Inelastic neutron scattering experiment on deuterated halogen-bridged nickel complex

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The halogen-bridged nickel complex, [Ni(chxn)2Br]Br2 (chxn=1R,2R-cyclohexandiamine), has a 1D structure, -Br-Ni(III)-Br-Ni(III)-Br-, along the b-axis [1-2]. This spin structure implies the formation of antiferromagnetically coupled S=1/2 Heisenberg chains of Ni(III). Recently, this system has been suggested to be the second d-electron spin-Peiers system following CuGeO3, and the first example of organic d-electron spin-Peiers system (TTF-CuBDT is a p-electron system). In fact, a clear splitting of the spectrum below 40 K has been observed in the Br-81 NQR study [3].

We have initiated inelastic neutron scattering experiments in [Ni(chxn)2Br]Br2, in order to detect magnetic excitations. In the early stage of our investigations, we grew single crystals and tried inelastic neutron scattering experiments. However, since the sample was not deuterated, local modes originating from hydrogen were too strong to detect magnetic excitations.

Very recently, we have successfully synthesized 95%-deuterated polycrystals of [Ni(chxn)2Br]Br2. We measured inelastic neutron scattering spectra from the 95%-deuterated polycrystalline sample on the triple axis spectrometer PONTA (5G) at JRR3M in JAEA (Tokai), with Ef = 14.7 meV, by using the collimation, open-80 '-80 '-open, at 10 K and 100 K (below and above the transition temperature). Although we used 95%-deuterated crystals, the background noise was still high as shown in Fig. 1(a) (1Mmon roughly corresponds to 5 minutes). In order to reduce the background noise, fully-deuterated crystals are required. The antiferromagnetic zone center is located at Q = 0.6 A-1. Assuming the signals at Q = 0.8 A-1 to be the background, the spectrum of S(E) = I(Q=0.6,E) - I(Q=0.8,E) was deduced, and the difference of S(E,T=10K) - S(E,T=100K) is plotted in Fig. 1(b). The spectrum in Fig. 1(b) should be magnetic signals at the magnetic zone center if magnetic response is detected.

[1] K. Toriumi et al., J. Am. Chem. Soc. 111 (1989)2341.
[2] H. Okamoto et al., PRB 54 (1996) 8438.
[3] S. Takaishi et al., J. Am. Chem. Soc. 126 (2004) 1614.

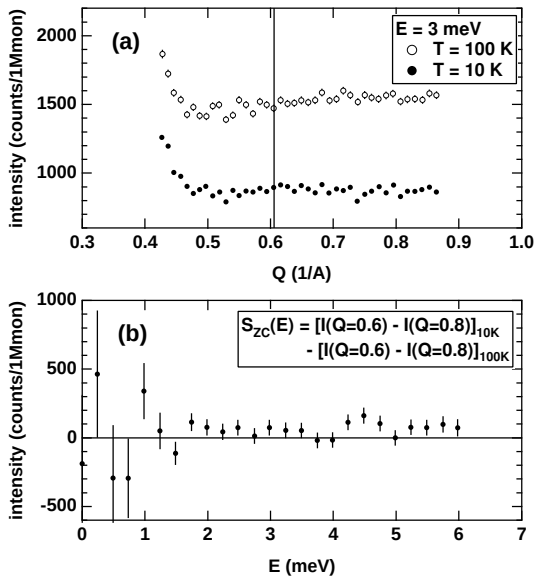

Fig. 1. Fig. 1 Inelastic neutron scattering spectra from deterated [Ni(chxn)2Br]Br2 measured on PONTA with Ef =14.7 meV.