MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2017A0143 実験課題名 Title of experiment Detailed structure analysis on perfect kagome compound $Li_2Cr_3SbO_8$ 実験責任者名 Name of principal investigator Kazuki Iida 所属 Affiliation CROSS	装置責任者 Name of responsible person Takashi Kamiyama 装置名 Name of Instrument/(BL No.) SuperHRPD (BL08) 実施日 Date of Experiment 2017/4/14 – 2017/4/18

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.

Polycrystalline Li2Cr3SbO8.

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.

Macroscopic ground-state degeneracy in highly frustrated magnets can lead to unconventional magnetic behaviors such as the classical/quantum spin liquid. Recently, we succeeded in making a new kagome compound $Li_2Cr_3SbO_8$, and $Li_2Cr_3SbO_8$ undergoes so-called $\sqrt{3} \times \sqrt{3}$ long-range magnetic order below T_N = 4.5 K. We already performed neutron diffraction measurements, but the resolution was not sufficient to determine the detailed "crystal" structure. Since the detailed crystal structure is important to discuss the properties of frustrated systems, investigation on the detailed crystal structure of $Li_2Cr_3SbO_8$ using SuperHRPD is purpose of this experiment.

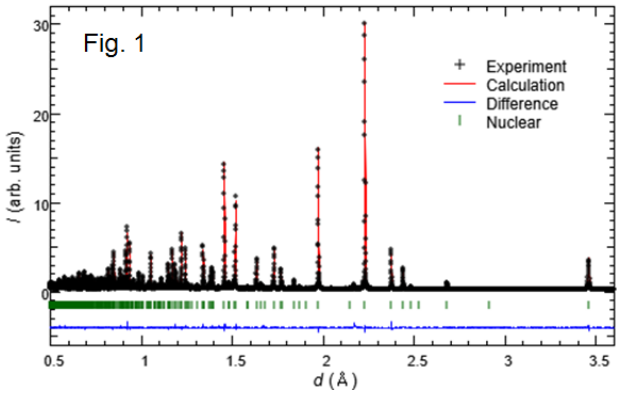
We prepared 2.2 g high-quality polycrystalline $Li_2Cr_3SbO_8$ sample for the neutron diffraction measurements. The sample was put into the vanadium can, which was attached to the bottom loading cryostat. The measurements were performed at T = 4.7, 7, 10, 20, 60, 100, 150, 200, and 300 K. We mainly used the data obtained by the backscattering (BS) bank. Data was analyzed by the ZRietveld software.

Figure 1 shows the neutron diffraction result from the BS bank at 4.7 K together with the Rietveld refinement results. The refined crystal parameters are summarized at Table I, and the obtained crystal structure is described in

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

Fig. 2. The results show that the kagome lattice in $Li_2Cr_3SbO_8$ is not a perfect kagome but slightly distorted. The difference between the two different nearest neighbor distances is about 5.02%. Interestingly, the crystal structure is a so-called breathing kagome, where the small and large triangles align alternatively. Furthermore, the weathervane mode which is the most interesting features of $\sqrt{3} \times \sqrt{3}$ kagome structures still exists in the breathing kagome structure realized in $Li_2Cr_3SbO_8$. Therefore, although the kagome lattice in $Li_2Cr_3SbO_8$ is slightly distorted, $Li_2Cr_3SbO_8$ still has the most important feature originating from the geometrical frustration.

Finally, we appreciate the local contacts at SuperHRPD for their kindness support.



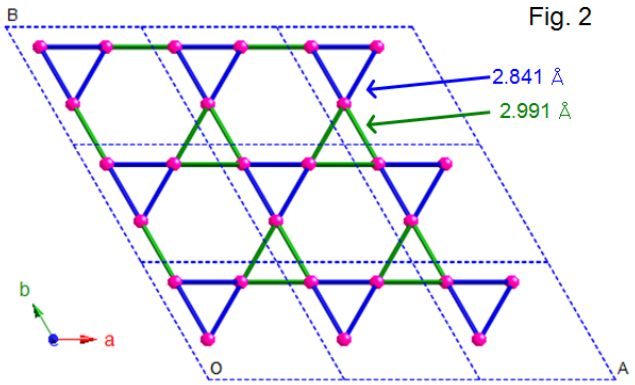


Figure 1. The neutron powder diffraction pattern at 4.7 K in $Li_2Cr_3SbO_8$ obtained from the BS bank at SuperHRPD together with the Rietveld refinement results using ZRietveld. Figure 2. Obtained crystal structure of $Li_2Cr_3SbO_8$. Only the Cr site is shown.

Atom	Occupancy	*x*	*y*	*z*	B_{iso} (Å^2)
Cr	1	0.17095(7)	0.82905(7)	0.2478(7)	0.377539
Li1	1	0.33333	0.66667	0.93649(3)	0.734892
Li2	1	0	0	0.52546(3)	0.963648
O1	1	0	0	0.34047(10)	0.397386
O2	1	0.33333	0.66667	0.13955(9)	0.498587
O3	1	0.48167(4)	0.51833(4)	0.37779(6)	0.450468
O4	1	0.16604(10)	0.83396(10)	0.62995(7)	0.436658
Sb	1	0.33333	0.66667	0.5228(10)	0.326869

Table I. The refined crystal structure parameters at 4.7 K in $Li_2Cr_3SbO_8$. We assumed the $P6_3mc$ space group. The refined crystal parameters are $a = b = 5.83269(1)$ Å and $c = 9.504188(3)$ Å.