Investigation of the Antiferromagnetic Coupling between Chromium(III) Ions Mediated by -O-Nb^{V}-O- Bridges

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Magnetic behavior of novel heterotetranuclear compound $[Cr_2(bpy)_4(\mu\text{-}O)_4Nb_2(C_2O_4)_4]\cdot 3H_2O$ (1; bpy = 2,2'-bipyridine) was investigated by magnetization measurements, EPR (X-, Q-band and and high-field) spectroscopy and DFT calculations. Results of $M(T)$ measurements show antiferromagnetic interaction of Cr^{III} ions through two diamagnetic bridges -O-Nb^{V}-O- with parameter of interaction $J = -12.77 cm^{-1}$ and ZFS parameter $D = -0.17 cm^{-1}$. The EPR spectra simulations and DFT calculations reveal the presence of a single-ion anisotropy that is close to being uniaxial, $D = -0.31 cm^{-1}$ and $E = 0.024 cm^{-1}$.