A new copper(II) di-?2-carboxylato bridged dinuclear complex: [Cu(oda)phen]2 · 6H2O (oda = oxydiacetate, phen = phenanthroline)

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The oxydiacetate-bridged copper(II) complex [Cu(oda)(1,10-phen)] \cdot 3H2O (oda = oxydiacetate dianion, 1,10-phen = 1,10-phenanthroline) has been characterized. The complex is dinuclear and centrosymmetric with each copper atom residing in a CuN2O4 octahedral environment. The Cu(II) ions are bridged by two carboxylate-oxygen atoms in a strictly planar Cu2O2 core with a Cu-Cu distance of 3.417(2) Å. The magnetic susceptibility measurements (2-300 K) show weak ferromagnetic coupling between the copper ions with J = 3.3 cm-1. The results are compared with those of the homologous [Cu(tda)(1,10-phen)]2tda (tda = thiodiacetate dianion). A model proposed for the electronic structures of the complexes based on the density functional theory (DFT) satisfactorily accounts for the magnetic results. © 2007 Elsevier B.V. All rights reserved.