EXECUTIVE SUMMARY

The heterocyclic compounds are important class of organic compounds which play an important role in living organism whether they are naturally occurred or prepared on a commercial scale. Since the function of all compounds are depending on their three dimensional structure of the molecules, it becomes unavoidable to know their structures which are determined by X-Ray Diffraction Technique. In the present project, the three dimensional structures of two molecules have been studied which revealed that the stability of the crystallographic structures, even in the absence of strong interactive forces, are due to many important intra and intermolecular interactions in them. Many crystallographic parameters like bond lengths, bond angles, torsional angles are compared with those obtained using the DFT study using Gaussian 09 programme employing RHF and B3LYP methods and found to be in good agreement with the X-ray result. In addition to this, the dihedral angles, HOMO-LUMO energies, the dipole moments and Mulliken charges of both the molecules are also calculated. The Mulliken charge calculations show the binding affinity of an individual atom with the other atoms in the same or the other molecules. The HOMO-LUMO energy of both the molecules is showing total binding of all the atoms in the molecules. The results found here along with both ORTEP diagrams of the molecules, unit cell, packing diagrams, various molecular interactions which would be more useful to end-users working in areas like synthesis, characterization, structure-function relationship determination, testing of biological activity, drug designing, molecular docking studies and crystal engineering etc.