ABSTRACT

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The thesis entitled "Structural Investigation of Some Organic Molecules Using Single Crystal X-ray Crystallography" is divided into five chapters as follows.

Chapter I: General Introduction

Chapter II: Crystal structure analysis of three different chalcones

Chapter III: Crystal structure analysis of substituted hydroxy piperidine derivatives

Chapter IV: Crystal structure analysis of two oxazolidinone derivatives

Chapter V: Crystal structure analysis of *N*-sodio,*N*-bromo-*p*-toluene sulfonamide

Chapter I

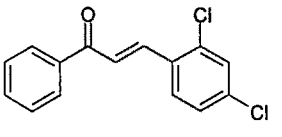
General Introduction

A general introduction about basic principles involved in X-ray crystallographic technique is given in chapter I.

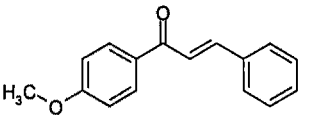
Chapter II

Crystal structure analysis of three different chalcones

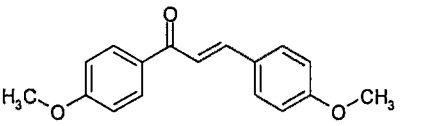
Chapter II deals with the X-ray crystal structure analysis of three different chalcones namely, 2′.4′-dichlorochalcone (1), 4-methoxychalcone (2) and 4,4′-dimethoxychalcone (3).



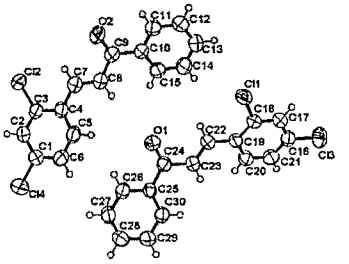
2',4'-Dichlorochalcone

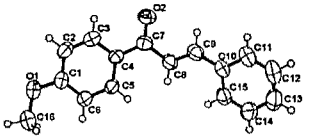


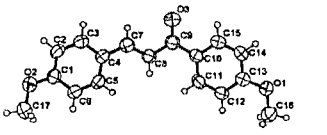
4-Methoxychalcone



4,4'-Dimethoxychalcone





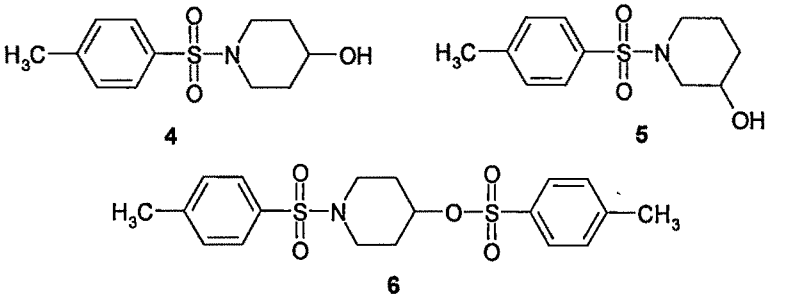


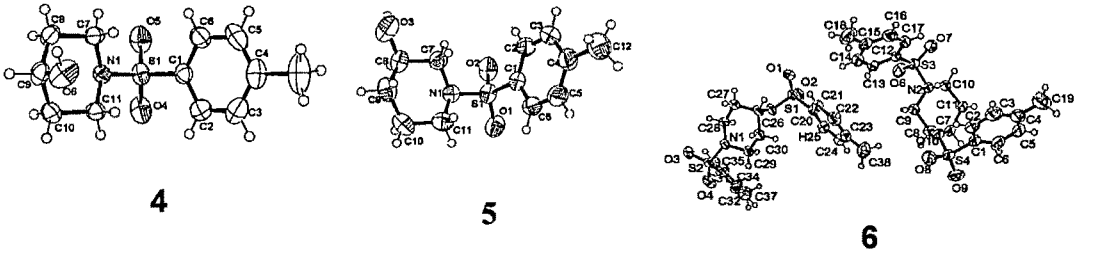
Chalcone 1 contains two formula units in its asymmetric unit whereas the other two chalcone contain only one formula unit. Packing in the crystal lattice is because of two kinds of interactions, namely, C–H···O and π-π – interactions. The dihedral angle between the rings in each case is different from the other. When both the benzene rings of a chalcone are symmetrically substituted by the same functional group, the compound orients itself in planner geometry, whereas compound having mono substitution have a bent structure having a higher dihedral angle between the plans of the phenyl rings. A detail structural analysis of the three chalcones is given in this chapter.

Chapter III

Crystal structure analysis of substituted hydroxy piperidine derivatives

Structural analysis of three substituted hydroxy piperidine derivatives is presented in chapter III. Structural variation was introduced by taking 3-hydroxy and 4-hydroxy piperidine as principal constituent.





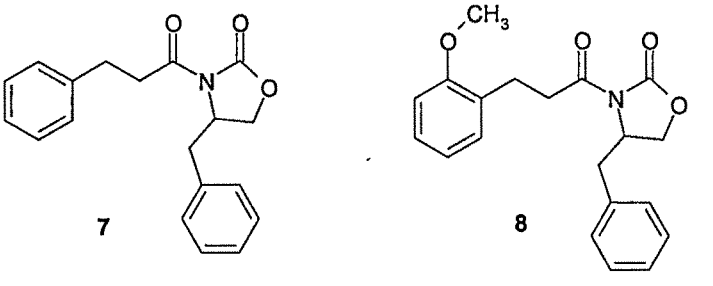
In first two cases (compound 4 & 5), a -*p*-toluene sulfonyl group is attached in the nitrogen atom of the skeletal molecule. The difference in the structural packing for these two compounds results from the position of the hydroxyl group in the piperidine skeleton. Hydrogen bonding in compound 4 results in the formation of catemer whereas compound 5 exists as a dimer due to intermolecular hydrogen bonding. The other molecule (6) has – p-toluene sulfonyl substitution on both nitrogen and oxygen atom of the skeletal

molecule. Compound 6 has two molecules in the asymmetric unit. The difference in orientation and packing parameters are analyzed for comparison.

Chapter IV

Crystal structure analysis of two oxazolidinone derivatives

Chapter IV deals with the X-ray crystal structure analysis of two different oxazolidinones (7 & 8). Two similar types of 4-benzyl-1,3-oxazolidin-2-one were taken for this study. Structural variation was included by introducing 3-phenylpropanoyl group at nitrogen atom of the oxazolidinone ring. In case of molecule 8, there is a methoxy group in phenyl ring of the 3-phenylpropanoyl group of the molecule.



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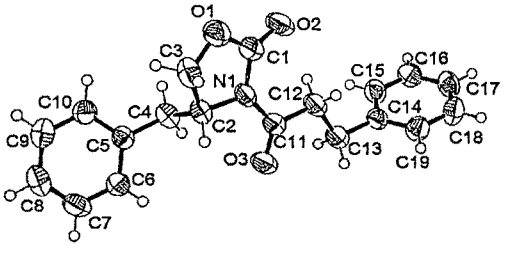
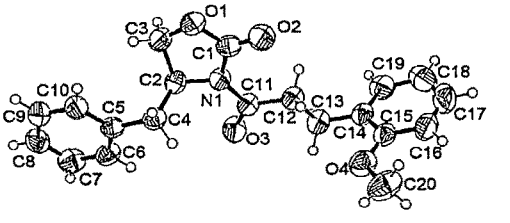




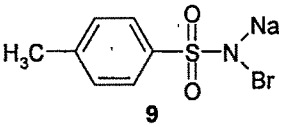
The impact of the substitution on crystal packing, bond length, bond angle etc. were analyzed by determining the single crystal x-ray structure. A

staircase type stacking is seen in case compound 8 due to short contact between hydrogen of methoxy group of one molecule and the same phenyl group of the other. Second interaction is seen between the other phenyl ring and C3-hydrogen of the oxazolidinone ring. These two interactions in oxazolidinone 8 creates a step type structure in the crystalline lattice. However, different orientations are seen in case of the other oxazolidinone (7). A detail discussion regarding all the interactions is presented in this chapter.

Chapter V

Crystal structure analysis of *N*-sodio,*N*-bromo-*p*-toluene sulfonamide

This chapter involves the crystal structure analysis of N-sodio-N-bromo-p-toluene sulfonamide.



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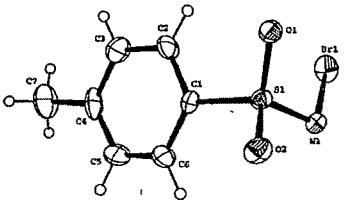

The compound was crystallized from water. Three waters of crystallization were seen in the crystal structure of the compound. Due to the present of these solvent of crystallization, sodium atom was detected far away from the main skeleton. A detail structural analysis of the compound is given in this chapter.