Structure determination of novel quantum spin liquid crystal at NSF's ChemMatCARS

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NSF's ChemMatCARS is a third-generation synchrotron user facility. It is located at Advanced Photon Source, Argonne National Laboratory, IL. NSF's ChemMatCARS is founded by National Science Foundation and operated by the University of Chicago. Advanced Crystallography Program at NSF's ChemMatCARS is dedicated to small-molecule crystallography. It provides high brilliance X-ray resources to explore novel structures of small molecular materials. Here we studied the structure of a new compound Cs14Cu4V16Cl8O48 crystallized from the quantum spin liquid system CsCl-V2O5-CuO. This system has potential applications such as quantum computing, and it's a candidate of high-temperature superconductive materials. Since the crystal is easy to deform and has large units, it will be benefited from the high-energy and high-resolution single crystal diffraction experiment performed at NSF's ChemMatCARS. A green single crystal Cs14Cu4V16Cl8O48 with size of 50×40×10 μm3 was mounted on the tip of fiber. Single crystal diffraction experiment was performed with Pilatus 1M (CdTe) detector at 30 keV. We succeeded in solving the crystal structure, which belongs to the monoclinic P2/n space group with lattice parameters of a=7.7669(3) Å, b=7.7610(3) Å, c=33.5028(12) Å, and β=96.608(1)°. Each V atom is coordinated with four oxygen atoms to form VO4 polyhedra, and each Cu is surrounded by five oxygen atoms. This quasi-two-dimensional structure shows interesting V4O12 rings, which are formed by VO4 polyhedra, and these rings are linked by CuO5.