

Accepted Manuscript

Research paper

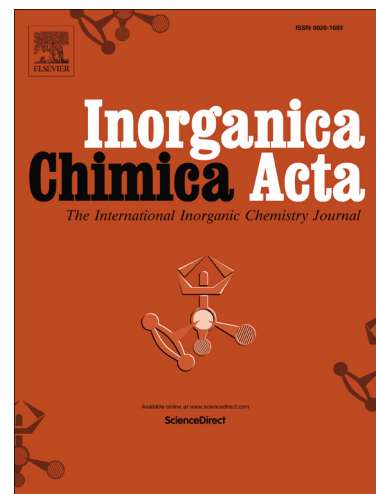
Tris(3,5-dimethylpyrazolyl)methane copper(I) complexes featuring one disubstituted cyanamide ligand

Anna A. Melekhova, Alexander S. Novikov, Alexey Yu. Dubovtsev, Andrey A. Zolotarev, Nadezhda A. Bokach

PII: S0020-1693(18)30609-1
DOI: <https://doi.org/10.1016/j.ica.2018.09.024>
Reference: ICA 18482

To appear in: *Inorganica Chimica Acta*

Received Date: 23 April 2018
Revised Date: 5 August 2018
Accepted Date: 8 September 2018



Please cite this article as: A.A. Melekhova, A.S. Novikov, A.Y. Dubovtsev, A.A. Zolotarev, N.A. Bokach, Tris(3,5-dimethylpyrazolyl)methane copper(I) complexes featuring one disubstituted cyanamide ligand, *Inorganica Chimica Acta* (2018), doi: <https://doi.org/10.1016/j.ica.2018.09.024>

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

Anna A. Melekhova, Alexander S. Novikov, Alexey Yu. Dubovtsev, Andrey A. Zolotarev,
Nadezhda A. Bokach*

Saint Petersburg State University, Universitetskaya Nab. 7/9, 199034 Saint Petersburg, Russian
Federation

Abstract. The complexes $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{NCNR}_2)][\text{BF}_4]$ (**1–8**; $\text{R}_2 = \text{Me}_2$ **1**, Et_2 **2**, C_5H_{10} **3**, $\text{C}_4\text{H}_8\text{O}$ **4**, C_4H_8 **5**, $\text{C}_3\text{H}_6\text{C}_6\text{H}_4$ [NC₃H₆C₆H₄ is 1,2,3,4-dihydroisoquinoline-2-yl] **6**, $(\text{CH}_2\text{Ph})_2$ **7**, $(\text{Me})\text{Ph}$ **8**) were prepared by the reaction of $[\text{Cu}(\text{NCMe})_4][\text{BF}_4]$ with $\text{HC}(3,5\text{-Me}_2\text{pz})_3$ 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 , $^{13}\text{C}\{^1\text{H}\}$ 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 $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{NCNMe}_2)]^+$, $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{NCMe})]^+$, and $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{CNMe})]^+$ model species. The nature of Cu–N coordination bonds in $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{NCNMe}_2)]^+$ and $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{NCMe})]^+$ is very similar, whereas Cu–C contact in $[\text{Cu}\{\text{HC}(3,5\text{-Me}_2\text{pz})_3\}(\text{CNMe})]^+$ is relatively more

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