

High-field EPR and magnetic susceptibility studies on binuclear and tetranuclear copper trifluoroacetate complexes. X-ray structure determination of three tetranuclear quinoline adducts of copper(II) trifluoroacetate.

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Streszczenie

Magnetic properties and high-field EPR spectra of three previously unknown tetranuclear quinoline adducts of copper(II) trifluoroacetate were studied, and their X-ray structures were determined. Two green complexes containing a μ_4 -oxo bridge, $\text{Cu}_4\text{O}(\text{CF}_3\text{COO})_6(\text{quin})_4 \cdot (\text{C}_6\text{H}_5\text{CH}_3)_{0.6}$ (orthorhombic, *Pbca*, $a = 15.278(3)$, $b = 23.227(5)$, $c = 34.895(7)$ Å) and $\text{Cu}_4\text{O}(\text{CF}_3\text{COO})_6(\text{quin})_4 \cdot (\text{C}_6\text{H}_6)_{0.8}$ (monoclinic, *P2/c*, $a = 21.933(4)$, $b = 11.176(2)$, $c = 23.927(5)$ Å, $\beta = 97.41(3)^\circ$) are ferromagnetic, whereas the blue complex $[\text{Cu}_4(\text{OH})_2(\text{CF}_3\text{COO})_8(\text{quin})_2]^{2-}(\text{quinH}^+)_2$ (monoclinic, $a = 21.933(4)$, $b = 11.176(2)$, $c = 23.927(5)$ Å, $\beta = 97.41(3)^\circ$), formed in humid air from the solid dimeric $[\text{Cu}(\text{CF}_3\text{COO})_2 \cdot (\text{quin})]_2$, is antiferromagnetic, as is the tetranuclear blue product formed in humid air of the μ_4 -oxo tetramers. High-field EPR spectra allowed determination of the spin Hamiltonian parameters for the spin quintet state ($S = 2$) in the ferromagnetic complexes, which facilitated accurate interpretation of their magnetic susceptibility data. "Broken symmetry" DFT calculations were performed to estimate the exchange integrals in all three tetranuclear complexes, showing surprisingly good agreement with experimental results. Negative sign of the zero-field splitting parameter D in two binuclear complexes, $[\text{Cu}(\text{CF}_3\text{COO})_2 \cdot \text{CH}_3\text{CN}]_2$ and $[\text{Cu}(\text{CF}_3\text{COO})_2 \cdot (\text{quin})]_2$, was found from single-crystal high-field EPR spectra, confirming recent results for nonhalogenated dimeric copper carboxylates.

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