

# Water Dissociation of a Dinuclear Bis(3,5-dimethylpyrazolyl)methane Copper(II) Complex: X-ray Diffraction Structure, Magnetic Properties, and Characteristic Absorption of the $(\text{CuN}_2\text{Cl}_2)_2$ Core

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A complex of formula  $[\{\text{CuCl}\{\text{H}_2\text{C}(3,5\text{-Me}_2\text{pz})\}\}_2(\mu\text{-Cl})_2]$  (1) is obtained and its structure is determined by single-crystal X-ray diffraction crystallography, revealing dinuclear character supporting a  $(\text{CuN}_2\text{Cl}_2)_2$  core. Compound 1 undergoes water dissociation that generates a change in the coordination sphere of the metals, yielding a mononuclear  $\text{CuII}$  complex of the formula  $[\text{CuCl}\{\text{H}_2\text{C}(3,5\text{-Me}_2\text{pz})_2\}_2]\text{Cl}\cdot 3\text{H}_2\text{O}$  (2), as supported by LeBail analysis and visible absorption spectroscopy. Interestingly, the optical features of 1 unravel characteristic patterns in the absorption spectrum, attributed solely to the formation of the  $(\text{CuN}_2\text{Cl}_2)_2$  core. The study of the magnetic properties of 1 reveals weak antiferromagnetic exchange coupling between the two  $\text{CuII}$  ions that is transmitted through the double-chloro bridge, which is supported by broken-symmetry DFT calculations. © 2018 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Antiferromagnetic coupling

Copper

$\text{Cu}_2\text{Cl}_2$  absorption

Density functional calculations

Water splitting