MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2015A0162 実験課題名 Title of experiment Weak Ferromagnetism of Honeycomb Lattice with *S*=3/2 for Co^{2+} Spins 実験責任者名 Name of principal investigator Yasui, Yukio 所属 Affiliation Meiji University	装置責任者 Name of responsible person Ishigaki, Toru 装置名 Name of Instrument/（BL No.） iMATERIA 実施日 Date of Experiment 2016/5/7 ～ 2016/5/8

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

$Li_3Co_2SbO_6$

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

We investigate the crystal structure and the magnetic structure of spin system $Li_3Co_2SbO_6$, where the system has Co^{2+} ions with spin S=3/2 and is Mott insulator. Similar compound $Na_3Co_2SbO_6$ forms the Co^{2+} honneycomb lattice, which is composed of Co_2SbO_6 layers and Na layers, and Co_2SbO_6 layers consist of edge-sharing CoO_6 and SbO_6 octahedra (space group $C2/m$: monoclinic). Because the ionic radius of Li^+ ion is significantly smaller than that of Na^+ ion, the lattice constant and the Co^{2+}-Co^{2+} distance of $Li_3Co_2SbO_6$ are shrunk, and interactions between Co^{2+} spins of $Li_3Co_2SbO_6$ are expected to be significantly different from that of $Na_3Co_2SbO_6$. There is not a report about detailed crystal structure of $Li_3Co_2SbO_6$. We have prepared polycrystalline sample of $Li_3Co_2SbO_6$, and carried out measurements of the magnetic susceptibility, and specific heat. Although $Na_3Co_2SbO_6$ exhibits the antiferromagnetic transition at T_N =7 K, the behavior of magnetic susceptibility and specific heat of $Li_3Co_2SbO_6$ indicates that the spin system exhibits the ferromagnetic transition at T_C=113K. Note that the magnetic transition of $Li_3Co_2SbO_6$ corresponds to a weak ferromagnetic or canted antiferromagnetic transition according to the behavior of magnetization curves below T_C. It is interesting that the transition

2. 実験方法及び結果（つづき） Experimental method and results (continued)

temperature rises to 16 times by Li-substitution on Na sites. In understanding this result, determination of the magnetic structure and the crystal structure of $Li_3Co_2SbO_6$ brings important information. We investigated to the magnetic structure and the crystal structure of $Li_3Co_2SbO_6$ by the neutron powder diffraction measurements using the iMATERIA at MLF.

Examples of neutron diffraction profiles of $Li_3Co_2SbO_6$ taken at various temperatures are shown in Figs. 1(a)-1(c). We can see the growth of intensities of the magnetic reflections. As a result of preliminary crystal structure analysis, we obtained the crystal structure of $Li_3Co_2SbO_6$ shown in Fig. 2(a), which is similar to that of $Na_3Ca_2TaO_6$ called as *Fddd* structure [1]. It is not honneycomb lattice. Because there is not a report about magnetic behavior of the *Fddd* structure compounds such as $Li_3Co_2TaO_6$, we interest in the magnetic behavior and magnetic structure of $Li_3Co_2SbO_6$.

Figure 2(b) shows the magnetic ordering pattern which can reproduce the observed magnetic scattering intensities of $Li_3Co_2SbO_6$ taken at 4 K. The Co^{2+}-moments align parallel to the *b* axis (collinear), which is consistent with the magnetization behavior of magnetic-field aligned samples. The crystal structure of $Li_3Co_2SbO_6$ has the corner-sharing CoO_6 octahedra and the edge-sharing CoO_6 octahedra as shown in Fig. 2(a). The obtained magnetic structure indicates that the Co^{2+}-moments of the corner-sharing CoO_6 octahedra align antiferromagnetic and those of the edge-sharing CoO_6 octahedra align ferromagnetic. However, because we are not satisfied with fitting, we are going to continue analyzing neutron diffraction data.

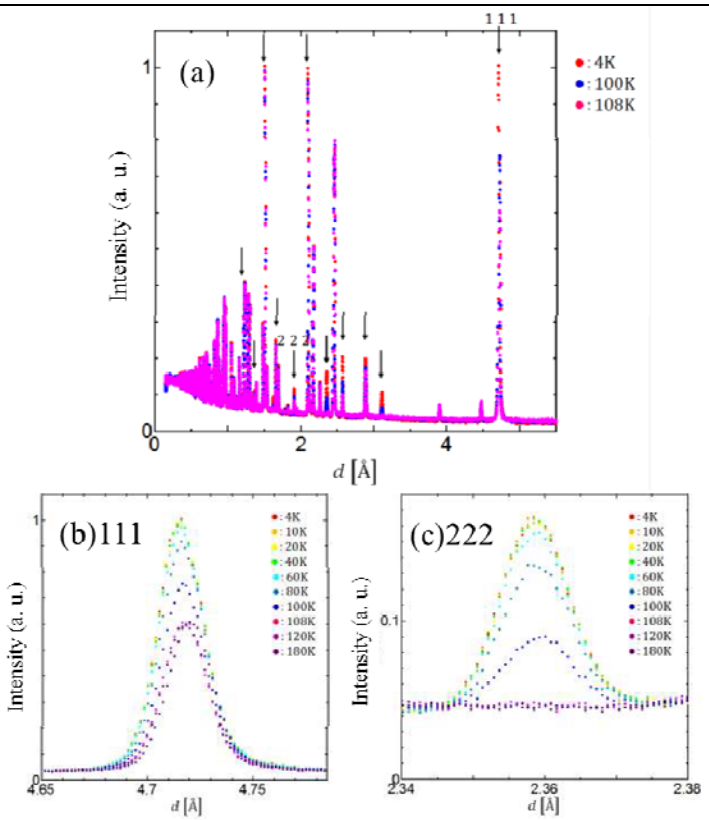

Fig. 1: (a) Profiles of the neutron diffraction of $Li_3Co_2SbO_6$ taken at various temperatures. Arrows indicate the magnetic reflections. (b-c) Profiles of the neutron diffraction of $Li_3Co_2SbO_6$ plot on the enlarged scale.

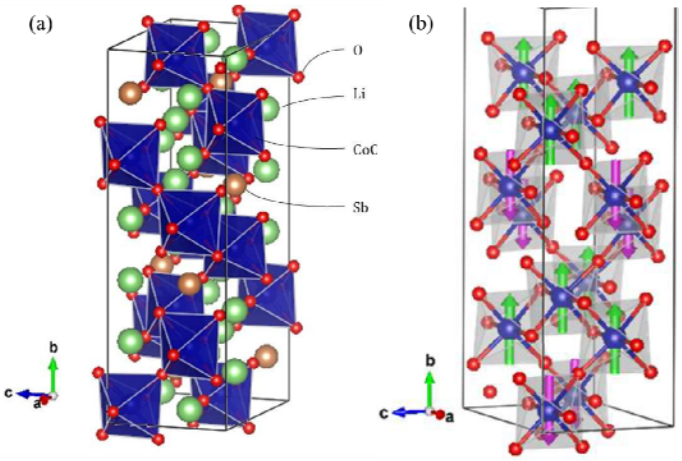

Fig. 2: (a) Schematic figure of the determined crystal structure of $Li_3Co_2SbO_6$ which is similar to that of $Na_3Ca_2TaO_6$ called as *Fddd* structure [1]. (b) The magnetic ordering pattern which can reproduce the observed magnetic diffraction intensities of $Li_3Co_2SbO_6$ taken at 4 K.

[1] H.Yamane *et al.*, Acta Cryst. C **56** (2000) 1177.