



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title: SYNTHESSES of HETEROCYCLES and AROYLHYDRAZONES USING ORGANIC NITRILES:  
MOLECCULAR STRUCTURES and SELF-ASSEMBLY of THEIR TRANSITION METAL COMPLEXES

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Thesis Submitted to the Department/ Center : CHEMISTRY

Date of completion of Thesis Viva-Voce Exam : 21/ 07/ 2017

Key words for description of Thesis Work : N-heterocycles, Nitrile, Aroylhydrazone, Weak interactions, Hydrogen bond, Halogen bond

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**SHORT ABSTRACT**

The thesis describes the syntheses of different *N*-heterocycles including 1,2-dihydroquinazolinones, 1, 2, 4-triazoles and aroylhydrazones using organic nitriles and hydrazides. The introduction chapter discusses self-assemblies of metal complexes driven by different non-covalent interactions. The reactions of organic nitriles with special emphasis on electrophilic nature of nitrile functional group have also been elaborated. The thesis contains four working chapters. The first chapter highlights tautomeric polymorphism induced by transition metal ions in a hydrazoneamide / hydrazone system. The occurrence of tautomeric polymorphism is depicted by crystal structure studies as well as computational methods including DFT and NBO analyses. The second chapter discusses supramolecular assemblies of Zn(II) complexes of *o*-halophenyl substituted hydrazides. Rare intramolecular halogen...oxygen and N-H...F interactions played an important role in determining the molecular conformations. The difference between the electronic nature of organic and inorganic halogens are also highlighted. The third chapter contains discussion on crystal structures and fluorescence property of Zn(II) / Cd (II) complexes of few 3-pyridyl-5-aryl substituted 1, 2, 4-triazoles. The detailed structural analyses of the complexes have been carried out using DFT and NBO analyses. In addition, fluorescence property of the ligands and the complexes has been studied by TD-DFT studies. The last chapter discusses an environment friendly synthetic protocol for efficient one-pot synthesis of a series of 2-aryl-3-imidamide-substituted 1, 2-dihydroquinazolin-4(1*H*)-ones. In all cases, the synthesized organic compounds as well as the metal complexes have been characterized by IR, NMR, UV-Vis, mass spectroscopy and single crystal XRD.