

ABSTRACT

A series of Copper(I) complexes with thiones of the general formula $[Cu_aL_bS_cX_d](H_2O)_e$ and $[Cu_aL_bS_c]X_d.(H_2O)_e$ (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 ^{13}C) spectroscopic methods. Crystal structures of nine complexes, $[Cu(Metu)_4]Cl$ **1**, $[Cu_4(Dmtu)_4(S)(\mu-S)Cl]Cl.(H_2O)$ **2**, $[Cu(DeTu)Cl]_3$ **3**, $[Cu(Metu)_4]Br$ **4**, $[Cu(Dphtu)_2Br]H_2O$ **5**, $[[Cu(Metu)]I]_6$ **6**, $[Cu(Mtu)_4]I$ **7**, $[Cu(Detu)_3]I$ **8** and $[Cu(Dbtu)_3]I \cdot 0.6(H_2O)$ **9** were determined by single crystal x-ray diffraction. An upfield shift in the $>C=S$ resonance of thiones in ^{13}C -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 planar. $[Cu(Detu)Cl]_3$ is a trinuclear complex consisting of Cu_3S_3 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/and 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.