Abstract Submitted for the MAR17 Meeting of The American Physical Society

Coupled antiferromagnetic spin-1/2 chains in green dioptase, $\mathbf{Cu}_{6}[\mathbf{Si}_{6}\mathbf{O}_{18}] \cdot 6\mathbf{H}_{2}\mathbf{O}^{1}$ ANDREY PODLESNYAK, L. M. ANOVITZ, A. I. KOLESNIKOV, M. MATSUDA, T. R. PRISK, G. EHLERS, Oak Ridge National Laboratory, S. TOTH, Paul Scherrer Institute — Gem crystals of natural dioptase with colors ranging from emerald-green to bluish have delighted people since ancient times and still attract attention of mineral collectors around the globe. The crystal structure of green dioptase (space group $R\bar{3}$) consists of corrugated silicate rings Si_6O_{18} interconnected by Cu^{2+} ions. Oxygen atoms form axially-elongated octahedral of $CuO_4(H_2O)_2$. The magnetic ground state of green dioptase remains controversial. We report inelastic neutron scattering measurements of the magnetic excitations of green dioptase $Cu_6[Si_6O_{18}] \cdot 6H_2O$. The observed spectrum contains two magnetic modes and a prominent spin gap that is consistent with the ordered ground state of Cu moments coupled antiferromagnetically in spiral chains along the c axis and ferromagnetically in ab planes on the hexagonal cell. The data are in excellent agreement with a spin-1/2 Hamiltonian that includes AFM nearestneighbor intra-chain coupling $J_c = 10.6(1)$ meV, ferromagnetic inter-chain coupling $J_{ab} = -1.2(1)$ meV and exchange anisotropy $\Delta J_c = 0.14(1)$ meV. This appears compatible with reduced Nèel temperature, $T_{N=14.5}$ K $\ll J_c$, and can be explained by a presence of quantum spin fluctuations.

¹Research at Oak Ridge National Laboratory's Spallation Neutron Source and High Flux Isotope Reactor was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

> Andrey Podlesnyak Oak Ridge National Laboratory

Date submitted: 13 Nov 2016

Electronic form version 1.4