

Metal–metal interactions in trinuclear copper(II) complexes  $[\text{Cu}_3(\text{RCOO})_4(\text{H}_2\text{TEA})_2]$  and binuclear  $[\text{Cu}_2(\text{RCOO})_2(\text{H}_2\text{TEA})_2]$ . Syntheses and combined structural, magnetic, high-field electron paramagnetic resonance, and theoretical studies.

Autorzy

Andrew Ozarowski

Carmen J. Calzado

Raj Pal Sharma

Santosh Kumar

Julia Jezierska

Celestino Angeli

Federico Spizzo

Valeria Ferretti

Rok wydania

2015

Czasopismo

Inorganic Chemistry

Numer woluminu

54

Strony

11916-11934

DOI

10.1021/acs.inorgchem.5b02199

Kolekcja

Naukowa

Język

Angielski

Streszczenie

The trinuclear  $[\text{Cu}_3(\text{RCOO})_4(\text{H}_2\text{TEA})_2]$  copper(II) complexes, where  $\text{RCOO}^-$  = 2-furoate (**1**), 2-methoxybenzoate (**2**), and 3-methoxybenzoate (**3**, **4**), as well as dimeric species  $[\text{Cu}_2(\text{H}_2\text{TEA})_2(\text{RCOO})_2] \cdot 2\text{H}_2\text{O}$ , have been prepared by adding triethanolamine ( $\text{H}_3\text{TEA}$ ) at ambient conditions to hydrated  $\text{Cu}(\text{RCOO})_2$  salts. The newly synthesized complexes have been characterized by elemental analyses, spectroscopic techniques (IR and UV–visible), magnetic susceptibility, single crystal X-ray structure determination and theoretical calculations, using a Difference Dedicated Configuration Interaction approach for the evaluation of magnetic coupling constants. In **1** and **2**, the central copper atom lies on an inversion center, while in the polymorphs **3** and **4**, the three metal centers are crystallographically independent. The zero-field splitting parameters of the trimeric compounds,  $D$  and  $E$ , were derived from high-field, high-frequency electron paramagnetic resonance spectra at temperatures ranging from 3 to 290 K and were used for the interpretation of the magnetic data. It was found that the dominant interaction between the terminal and central Cu sites  $J_{12}$  is ferromagnetic in nature in all complexes, even though differences have been found between the symmetrical or quasi-symmetrical complexes **1–3** and non-symmetrical complex **4**, while the interaction between the terminal centers,  $J_{23}$ , is negligible.

Adres publiczny<http://dx.doi.org/10.1021/acs.inorgchem.5b02199>Strona internetowa wydawcy<https://www.acs.org/content/acs/en.html>

Typ publikacji

---

Artykuł

Plik został wygenerowany dnia 2026-05-06 06:47:51

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/VadtckL>.