

Structure and bonding in the hydrothermally synthesized copper(I) complex $\text{Cu}_4(\mu_2\text{-Cl})_4(\text{BIPY})_2$

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The title compound corresponds to a molecular product of the hydrothermal reaction of CuCl_2 , Zn, and BIPY (BIPY=2,2'-bipyridine) in the presence of phosphoric acid. The structure of the neutral complex $\text{Cu}_4(\mu_2\text{-Cl})_4(\text{BIPY})_2$ determined by means of X-ray diffraction consists of molecular units constructed around a Cu_4 parallelogram, with diagonally opposed tetrahedral and linear copper centers. DFT calculations provide a rationalization of the bonding in this molecule. © 2003 Elsevier Science B.V. All rights reserved.