

**Title:** Reactivity of bulky tris(phenylpyrazolyl)methanesulfonate copper(I) complexes towards small unsaturated molecules

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**Abstract:** Reaction of the tris(3-phenylpyrazolyl)methane sulfonate species ( $\text{Tpms}(\text{Ph})\text{Li}$ ) with the copper(I) complex  $[\text{Cu}(\text{MeCN})(4)][\text{PF}_6]$  affords  $[\text{Cu}(\text{Tpms}(\text{Ph}))(\text{MeCN})]$  1. The latter, upon reaction with equimolar amounts of cyclohexyl-(CyNC) or 2,6-dimethylphenyl (XylNC) isocyanides, or excess CO, furnishes the corresponding Cu(I)complexes  $[\text{Cu}(\text{Tpms}(\text{Ph}))(\text{CNR})]$  (R = Cy 2, Xyl 3) or  $[\text{Cu}(\text{Tpms}(\text{Ph}))(\text{CO})]$  4. The ligated isocyanide in 2 or 3 (or the acetonitrile ligand in 1)is displaced by 3-iminoisoindolin-1-one to afford 5, the first copper(I) complex containing an 3-iminoisoindolin-1-one ligand. The ligated acetonitrile in 1 undergoes nucleophilic attack by methylamine to give the amidine complex  $[\text{Cu}(\text{Tpms}(\text{Ph}))\{\text{MeC}(\text{NH})\text{NHMe}\}]$  6, whereas only the starting materials were recovered from the attempted corresponding reactions of 2 and 3 with methylamine. Complexes 1 or 6 form the trinuclear hydroxo-copper(II)species  $[(\mu\text{-Cu})\{\text{Cu}(\mu\text{-OH})_2(\text{Tpms}(\text{Ph}))\}_2]$  7 upon air oxidation in moist methanol. In all the complexes the scorpionate ligand facially caps the metal in the N,N,O-coordination mode. (C) 2012 Elsevier B. V. All rights reserved.

**Author Keywords:** Tris(pyrazolyl)methanesulfonate Ligand; Copper Complexes; Isocyanide; Carbon Monoxide; 3-Iminoisoindolin-1-one

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