Magnetic Interaction between Adsorbed O_2 Molecules in $[Cu_2(bza)_4(pyz)]_n$

Minoru Soda and Takatsugu Masuda
Neutron Science Laboratory, Institute for Solid State Physics, University of Tokyo, Tokai, Ibaraki 319-1106, Japan

Recently, $[Cu_2(bza)_4(pyz)]_n$ (bza=benzoate, pyz=pyrazine), which can generate stable O_2-inclusion crystals at low temperature using forcible adsorption conditions, has been extensively investigated.[1,2] In this system, interesting magnetization was found, and the trimer induced by magnetic interactions between adsorbed O_2 molecules in the nano-porous cavity was expected. In the present work, we carried out neutron scattering measurements on $[Cu_2(bza)_4(pyz)]_n$ to clarify the magnetic interaction between adsorbed O_2 molecules. Neutron measurements were carried out using the cold neutron multi-chopper spectrometer Let installed at ISIS. After measurements on the $[Cu_2(bza)_4(pyz)]_n$ polycrystalline sample sealed with high pressure oxygen gas (60 atm at room temperature), the measurements on the $[Cu_2(bza)_4(pyz)]_n$ having no O_2 were also performed.

$S(Q,E)$ measured at 1.8 K for $[Cu_2(bza)_4(pyz)]_n$ polycrystalline sample sealed with 60 atm oxygen gas indicates the dispersion-less excitations at $E\sim0.4$ meV and 4 meV. Since these excitations were not observed for the $[Cu_2(bza)_4(pyz)]_n$ having no O_2, these are originated from the magnetic moments of O_2. The constant-E scans show that both excitations have the peaks at $Q\sim1.1$ Å^{-1}.

We study the observed magnetic excitations using the trimer model. The spin Hamiltonian is

$$\mathcal{H}_{trimer} = J_1 \boldsymbol{S_1}\cdot\boldsymbol{S_2} + J_2 \boldsymbol{S_2}\cdot\boldsymbol{S_3} + D\sum_l (S_l^z)^2 . \quad (1)$$

As the result of the fitting, we obtained the exchange interactions J_1=3.98 meV, J_2=0.79 meV, and the uniaxial anisotropy D=0.44 meV. The magnetic excitation can be reasonably explained by the trimer model. Although there is the large difference between the values of J_1 and J_2, the similar difference has been reported in the theory about the Rh-system having the randomness of S_2 site.[2] On the other hand, the temperature dependence of observed excitations is no simple. At this moment, we try to make the analyses of the T-dependence in order to clarify the magnetic correlation of trimer.

[1] S. Takamizawa, E. Nakata, and T. Akutsuka, Andew. Chem., Int. Ed. 45 (2006) 2216.

[2] S. Takamizawa et al., J. AM. CHEM. SOC. 130 (2008) 17883.