実験報告書様式（一般利用課題・成果公開利用）

（ ※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。 ）

MLF Experimental Report	提出日 Date of Report 2017/1/4
課題番号 Project No. 2017A0070 実験課題名 Title of experiment Probing magnetic ground state in Zn-Ln-Zn single ion magnets 実験責任者名 Name of principal investigator Maiko Kofu 所属 Affiliation J-PARC Center, JAEA	装置責任者 Name of responsible person Jun-ichi Suzuki 装置名 Name of Instrument/(BL No.) TAIKAN (BL15) 実施日 Date of Experiment 2017/5/13 – 2017/5/15 2017/6/8 – 2017/6/9

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.

Nd complex ($C_{40}D_{39}NdN_8O_{11}S_2Zn_2$)

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.

A single-molecule magnet (SMM) is a metal complex that behaves as an individual nanomagnet. Each molecule, containing several metal centers with unpaired electrons, possesses a giant resultant spin. Given that the giant spin exhibits easy-axis anisotropy ($D < 0$), the magnetization reversal between the ground states with $S_z = \pm S$ is hindered by the potential barrier of DS_z^2. The barrier yields a slow relaxation of the magnetization reversal that is characteristic of SMMs. Early SMM researches have focused on the complexes containing multiple transition metal atoms. During the past decade, lanthanide SMMs have received much attention as promising materials with high blocking temperature, i.e. stable SMMs [1]. Owing to a large contribution of angular momentum, lanthanide complexes can become SMMs containing only one or two magnetic ions. However, the relaxation behaviors of lanthanide SMMs are rather complicated and several types of mechanisms are discussed, for example Raman, direct and quantum tunneling processes. Clarifying the mechanism of magnetic relaxation is a key issue in lanthanide SMMs and assists formulation of designing strategies for engineering long-living SMMs.

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

We have first studied a Tb–Cu dinuclear SMM by means of inelastic (INS) and quasielastic neutron scattering (QENS) [2,3]. We are now investigating trinuclear Zn–Ln–Zn complexes (Ln = Ce, Pr, Nd). The system has only one magnetic center in a molecule, which can be regarded as "single ion magnet". Interestingly, the complexes with Kramers ion (Ce : J=5/2 and Nd : J=9/2) exhibit the SMM behavior while that with non-Kramers ion (Pr : J=4) does not [4]. It is noted that both Ce and Nd complexes are field-induced SMMs; magnetic relaxation is observed in ac susceptibility measurements under dc magnetic field as small as 500G (see Fig. 1). This indicates that the hybridization between the ground states (in ideal case, $J_z = \pm J$) is changed by applying a magnetic field.

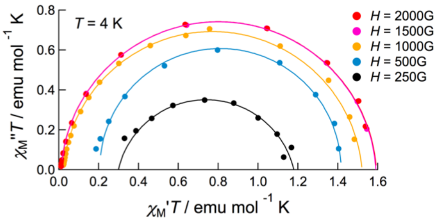

Fig. 1: Cole-Cole plots for the Nd complex.

The purpose of this experiment was to probe magnetic elastic scattering to gain information regarding the magnetic ground state of this system. The Zn–Ln–Zn complexes are purely zero-dimensional and do not exhibit any peak in Q. Therefore, a measurement utilizing polarized neutron is necessary. However, we have recognized on the day of the experiment that a xyz polarization analysis was currently impossible at TAIKAN. We have changed our experimental plan and decided to measure the field dependence of $S(Q)$ using unpolarized beam. Figure 2 shows the static structure factors $S(Q)$ of the Nd complex under H = 0G and 1500G and the difference between them. Unfortunately, field-dependent signals were not detected. After this experiment, we have made a xyz polarization analysis using a spin-echo instrument at NIST and found that the fraction of elastic magnetic scattering is 1.1 ± 0.3 %. The magnetic scattering is too weak to observe the effect of magnetic field on the intensity.

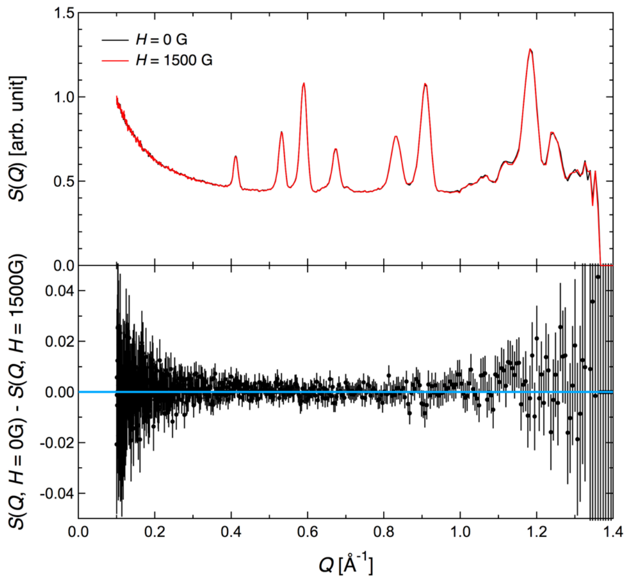

Fig. 2: (top) $S(Q)$ of Nd complex under magnetic field of H = 0G and 1500G. (bottom) Difference in $S(Q)$ between H = 0G and 1500G.

[1] R. Sessoli et al., Coordin. Chem. Rev., 253, 2328 (2013). [2] M. Kofu et al., Phys. Rev. B, 88, 064405 (2013). [3] M. Kofu et al., Chem. Phys., 427, 147–152 (2013).