

Exchange interactions through π - π Stacking in the lamellar compound



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Structural, magnetic, and powder and single-crystal electron paramagnetic resonance (EPR) studies were performed on $[\{\text{Cu}(\text{bipy})(\text{en})\}\{\text{Cu}(\text{bipy})(\text{H}_2\text{O})\}\{\text{VO}_3\}_4]_n$ (bipy = 2,2'-bipyridine, en = ethylenediamine), which is a new copper-vanadium hybrid organic-inorganic compound containing CuII and VV centers. The oxovanadium units provide an anionic scaffolding to the structure, where two types of CuII coordination modes, octahedral (Cu1) and square pyramidal (Cu2), contribute to the magnetic properties. The crystal structure contains layers including Cu1 and Cu2 ions, separated by stacked arrangements of 2,2'-bipyridine molecules. Each type of CuII ion in these layers forms parallel spin chains described by exchange coupling parameters J_1 and J_2 for Cu1 and Cu2, respectively (exchange couplings defined as $\text{Hex}(i,j) = -J_{ij}S_iS_j$), which, for necessity, are assumed to be equal to J . These chains are coupled by much weaker Cu1-Cu2 exchange interactions J_3 connecting neighbor Cu1 and Cu2 ions within