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

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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 absorbed 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 absorbed 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~0.4 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~1.1 Å.

We study the observed magnetic excitations using the trimer model shown in Fig. 1

$$H=J_1\boldsymbol{S}_1\cdot\boldsymbol{S}_2+J_2\boldsymbol{S}_2\cdot\boldsymbol{S}_3+D\{(S_1^z)^2+(S_2^z)^2+(S_3^z)^2\}.$$

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]

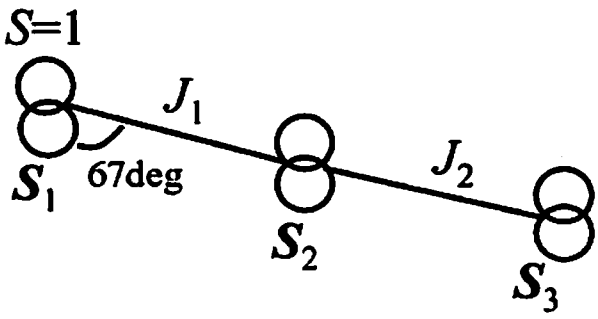

Fig. 1 Trimer model of oxygen molecules.

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.