

Poster Presentation

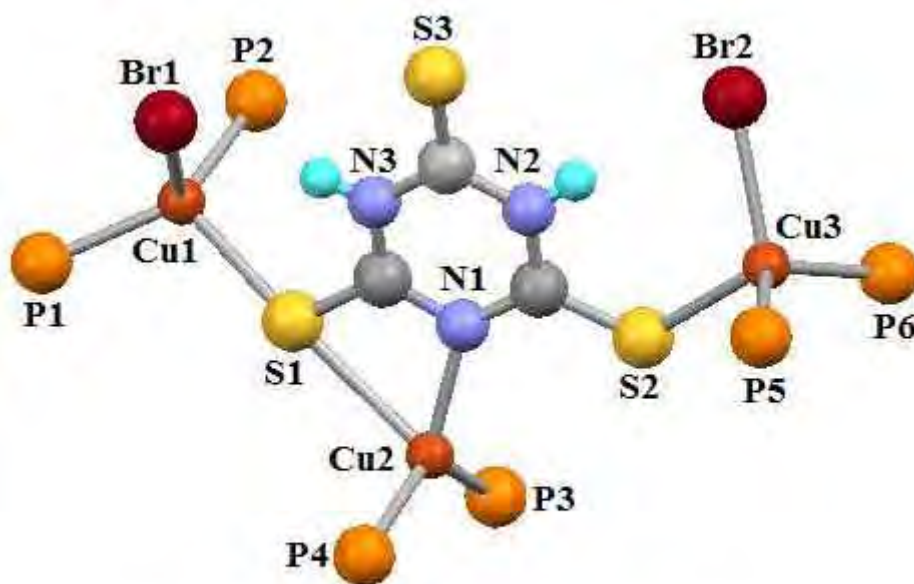
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Coordination variability of Copper(I) in multidonor heterocyclic thioamides.

T. Lobana¹, A. Kaur¹

¹Guru Nanak Dev University, Department of Chemistry, Amritsar, India

The chemistry of copper(I) with scarcely studied heterocyclic thioamides, namely, 2,4,6-trimercaptotriazine, purine-6-thione, 2,4-dithiouracil, 2-thiouracil and pyrimidine-2-thione is described. The interaction of 2,4,6-trimercaptotriazine (tmtH3) with [Cu(CH₃COO)(PPh₃)₂] gave rise to a pair of bond isomers: [Cu(κ¹N-tmtH₂)(PPh₃)₂] (6a), [Cu(κ¹N,κ¹S-tmtH₂)(PPh₃)₂] (6b) and with copper(I) bromide and PPh₃, it has formed a trinuclear complex, [Cu₃Br₂(κ¹N,κ¹S,κ²S-tmtH₂)(PPh₃)₆] (7) with anionic tmtH₂⁻ in these complexes. The 2,4-dithiouracil with copper halides (CuCl, CuBr) and PPh₃ yielded dinuclear complexes: [Cu₂(κ²Cl)(κ¹S,κ¹S-dtuch)(PPh₃)₄] (4) and [Cu₂(κ²Br)(κ¹S,κ¹S-dtuch)(PPh₃)₄] (5) with unusual eight membered metallacyclic rings. Pyrimidine-2-thione (pymSH) coordinated to CuI as N,S-chelated anion yielding mononuclear complex, [Cu(κ¹N,κ¹S-pymS)(PPh₃)₂] (1), while 2-thiouracil (tuch₂) with copper(I) chloride and PPh₃ yielded a tetrahedral complex, [CuCl(κ¹S-tuch₂)(PPh₃)₂] (3). Purine-6-thione (purSH₂) coordinated to CuI in two different modes yielding mono- and di-nuclear complexes, [Cu(κ¹N,κ¹S-purS)(PPh₃)₂].CH₃OH (2a) and [Cu₂(κ¹N,κ²S-purS)₂(PPh₃)₂] (2b). The existence of bond isomers (6a and 6b), synthesis of novel dinuclear (4 and 5) and rare trinuclear (7) complexes with unusual bonding patterns and uncommon chelation to CuI by pymS⁻ in 1 are the novel features of the present study. Complexes have shown intense emission bands in the visible region, λ_{max} 490 to 495 nm.



Skeletal view of 7 (phenyl rings omitted)

Keywords: 2,4,6-trimercaptotriazine, purine-6-thione