

Crystal and magnetic structures of 12L-perovskites Ba₄LnRu₃O₁₂ (Ln = Pr and Tb)

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Crystal structure and magnetic properties of new perovskites Ba₄LnRu₃O₁₂ (Ln = Pr and Tb) were investigated. The schematic crystal structure is illustrated in Fig. 1. In this structure, two kinds of the B site ions, Ru and M, occupy the face-sharing octahedral sites (Ru₃O₁₂ trimer) and the corner-sharing octahedral ones (LnO₆ octahedron), respectively. From the magnetic susceptibility and specific heat measurements, it is found that both compounds show magnetic anomalies at low temperatures.

In order to determine their crystal and magnetic structures, the neutron diffraction measurements were performed using the high efficiency and resolution powder diffractometer, HERMES, of Institute for Materials Research, Tohoku University, installed at the JRR-3M Reactor in JAEA (Tokai). The wavelength of a neutron incident is 1.82035 Å. The data were analyzed by the Rietveld technique.

As results of the Rietveld analyses of the neutron diffraction data at room temperature, the crystal structures of Ba₄LnRu₃O₁₂ (Ln = Pr and Tb) were determined. Both compounds have a perovskite-related structure which consists of the 12-layer (12L) of the BaO₃ sheets. The Ba₄TbRu₃O₁₂ has a hexagonal unit cell with space group R-3/m; the cell parameters are a = 5.8314 Å and c = 29.0212 Å. On the other hand, the crystal structure of the Ba₄PrRu₃O₁₂ is monoclinically (space group C2/m) distorted with a = 10.157 Å, b = 5.869 Å, c = 29.315 Å, and beta = 90.910 degree.

The neutron diffraction measurements at low temperatures were performed for Ba₄TbRu₃O₁₂. In the diffraction profile at 2.5 K, some additional reflection peaks were found at lower angles, which were

not observed at room temperature. These peaks can be indexed using a propagation vector $k = (0, 0, 3/2)$. The magnetic structure was by the Rietveld analysis of the data. In this magnetic structure, the magnetic moments of Ru ions in the Ru₃O₁₂ trimer order antiferromagnetically (up-down-up). The ferrimagnetic moments remaining in the Ru₃O₁₂ trimers and magnetic moments of Tb ions order antiferromagnetically along the c-axis.