## Chapter II : Scope and Objectives

In spite of a large volume of literature existing on the study of molecular complexes[1-4] there is enough scope for studying such complexes involving pharmaceutical molecules. Most of the studies on charge transfer complexes have so far been carried out in non-polar media which are not bio- or environment-friendly. The objectives of the works described in the present thesis are to study molecular complexes of some drug and vitamin molecules in aqueous ethanol media of varying composition. Such media are close to body fluid in living beings and hence the results are expected to have some relevance to pharmacology. The results are described in the next five chapters (Chapters III to VII). Each chapter begins with an introductory section where the scope and objectives of the work described in that chapter have been clearly stated. The materials used and methods of their purification have also been described in the experimental section of the respective chapters. In chapter VII a computational study using the density functional theory (DFT)[6,7] has been carried out which confirms the CT nature of the transitions observed with the complexes mentioned in the earlier chapters. The DFT requires reasonably less computer time than other *ab initio* methods for molecules of moderate size. With a given donor and a series of electron acceptors, the CT transition energies should show a decreasing trend with increase in vertical electron affinity of the acceptors according to Mulliken's theory.[5] This has been verified in chapter VII for the transition energies of the cloxacillin sodium complexes with the series of acceptors used in the experimental work

reported in chapter III. The thesis ends with a summary of the results (chapter VIII).

**References**


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