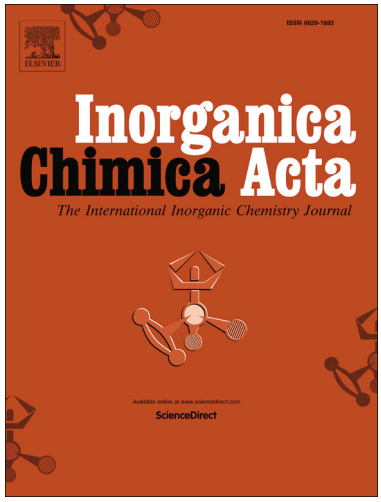

Research paper

Tris(3,5-dimethylpyralzoly)methane copper(I) complexes featuring one disubstituted cyanamide ligand

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Tris(3,5-dimethylpyralzoly)methane copper(I) complexes featuring one disubstituted cyanamide ligand

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Abstract. The complexes $[Cu\{HC(3,5\text{-}Me_2pz)_3\}(NCNR_2)][BF_4]$ (**1**–**8**; R_2 = Me_2 **1**, Et_2 **2**, C_5H_{10} **3**, C_4H_8O **4**, C_4H_8 **5**, $C_3H_6C_6H_4$ [$NC_3H_6C_6H_4$ is1,2,3,4-dihydroisoquinoline-2-yl] **6**, $(CH_2Ph)_2$ **7**, (Me)Ph **8**) were prepared by the reaction of $[Cu(NCMe)_4][BF_4]$ with $HC(3,5\text{-}Me_2pz)_3$ and $NCNR_2$ (CH_2Cl_2, 20–25 °C) and these species were characterized by C, H, N analyses, high resolution mass-spectrometry with electrospray ionization, ^1H, $^{13}C\{^1H\}$ NMR and FTIR spectroscopic techniques, molar conductivity measurements, thermogravimetry/differential thermal analysis, and also by single-crystal X-ray diffraction for **3**. The theoretical topological analysis of the electron density distribution (QTAIM method) together with the NBO analysis were applied to study the nature of Cu–N and Cu–C coordination bonds in $[Cu\{HC(3,5\text{-}Me_2pz)_3\}(NCNMe_2)]^+$, $[Cu\{HC(3,5\text{-}Me_2pz)_3\}(NCMe)]^+$, and $[Cu\{HC(3,5\text{-}Me_2pz)_3\}(CNMe)]^+$ model species. The nature of Cu–N coordination bonds in $[Cu\{HC(3,5\text{-}Me_2pz)_3\}(NCNMe_2)]^+$ and $[Cu\{HC(3,5\text{-}Me_2pz)_3\}(NCMe)]^+$ is very similar, whereas Cu–C contact in $[Cu(\{HC(3,5\text{-}Me_2pz)_3\}(CNMe)]^+$ is relatively more