Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Magnetic Ordering in the Frustrated Heisenberg Chain System $CuCl_2$ R. K. KREMER, M. G. BANKS, C. HOCH, A. SIMON, MPI fuer Festkoerperforschung, Heisnebergstarsse1, D-70569 Stuttgart, Germany, B. OULADDIAF, Institut Laue-Langevin, B.P. 156, 38043 Grenoble, France, J.-M. BROTO, H. RAKOTO, Lab. National des Champs Magnetiques Intenses, 143 Avenue de Rangueil, 31400 Toulouse, France, C. LEE, W.-H. WHANGBO, Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, U.S.A. — We report a detailed examination the magnetic structure of anhydrous cupric chloride $CuCl_2$ carried out by powder neutron diffraction, magnetic susceptibility and specific heat measurements as well as an evaluation of the spin exchange interactions by first principles density functional theory (DFT) calculations. Anhydrous $CuCl_2$ shows one dimensional antiferromagnetic behavior and long range antiferromagnetic ordering below a Néel temperature of 23.9 K. Neutron powder and single crystal diffraction reveal that, below 23.9 K, $CuCl_2$ undergoes a phase transition into an incommensurate magnetic structure (propagation vector (1,0.2257,0.5) with a spin-spiral propagating along *b* and the moments confined in the *bc* crystallographic plane. Our DFT calculations show that the spin-spiral results from competing ferromagnetic nearest neighbor and antiferromagnetic next-nearest neighbor spin-exchange interaction along the spin chains. Implications for possible multiferroic behavior of $CuCl_2$ are discussed.

Reinhard K. Kremer
MPI fuer Festkoerperforschung, Heisnebergstarsse1, D-70569 Stuttgart

Date submitted: 20 Nov 2009 Electronic form version 1.4