XRD and optical microscopic studies of Co(III) complexes containing 5-cyano-6-(4-pyridyl)-2-thiouracil, thymine and adenine bases

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Abstract. Multifunctional ligand 5-cyano-6-(4-pyridyl)-2-thiouracil (L) was prepared and allowed to react with trans [Co(en)₂Cl₂]⁺Cl⁻ resulting into [Co(en)₂LCl]⁵⁺·2Cl⁻ which upon further reaction with equimolar ratio of ligand [L] gave the complex [Co(en)₂L₂]³⁺·3Cl⁻. These metal complexes were then separately reacted with thymine and adenine bases. Complexes thus prepared after characterization by their elemental analysis, FAB mass and spectral (IR, ¹HNMR, UV-visible) data were studied for their powder X-ray diffraction and optical microscopic characteristics.

Keywords. Supramolecular; hydrogen-bonding; thymine; adenine.

1. Introduction

Self-assembly of molecules containing complementary hydrogen-bonding groups structurally related to those found in nucleotide bases are of current research interest in the area of supramolecular chemistry (Burrows et al 1995). Since non-covalent interactions play a special role in supramolecular chemistry (Lehn 1988, 1990), various supramolecular species have been synthesized by adopting the procedure of non-covalently assisted synthetic technique which primarily relies on the principle of stabilization provided by the interaction between recognition site incorporated within precursors (Muller-Dethlefs and Hobza 2000). In this context, the development of multifunctional ligand leading to the formation of the metal complexes capable of recognizing nucleotide bases by means of hydrogen-bonding have been considered quite promising. Metal based supramolecular complexes have also been used for inducing the formation of supramolecular mesophase and self-assembled nanostructure (Burrows et al 1995). Additionally, rhodium acetate dimer and related complexes have shown good antitumour activity (Clarke et al 1999), so cobalt being congener of rhodium was thought to be of great biological relevance.

Thus on the basis of above reports it was considered worthwhile to synthesize some Co(III) complexes bearing multifunctional ligand (L) scheme 1 and to attach them with adenine and thymine bases for their solid states structural studies using X-ray powder diffraction and optical microscopy techniques.

2. Experimental

5-Cyano-6-(4-pyridyl)-2-thiouracil (L) and trans [Co(en)₂Cl₂]²⁺Cl⁻ were prepared by the reported procedures of Upadhyay and Ram (1999) and Haworth and Elsen (1974) respectively.

Synthetic strategy reported by Mishra et al (2001) is shown in scheme 1. In this procedure, equimolar ratio of L and [Co(en)₂Cl₂]²⁺Cl⁻ were allowed to react in methanol (~10 ml) which gave the initial product identified as [Co(en)₂LCl]⁵⁺·2Cl⁻ which upon further reaction with equimolar ratio (1:1) of L in methanol containing few drops of DMSO gave another product identified as [Co(en)₂L₂]³⁺·3Cl⁻. These complexes were then further allowed to react separately with 1:1 and 1:2 molar ratio of thymine, however 1:3 molar ratio of the complexes [Co(en)₂LCl]⁵⁺·2Cl⁻ and adenine in similar condition yielded the complex [Co(en)₂LA₃]³⁺·3Cl⁻.

3. Results and discussion

Details of the instruments used for spectral (IR, UV-visible, ¹HNMR) studies have already been reported elsewhere (Mishra et al 2001), however, powder X-ray diffraction data were collected on PW1717 and optical microscopic study was done using Leitz optical microscope.

Synthetic strategy of the complexes as shown in scheme 1 indicated the different types of the complexes used in present study. The composition of the complexes has been assigned on the basis elemental analysis and FAB mass data (Mishra et al 2001). Complexes were found to decompose after heating above room temperature. The structure of the complexes, are however, supported by their spectroscopic data.

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Scheme 1. Synthetic strategy adopted for the preparation of the complexes.