MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2012B0251 実験課題名 Title of experiment Magnetic Excitations in 4f - 2p Orbital Exchange Coupled Molecular Nanomagnets 実験責任者名 Name of principal investigator Michael L. Baker 所属 Affiliation Institute for Materials Research, Tohoku University.	装置責任者 Name of responsible person Nakajima Kenji and Seiko Kawamura 装置名 Name of Instrument/（BL No.） BL14 実施日 Date of Experiment March 19 – March 27 2013

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 samples of chemical formula:

Tb(2pyNO) – $C_{24}H_4D_{12}F_{18}N_2O_7Tb$

Tb(DNN2) – $C_{29}H_{29}F_{18}N_4O_{10}Tb$

Samples were loaded into aluminum cells of hollow cylindrical geometry.

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.

Setup Measurements were performed in a closed cycle cryostat sample environment enabling a sample base temperature of 3.8 K. Various multi-E_i configurations were used to access different dynamical ranges.

Tb(2pyNO) We were successfully able to measure the Tb – radical spin flip excitation which characterizes the Tb radical exchange interaction. Figure 1 shows an Ei=7.743 meV setting spectrum integrated over Q. The magnetic excitation is found at 3.7 meV. Initial analysis suggests a flat Q-dependence for this excitation; however Vanadium correction is required before a final conclusion can be made. It is noted that spurious peaks are encountered within an energy range from 4.5 to 6.25 eV with the E_i = 7.743 meV neutron setting. The spurious nature of these features are clearly distinguished from the magnetic excitation as they shift in energy depending on the specific dynamical range chosen and exhibit no temperature dependence.

Tb(DNN2) Two excitations emanating from the ground state were probed with E_i settings of 3.13 and 5.18 meV. Figure 2 shows the E_i = 3.13 meV results, the intensity of the excitations are greater at 3.8 K than at 10 K confirming that the transitions come from the ground state. A background increases with

energy transfer due to the increased contribution of electrical background when converting from TOF to energy; this will be corrected with the relevant subtraction of background from the TOF spectra. Nevertheless it is clear from the raw data that the two excited states found are consistent with the expected excitations for the Tb(DNN)2, which carries two free radical spins per a molecule. Currently further analysis is required to correct for the sample cell contributions and vanadium normalization is necessary before full analysis of the Q dependence of the measured excitations can be performed. Hamiltonian simulations will then be applied to simulate state eigenvalues, oscillator strengths and Q-dependencies.

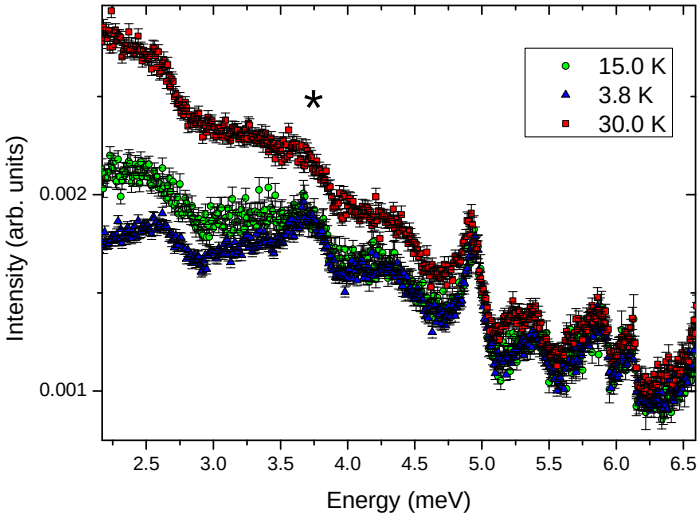

Figure 1. Tb(2pyNO) INS energy spectrum. E_i = 7.743 meV.

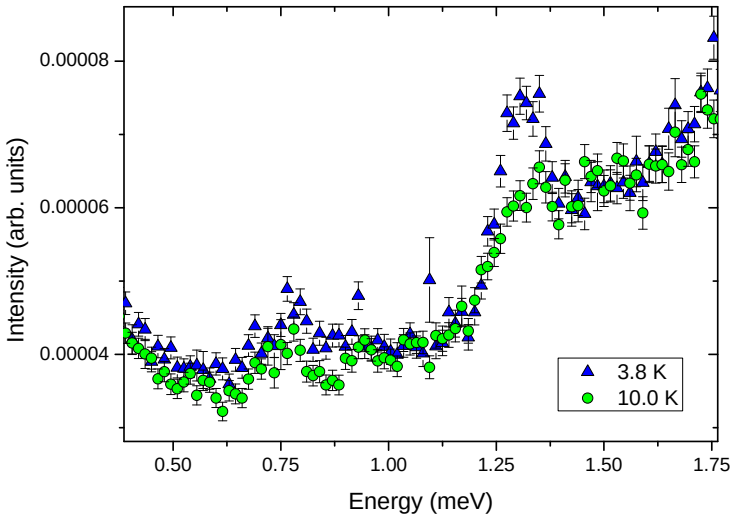

Figure 2. Tb(DNN)2 Energy spectrum. E_i = 3.13 meV.