

EPR-Einkristall-Untersuchungen an $(n\text{-Bu}_4\text{N})_2[\text{Cu}(\text{dmit})_2]$ im antiferromagnetisch gekoppelten Wirtsgitter $(n\text{-Bu}_4\text{N})_2[(\text{dmit})\text{Cu}(\text{tto})\text{Cu}(\text{dmit})]$: Ein Beitrag zur Aufklärung der sogenannten „paramagnetischen Verunreinigung“ im Wirtsgitter

A Single Crystal EPR Investigation on $(n\text{-Bu}_4\text{N})_2[\text{Cu}(\text{dmit})_2]$ in the Antiferromagnetically Coupled Host Lattice $(n\text{-Bu}_4\text{N})_2[(\text{dmit})\text{Cu}(\text{tto})\text{Cu}(\text{dmit})]$: A Contribution to the Nature of the So-called “Paramagnetic Impurities”

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Copper(II) Complexes, Single-Crystal EPR, DFT-MO Calculations

Single-crystal EPR investigations on the paramagnetic Cu^{II} impurity present in the binuclear antiferromagnetically coupled complex $(n\text{-Bu}_4\text{N})_2[(\text{dmit})\text{Cu}^{\text{II}}(\text{tto})\text{Cu}^{\text{II}}(\text{dmit})]$ (dmit = dimercaptoisotrithion, tto = tetrathiooxalate) identify the mononuclear $S = 1/2$ complex $[\text{Cu}^{\text{II}}(\text{dmit})_2]^{2-}$ as being responsible for the observed EPR spectra. The ^{63}Cu hyperfine structure data as well as the data obtained from density functional theory (DFT) and extended Hückel theory molecular orbital (EHT-MO) calculations were used to characterize the spin-density distribution of the copper complex.