Synthesis and structural characterization of 2Dioxane-\(2\text{H}_2\text{O}\cdot\text{CuCl}_2\): Metal-organic compound with Heisenberg antiferromagnetic \(S=1\ 2\) chains\(^1\) TAO HONG, R. CUSTECEAN, B.C. SALES, B. ROESSLIE, D.K. SINGH, A. ZHELUDEV, Neutron Scattering Science Division, Oak Ridge National Laboratory — A novel organometallic compound 2Dioxane-\(2\text{H}_2\text{O}\cdot\text{CuCl}_2\) (CuDCl) has been synthesized and structurally characterized by X-ray crystallography. Magnetic susceptibility and zero-field inelastic neutron scattering have also been used to study its magnetic properties. It turns out that this material is a weakly coupled one-dimensional \(S=1/2\) Heisenberg antiferromagnetic chain system with chain direction along the crystallographic \(c\) axis and the nearest-neighbor intra-chain exchange constant \(J=0.85(4)\) meV. The next-nearest-neighbor inter-chain exchange constant \(J'\) is also estimated to be 0.05 meV. Unlike other compounds, the Cl concentration in CuDCl can be arbitrarily tuned by Br substitution. As a result, the strength of superexchange coupling \(J\) changes dramatically with different Br concentrations \(x\).

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