Poster Presentation

Structural characterization of Mn - terpy - 5\'-IMP complex

<u>Dineshchakravarthy Senthurpandi</u>¹, Munirathinam Nethaji¹ ¹Inorganic and Physical Chemistry, Bangalore, India E-mail: dineshapothecary@gmail.com

Metal-nucleotide-aromatic amine ternary complexes would be a suitable candidate to unravel the interactions between metalprotein-nucleotide interactions. In the present work, we report two complexes of Mn + 5'-IMP + terpy, wherein one is 1D (linear)coordination polymer(A) and other is mononuclear complex(B). Both complexes have found in the same reaction vessel(concomitant polymorphs) and exhibit two different habits i.e., needle(A) and block(B). In polymer A, the metal ions are bridged by phosphate oxygens in two different manner i.e., doubly and terminal bridging. Doubly bridging and terminal bridging centers exhibit octahedral and square pyramidal geometry respectively. Mononuclear complex B is hexa-coordinated with octahedral geometry. In both complexes(A and B) three sites are occupied by the co-ligand terpy and other sites are occupied by phosphate oxygens in A and solvent water molecules in B. Both complexes are crystallised in chiral space group P21 with 18(A) and 11(B) spectator water molecules respectively. There are 2 units of 5'-IMP(binding to metal) in A and 4 units of 5'-IMP (Uncoordinated to metal) in B present in asymmetric unit. 5'-IMP adopts the most favoured conformational features like "anti" about the glycosyl bonds and ribose ring C3'- and C2'-endo conformation but the conformation about the C4'-C5' bond shows the rare form of gauche-trans(A) and trans-gauche(B). Both structures are stabilised by hydrogen-bonding and pi-pi stacking interactions.

Abbreviations Used:

5-IMP - 5'-Inosine MonoPhosphate
terpy - 2,2':6'-2"-terpyridine
complex A - [Mn(5'-IMP)tpy]2. 18H2O
complex B - [Mn(H2O)3 tpy]2. (5'-IMP)4. 11H2O
Sabat,M. et al.(1983). J. Am. Chem. Soc., 104, 976-980.
Zhou,P. et al.(2015). Coord. Chem. Rev., 292, 107-143.
Keywords: Metal-nucleotide coordination, Single crystal structure, complexes