INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Synthesis and Characterization of Some Nitrogen Heterocycles and Their Coordination Complexes**

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SHORT ABSTRACT

In this thesis, new synthetic methods and the coordination behavior of some multidentate nitrogen heterocyclic ligands have been reported. Firstly, a new efficient route for the synthesis of three 2,4,-bis(2-pyridyl)-6-(pyridyl)pyrimidines, by employing respective acetylpyridine, sodium hydroxide and 2-cyanopyridine as well as coordination behavior of thus synthesized 2,4,6-tris(2-pyridyl)pyrimidine (**L1**) have been described. Structural characterization of complexes $[Ni(\mathbf{L1})(H_2O)_3](NO_3)_2\cdot 4H_2O$, $[Ni(\mathbf{L1})_2](NO_3)_2\cdot 2H_2O$ and $[Co(\mathbf{L1})_2](NO_3)_2\cdot 1.5H_2O$, revealed that **L1** behaves as a tridentate ligand with Ni(II) and Co(II) ions having a distorted octahedral geometry. Here, the mono- and bis-chelated Ni(II) complexes were isolated by controlling the stoichiometry of the reactants and only the bis-chelated Co(II) complex formed, irrespective of the reactant ratios. Results of DFT calculations performed on all the three 2,4,-bis(2-pyridyl)-6-(pyridyl)pyrimidines were reported.

Two new binuclear complexes of composition $[Ni_2(\mathbf{L4})_2(Cl)_2(H_2O)_2]Cl_2\cdot 12H_2O$ (**4**), and $[Ni_2(\mathbf{L4})_2(N_3)_3](N_3)\cdot 5H_2O$, (**5**) were isolated using *N*-(3-(pyridine-2-yl)imidazo[1,5-a]pyridine-1-yl)picolinimidamide (**L4**). Complex **4** was obtained by treating **L4** with $NiCl_2\cdot 6H_2O$, in 1:1 ratios while **5** was isolated by using two equivalent of NaN_3 additionally. Structural characterization revealed that the nickel center has pseudo-octahedral coordination geometry in both the complexes with **L4** acting as a bridging bis(bidentate) ligand. In **5**, out of the three coordinated azide ions, two are bound as a monodentate fashion at each metal center and the third one in μ-1,3 (end-to-end) bridging fashion.

A method for the construction of imidazo[5,1-*a*]isoquinoline nucleus from 1-isoquinolinemethylamine, various aldehydes and selenium dioxide have been described. Using this method several 3-substituted imidazo[5,1-*a*]isoquinolines were synthesized and characterized using spectroscopic and single crystal X-ray diffraction methods. The 1-isoquinolinemethylamine alone afforded 3-(1-isoquinolinyl)imidazo[5,1-*a*]isoquinoline (**IQ-1**) as the only product in absence of aldehydes. The ligand **IQ-1** is fluorescent in nature in most of the common solvents. This developed synthetic method could be applicable to wide variety of substrates and believe that imidazo[5,1-*a*]isoquinoline moiety can easily be incorporated in substrates having a aldehyde group provided other functionalities are stable towards selenium dioxide. These compounds with suitably substituted groups could find their utility in various fields. As a continuation, utility of this method for the synthesis of 3-substituted imidazo[1,5-*a*]pyridines has also been described along with the scope and limitations. In this procedure, by reacting 2-picolylamine and different aldehydes in presence of selenium dioxide as the oxidant, a series of 3-substituted imidazo[1,5- *a*]pyridines were isolated in good yields.