Structural characterization of Cu-tpy-nucleotide ternary complexes

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Structural information on ternary metal-aromatic amine-nucleotide complexes is required to explicate the role of metal ions in proteinnucleotide interactions. In the present work, we report two ternary copper complexes i.e., Cu-tpy-GMP (A) and Cu-tpy-CMP (B) [tpy - 2, 2':6', 2" terpyridine, GMP – Guanosine 5'-monophosphate, CMP – Cytidine 5'-monophosphate], where both are 1D(linear) coordination polymers. They are crystallized in space groups $P2_1$(A), and $P2_12_12_1$(B) with habit block and rhombus, respectively. In polymer A, the monomer is hexanuclear and the metal ions are bridged by two 'O's of phosphate group, O6 and N7 of the heterocyclic base, giving distorted square pyramidal geometry to all the Cu centres. In tetranuclear monomeric unit of polymer B, the metal ions are bridged by one 'O' of the phosphate group, O2 and N3 of the heterocyclic base, giving two different geometries i.e., distorted octahedral to 2 Cu and distorted square pyramidal to 2 other Cu centres. Polymer A has 2 units of 5'-GMP and B has the same number of 5'-CMP units in the monomeric asymmetric unit. The spectator molecules are 6 perchlorates, 1 H_2O and 3MeOH in Polymer A, whereas Polymer B has 4 perchlorates and 16 H_2O. The point of polymeric chain extension is at O6 of one nucleotide and Cu ion in Polymer A, but in Polymer B it is at sugar ring OH of one nucleotide and Cu ion. Both the structures are stabilized by Hbonding and pi-pi stacking interactions.

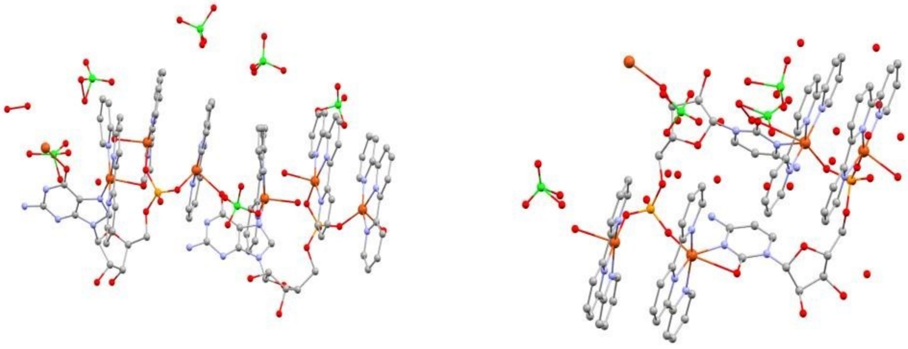

Fig 1. (left) Crystal structure of $[Cu_6(GMP)_2(tpy)_6]6ClO_4.H_2O.3MeOH$ (right), Crystal structure of -$[Cu_4(CMP)_2(tpy)_4]4ClO_4.16H_2O$

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Keywords: Metal-nucleotide interactions; ternary complex; coordination polymer; single crystal structure