# Supplementary material for "Antiferromagnetism and insulator-metal transition of alkali metal-loaded sodalite"

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Figure 1 shows the magnetization curve for $Na_4^{3+}$ clusters in sodalite measured at 300 K. The data obeys a straight line at high fields, while a step-like behavior is seen near the zero field. The latter is due to a tiny amount of ferromagnetic impurities, perhaps some transition metal elements. This is also seen in the non-loaded sodalite. Assuming that the intercept of the straight line is the spontaneous magnetization $M_s$, its value is 0.0051 G. This value corresponds to an average magnetic moment of $1.9 \times 10^{-4}$ $\mu_B$ per $\beta$-cage. This value is very small, but to eliminate its influence, the slope at high magnetic field should be used as the magnetic susceptibility, as explained in the main text.

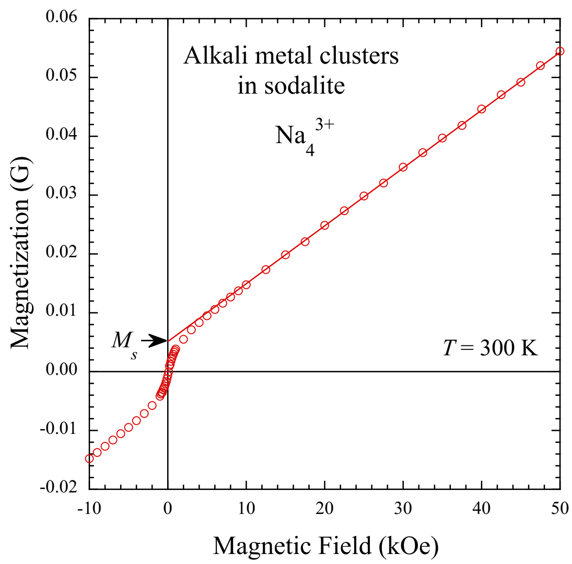


FIG. 1. Magnetization curve for $Na_4^{3+}$ clusters in sodalite measured at 300 K.

Figure 2 shows the temperature dependence of magnetic susceptibility for the $Na_4^{3+}$ sample. $\chi_{obs}$ is the experimental data, which show a peak at about 54 K and an upturn at lower temperatures. $\chi_{Curie}$ is a susceptibility calculated based on the Curie law $\chi_{Curie} = C/T$ with the Curie constant of $C = 0.008$ K emu/mol. For $\chi_{obs} - \chi_{Curie}$ the calculated value of the Curie law is subtracted from the experimental data. This result suggests that the low-temperature upturn originates from the Curie paramagnetic signal. Assuming that all $\beta$-cages accommodate magnetic moments with $g = 2$ and $S = 1/2$, $C$ is calculated to be 0.375 K emu/mol. The Curie component is only 2% of this value. Therefore, it can be concluded that the upturn at low temperatures is not intrinsic and originates from a small amount of paramagnetic impurities in the sample.

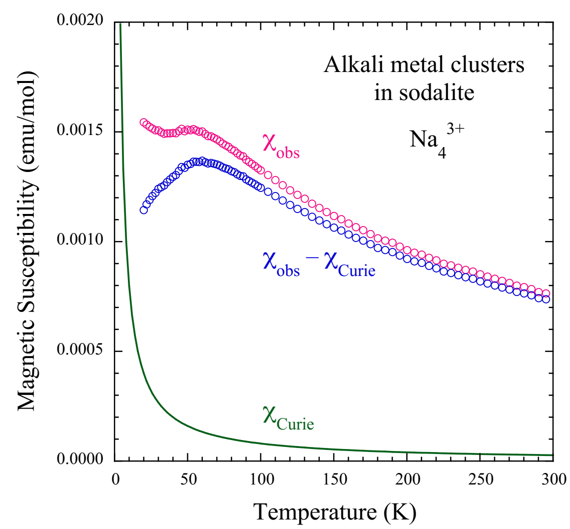


FIG. 2. Temperature dependence of magnetic susceptibility for $Na_4^{3+}$ clusters in sodalite. For analysis, see text.

Figure 3 shows the temperature of alkali-metal loaded sodalite as a function of the inter-cluster distance. The distance is given by $a\sqrt{3}/2$, where $a$ is the lattice constant of the bcc unit.

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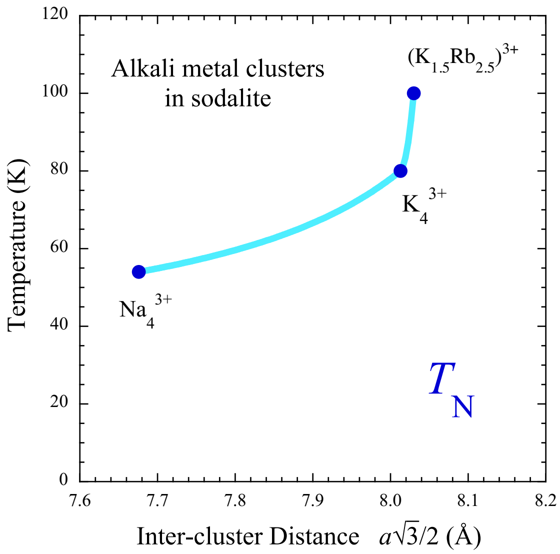


FIG. 3. Néel temperature of alkali-metal loaded sodalite as a function of the inter-cluster distance, which corresponds to the distance between the cluster located at the corner and the cluster located at the body center of the bcc unit.