Neutron scattering in O_2 adsorbed CPL-1

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Oxygen is a rare diatomic magnetic molecule. Recently trial to utilize the oxygen as magnetic entity has been conducted in some types of nanoporous metal-organic compounds. The physically adsorbed O_2 molecule forms magnetic framework and O_2 based magnet is realized. Among them in CPL-1 ($C_{16}H_{12}Cu_2N_6O_{10}$) [1], O_2 molecules forms ladder-like structure and the spin-gap behavior is expected. Indeed the magnetic susceptibility [1] and magnetization measurements [2] suggests the spin gap of 60 $\sim$ 88 K (5.2 $\sim$ 7.6 meV).

Hence we started the thermal neutron scattering study on the O_2 based magnet since the fiscal year of 2006. We succeeded in observing the magnetic signal of the adsorbed oxygen and obtained preliminary data set of constant q scans and constant E scans (Fig.1). The difficulty of the study was that we had to collect all the data set in one allocated machine time due to the following technical reason.

The sample contains many hydrogen atoms and the background is large. Therefore, we performed scans on non-O_2 adsorbed sample for background measurement and then we repeat the same scan on O_2 adsorbed sample. It is not until we finish a set of scans that we obtain the net magnetic excitation of the adsorbed oxygen. Usually we noticed that some additional scans were necessary in the end of experiment. In the next allocated experiment we found that the obtained background was slightly different from that in the previous one. This is probably due to slightly different instrumental configuration; e.g., effective volume of the sample in the specially designed Al can, detailed optical set up, and so on. Even though small the difference is, the absolute intensity of the background is large and we have to redo the background measurements. This is why we obtained only preliminary data in the year of 2006. Figure 1 was the best data.

In the year of 2007 we know exactly what we need and what we should do. We focused on obtaining publication quality data in (i) a series of constant q scans at T = 2 K (4 days), (ii) constant energy scan at 8 meV (4 days), and (iii) a constant q scans at various temperatures (4 days). We successfully collected the data set. The detail of this study will appear in a forthcoming publication.

Now we have some technique and budget to obtain deuterated samples. In the next fiscal year we will proceed the project more efficiently.

References

[1] R. Kitagawa, *et al.*, Science **20**, 2358 (2002).
[2] T. C. Kobayashi *et al.*, Prog. Theor. Phys. Suppl. **159**, 271 (2005).

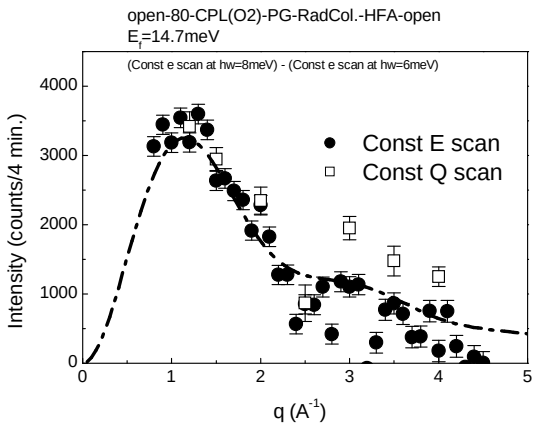

Fig. 1. Constant E scan.