# Magnetic order of Kitaev model candidate compound $Ru(Br,I)_3$

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Kitaev model has attracted interest since its ground state is exactly solvable and becomes a quantum spin liquid state [1]. According to a theoretical proposal [2], Kitaev interactions, bond-dependent Ising interactions, can be microscopically induced by orbital exchange mechanisms between pseudospins-1/2 from a $d^5$ electron configuration. $RuCl_3$ is known as a candidate Kitaev model compound with dominant Kitaev interactions (such as ref. [3]). We find that $RuBr_3$[4] and $RuI_3$ [5], where $Ru^{3+}$ ions form layered honeycomb structure as $RuCl_3$, are good model compounds to investigate anion substitution effect on Kitaev interactions. Magnetization measurements reveal that antiferromagnetic interactions are dominant in $RuBr_3$ ($\theta_W$ ~ -58 K), while ferromagnetic Kitaev interactions are dominant in RuCl3 ($\theta_W$ ~ +19 K). In addition, the magnetic susceptibility becomes almost independent on the temperature in $RuI_3$. The largely different physical properties among $RuCl_3$, $RuBr_3$, and $RuI_3$ should be due to the largely different anion contributions to the bonding between Ru atoms.

To investigate the anion substitution effect on the Kitaev interactions, systematic magnetization measurements have been performed on $Ru(Br_{1-x}I_x)_3$ [6]. The non-monotonic composition dependence of the magnetic susceptibility was observed around $x$ = 0.3, supporting the change in the magnetic structure at $x > 0.3$. To confirm this expectation, we have searched for magnetic reflections in $Ru(Br_{0.4}I_{0.6})_3$ by powder neutron diffraction experiments by using a general-purpose triple axis spectrometer GPTAS in JRR-3. The spectrometer was operated in a three-axis mode with a wavelength of 2.359 Å by using pyrolytic graphite (002) reflections and a collimation of 40’-40’-40’-80’.

First, we have performed $\theta$-$2\theta$ scans to look for magnetic reflections, and find that the magnetic reflections appear at the $2\theta$ angle of

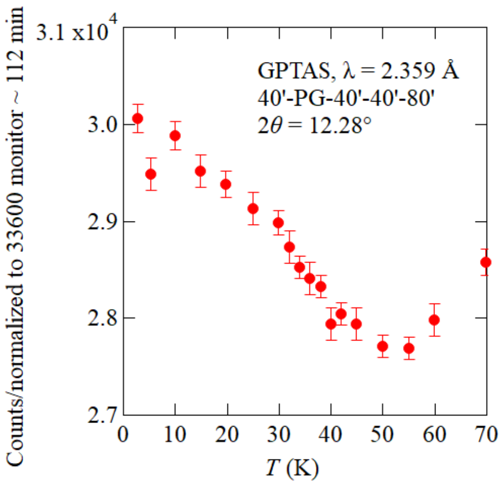


Figure Temperature dependence of the magnetic reflection.

12.3°, which is different from 13.9° expected from the (0, 1/2, 1) reflection observed in $RuBr_3$. Figure shows the temperature dependence of the observed magnetic reflection. The peak disappears above 40 K, which is close to the transition temperature of ~36 K $Ru(Br_{0.4}I_{0.6})_3$. We found that this reflection can be indexed as (1/2, 0, 1/2), suggesting that the stacking sequence of the magnetic moments is altered along the $c$-axis in $Ru(Br_{1-x}I_x)_3$. We have also performed the powder neutron diffraction experiments on iMATERIA diffractometer. The arrangement of magnetic moments within each honeycomb plane will be revealed by detailed magnetic structure analysis on the data collected by iMATERIA diffractometer.

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