

MS24-O3 New antiferromagnets [CuX(py_z)₂](BF₄) with X = Cl and Br.

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The structures of new compound [CuX(py_z)₂](BF₄) with X = Cl⁻ and Br⁻ and py_z = pyrazine were determined by single crystal X-ray diffraction. These tetragonal compounds crystallize in space group *P4/nbm*. They are built from [Cu(py_z)₂]²⁺ layers which are connected by X⁻ ions along the *c*-axis. Charge is compensated by BF₄⁻ ions in the voids of the 3D coordination compound. The antiferromagnetic interactions between the Cu²⁺ ions are mainly two-dimensional (2D) located within the [Cu(py_z)₂]²⁺ layers. This results in a broad maximum of the magnetic susceptibility around 9 K. Towards lower temperature a kink is observed at 4 K which indicates long-range 3D magnetic order. The magnetic unit cell is doubled along the *c*-axis (*k* = 0,0,1/2) and the ordered magnetic moment amounts to $\mu_x = 0.76(8) \mu_B/\text{Cu}^{2+}$ at 1.5 K. The moments are antiferromagnetically coupled along the *b*- and *c*-axes. Long-range 3D magnetic order is observed below $T_N = 3.9(1)$ K. A fit of a 2D Heisenberg model to the magnetic susceptibility data results in $J_{||} = 9.6$ K.

Keywords: 2D antiferromagnet, copper, pyrazine, DMC, XRD, ESR

MS24-O4 Structural and magnetic properties of the low dimensional fluoride $\beta\text{-FeF}_3 \cdot 3\text{H}_2\text{O}$

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The anisotropy inherent in low-dimensional (1-D) solid-state compounds leads to a variety of interesting magnetic, electronic, and optical properties, with applications including single-chain magnets for data storage, (1) multiferroics for bifunctional materials (2,3) and nonlinear optical materials for second harmonic generation (4,5). Certain types of 1-D materials containing isolated chains exhibit nearly ideal magnetic properties, acting as experimental models for Ising and Heisenberg spin chains, furthering our understanding of magnetic exchange in highly correlated systems (6). One of the strategies for building these 1-D magnetic materials is to incorporate small one- or three-atom linkers between magnetic centers to facilitate exchange along the chains or networks (7,8). Many of these compounds are known, but very few have been created using iron centers, and most rely on relatively large bridging ligands to separate the magnetically coupled components within the structure. We report on the structural and magnetic properties of the low-dimensional fluoride $\beta\text{-FeF}_3 \cdot 3\text{H}_2\text{O}$ using SQUID magnetometry, X-ray and neutron diffraction. The structure consists of 1D-chains of corner-linked Fe[F(H₂O)₆] octahedra running parallel to [001] and isolated wafer molecules. A dense network of hydrogen bonds strongly connects the Fe-F chains. The structural formula is Fe[F_{0.5}(H₂O)_{0.5}]₄H₂O. This material exhibits a very pronounced 1D character with a very broad maximum around 150 K in the magnetic susceptibility. Below TN = 20 K, long range magnetic order appears characterized by $k = (0 \ 0 \ 1/2)$. From magnetic susceptibility, the intrachain magnetic coupling is estimated to be 18 K, while the interchain magnetic interaction is estimated to be about 3 K. We discuss this non negligible interchain coupling in light of the crystal structure of this material.

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