ABSTRACT

A series of Copper(I) complexes with thiones of the general formula [CuₐL₅S₅Xₜ](H₂O)ₙ and [CuₐL₅S₅]Xₜ(H₂O)ₙ (where a = 1 - 6, b = 1 - 6, c = 0 - 6, d = 0 - 6, e = 0 - 1 and X = Cl, Br & I) were prepared and characterized by elemental, IR and NMR (¹H and ¹³C) spectroscopic methods. Crystal structures of nine complexes, [Cu(Metu)₄]Cl 1, [Cu₄(Dmtu)₄(S)(µ-S)Cl]Cl·(H₂O) 2, [Cu(DeTu)Cl]₃ 3, [Cu(Metu)₄]Br 4, [Cu(Dphtu)₂Br]H₂O 5, ([Cu(Metu)]I)₆ 6, [Cu(Mtu)₄]I 7, [Cu(DeTu)₂]I 8 and [Cu(Dbtu)₃]I0.6(H₂O) 9 were determined by single crystal x-ray diffraction. An upfield shift in the ≥C=S resonance of thiones in ¹³C-NMR and downfield shift in the N-H resonance in ¹H-NMR were consistent with the sulfur coordination of thiones to Copper(I). The crystal structures of 1, 4, 7, 8 and 9 show that they are monomeric having tetrahedral or distorted tetrahedral geometries at Copper(I) center. The crystal structure of 2 showed that it consists of a tetrameric cationic complex having terminal as well as doubly bridged Dmtu and S⁻ ligands. The complex has two kinds of coordination environments around four Copper atoms, a distorted tetrahedral and a trigonal planer. [Cu(DeTu)Cl]₃ is a trinuclear complex consisting of Cu₃S₃ six-membered ring possessing chair conformation. The geometry around each Cu center was nearly trigonal planar. In 5, the Cu(I) atom adopts a slightly distorted trigonal planar coordination. The X-ray studies of 6 showed that the complex was hexanuclear consisting of [Metu-Cu-I] units. The geometry around each Cu center was distorted tetrahedral. In all these complexes intra or intermolecular hydrogen bonding is present in 2-D or 3-D network. The antimicrobial activities of Copper(I) bromide complexes were evaluated by minimum inhibitory concentrations (MIC) and they showed wide range of activity against the test isolates.