Magnetic Structure of Antiferromagnetic Trimer System Cs2Cu4P4O14

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The complex spin system produced by ferromagnetic/antiferromagnetic coupled cluster (dimer, trimer, tetramer,⋯) attracts much attention because of a great variety of their fascinating quantum phenomena depending on various magnetic interactions between the clusters.

Cs2Cu3P4O14 is an S=1/2 antiferromagnetic trimer system described by the Hamiltonian $\mathcal{H}_{\mathrm{trimer}} = J\,(S_1 \cdot S_2 + S_2 \cdot S_3)$ with three-dimensional magnetic interaction between the trimers. Temperature dependence of magnetic susceptibility indicated that the antiferromagnetic trimer is formed at T_S=15K and there are antiferromagnetic interactions between trimers. Heat capacity showed the a long-range magnetic order at T_N=10K.

In these trimer systems, two different kinds of ground states are expected; one is the so-called trimer ground state, where total S=1/2 made of three trimer spins interact with each other, whereas the other is the so-called dimer-monomer ground state, where two out of three spins in a trimer form a non-magnetic singlet with one monomer (spin s=1/2) remaining as magnetic. One of the two ground states is selected by detailed balance of multiple inter-trimer interactions, and therefore similar situation is also expected for the interacting three-dimensional trimer system such as Cs2Cu3P4O14. These ground states cannot be distinguished from macroscopic measurement, since they have the same remaining spin 1/2. Moreover, the effective spin Seff = 1/2 (or monomer spin S = 1/2) remains at low temperatures, exhibiting a magnetic long-range magnetic order. If this ordered state is made of the trimer S=1/2 spins, then the nature of the ordered state, i.e. difference from the usual long-range order made of uniformly interacting spins, is also an intriguing issue to study. We, therefore, would like to perform elastic neutron scattering experiments to determine the magnetic structure.

The neutron powder diffraction experiment was performed on the powder diffractometer for high efficiency and high resolution measurements, HERMES. Figure 1 shows the powder pattern Cs2Cu3P4O14 at three temperatures. The pattern at 50 K was used for the nuclear scattering standard. At $|Q| = 0.71 \mathring{A}^{-1}$ with propagation vector of (1/2, 1, 0) or (0, 1, 1/2), the magnetic Bragg peak was observed at T=5K. From the inelastic neutron scattering experiments, we confirmed that the ground state of Cs2Cu3P4O14 is dimer-monomer state. So the magnetic structure is collinear magnetic structure with the magnetic moments of one monomer.

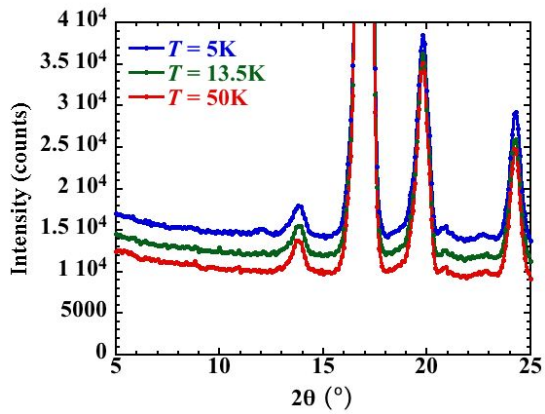

Fig. 1. The powder diffraction pattern of Cs2Cu3P4O14.