1D magnetic interactions in Cuⁱⁱ oxovanadium phosphates (VPO), magnetic susceptibility, DFT, and single-crystal EPR

Venegas-Yazigi, Diego

Spodine, Evgenia

Saldias, Marianela

Vega, Andrés

Paredes-García, Verónica

Calvo, Rafael

Santana, Ricardo Costa De

 We report the crystal face indexing and molecular spatial orientation, magnetic properties, electron paramagnetic resonance (EPR) spectra, and density functional theory (DFT) calculations of two previously reported oxovanadium phosphates functionalized with Cu^{II} complexes, namely, [Cu(bipy)(VO<inf>2</inf>)(PO<inf>4</inf>)]<inf>n</inf> (1) and [{Cu(phen)}<inf>2</inf>(VO<inf>2</inf>(H<inf>2</inf>O)<inf>2</inf>)(H<inf>2</inf>PO4)<inf>2</inf > (PO<inf>4</inf>)]<inf>n</inf> (2), where bipy = 2,2?-bipyridine and phen = 1,10-phenanthroline, obtained by a new synthetic route allowing the growth of single crystals appropriate for the EPR measurements. Compounds 1 and 2 crystallize in the triclinic group P1¯and in the orthorhombic Pccn group, respectively, containing dinuclear copper units connected by two -O-P-O- bridges in 1 and by a single -O-P-O- bridge in 2, further connected through -O-P-O-V-O- bridges. We emphasize in our work the structural asp