

Abstract Submitted
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**Synthesis and structural
characterization of 2Dioxane·2H₂O·CuCl₂: Metal-organic compound with
Heisenberg antiferromagnetic S= 1 2 chains¹** TAO HONG, R. CUSTEL-

CEAN, B.C. SALES, B. ROESSLIE, D.K. SINGH, A. ZHELUDEV, Neutron Scattering Science Division, Oak Ridge National Laboratory — A novel organometallic compound 2Dioxane·2H₂O·CuCl₂ (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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