93 (Sheldrick, 1993); SHELXL-97 (Sheldrick, 1997).

Five chemical compounds were chosen for this work of which four have reported to be of medicinal interest. The structure determination of these compounds assumes importance in view of the fact that any structural changes observed in the conformation of these molecules, due to different substituents can lead to the better understanding of their biological activities. Hence, each structure has been studied and discussed with the other compounds of the same group, taking the available information on structures so far reported and published.

In the chapter I, the basic principles involved and methods used in the determination of crystal structure, particularly those employed in the present work, together with the computer programs used, have been described.

Chapter II describes the determination of crystal and molecular structure of " benzyl phenyl ketoxime - $C_{14}H_{13}NO$ ".

Chapter III is concerned with the crystal and molecular structure of " hexahydro-1,3,5-tri(p-chloro-phenyl)-s-triazine - $C_{21}H_{18}N_3Cl_3$ ".

Chapter IV deals with the crystal and molecular structure of " hexahydro-1,3,5-tri(p-methoxy-phenyl)-s-triazine - $C_{24}H_{27}O_3N_3$ ".

Chapter V is an account of the crystal and molecular structure determination of " dichlorobis (4-cyanopyridine)copper(II) - $CuC_{12}H_8N_4Cl_2$ ".

Chapter VI contains determination of the crystal and molecular structure of "tetrakis(imidazole)copper(II) bromide - $CuBr_2C_{12}N_8H_{12}$ ".