

# Neutron Diffraction Study of Antiferromagnetic Na and K Nanoclusters Incorporated into Sodalite

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Various kinds of magnetic orderings have been found in alkali-metal clusters arrayed in aluminosilicate zeolite crystals. They are novel magnetic materials because they contain no magnetic element and the magnetic orderings are realized by s-electrons confined in the regular nanospace of zeolites [1]. Sodalite is a kind of zeolites where cages with the inner diameter of 0.7 nm are arrayed in a bcc structure as shown in Fig. 1.  $\text{Na}_4^{3+}$  and  $\text{K}_4^{3+}$  clusters arrayed in sodalite are known to show antiferromagnetism (AFM) below  $T_N$  of 48 K and 72 K, respectively. The cluster accommodates an unpaired s-electron shared by four cations in the cage. We performed neutron diffraction (ND) measurements and succeeded in observing the magnetic Bragg peaks [2]. This is the first direct observation of long range ordering in s-electron systems by using ND. The AFM order is given by the antiparallel coupling of the spins in the body center and the corner clusters. The magnetic form factor coincides well with the s-electron wave function confined in the nanometer-sized cage. It is also found that the form factor dumps quicker in K clusters than that in Na ones as a function of  $Q$ . We also measured optical reflection spectra. A significant red shift is observed in s-p transition in the K clusters. These results clearly indicate that the wave function of K cluster is larger than that of Na cluster. This leads to a decrease in  $U/t$  and the increase in  $T_N$  in the Mott-Hubbard picture.

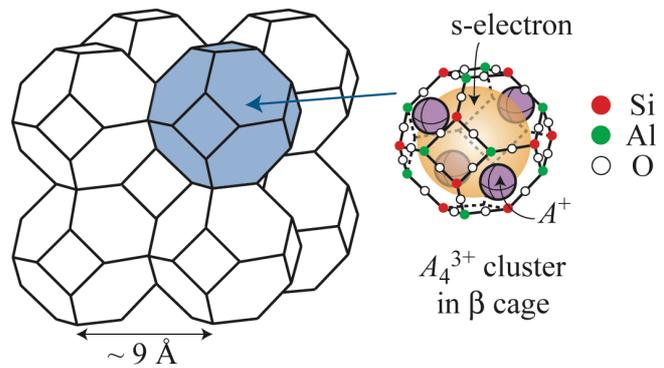


Fig. 1. Schematic illustrations of crystal structure of aluminosilicate sodalite and  $A_4^{3+}$  cluster formed in the  $\beta$ -cage ( $A$ : alkali atom).

## References

- [1] T. Nakano, D. T. Hanh, Y. Nozue, N. H. Nam, T. C. Duan, and S. Araki, *J. Kor. Phys. Soc.* **63**, 699 (2013), and the references therein.
- [2] T. Nakano, M. Matsuura, A. Hanazawa, K. Hirota, and Y. Nozue, *Phys. Rev. Lett.* **109**, 167208 (2012).