

MS30-P35 Novel coordination modes of 2,6-diacetylpyridine bis(*S*-methylisothiosemicarbazone)

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Thiosemicarbazones (tsc) are important class of *S*-donor ligands [1]. Their transition- and non-transition metal complexes are studied for many years, mainly due to wide variety of their biological activity. Their *S*-alkylated derivatives—*isothiosemicarbazones* (itsc)—are less studied, although they show interesting structural and electrochemical features. As a rule, *isothiosemicarbazones* are coordinated through the azomethine and *isothioamide* nitrogen atoms, which was also the case with pentadentate (*N*₅) 2,6-diacetylpyridine bis(*S*-methylisothiosemicarbazone) (*H*₂*L*) [2]. However, in [Ni(HL)I] [3], one thiosemicarbazide moiety of the tetradentate HL is coordinated in described way, whereas the other uses nitrogen N3 instead of azomethine nitrogen.

Here we present crystal structures of two copper complexes with this ligand of the formula [Cu(*H*₂*L*)Cl₂Py] (1) and [Cu^{II}₂(*H*₂*L*)₂Br₁₀Cu^I₆] (2) (Fig. 1), where novel coordination modes of this ligand are observed. In 1, ligand acts as *NNN* tridentate through the pyridine and both azomethine nitrogen atoms, so that both *isothioamide* nitrogen atoms remain uncoordinated. The distorted octahedral coordination polyhedron of Cu(II) is completed by coordination of the pyridine in equatorial, and chloride ligands in axial positions. Unsymmetrical coordination of *H*₂*L* is observed in 2: one itsc moiety is coordinated usually through the azomethine and *isothioamide* nitrogen atoms, whereas the other uses azomethine nitrogen to bind to the Cu(II) atom, and methylated sulfur to bind to the other Cu(I) atom. This complex has centrosymmetrical octanuclear structure, with Cu(II) atoms in square-pyramidal environment, and Cu(I) atoms in trigonal planar environment. It appears that coordination of terminal *isothioamide* groups can be avoided by introducing co-ligands with good donor capabilities; that coordination of alkylated sulfur atom is possible when acceptors are soft Pearson acids.

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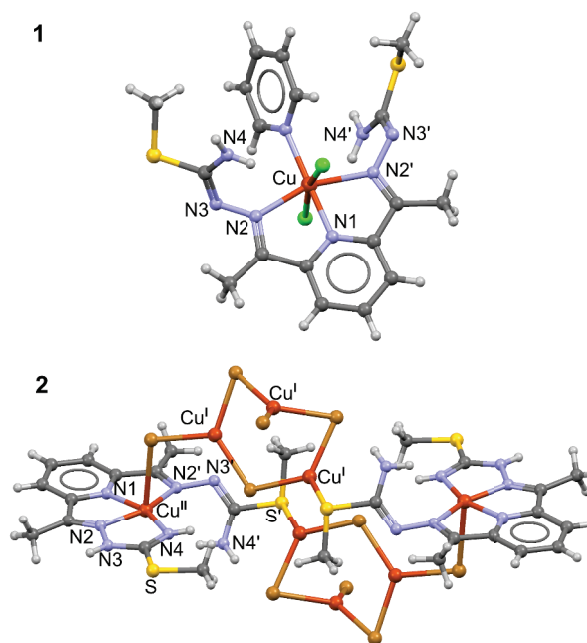


Figure 1. Molecular structures of the complexes Cu(*H*₂*L*)Cl₂Py (1) and [Cu^{II}₂(*H*₂*L*)₂Br₁₀Cu^I₆] (2)

Keywords: crystal structure, Copper(II) complex, *isothiosemicarbazone*, 2,6-diacetylpyridine