Spin singlet state due to heptamer formation in AlV$_2$O$_4$ KEISUKE MATSUDA, NOBUO FURUKAWA, Aoyama Gakuin University, YUKITOSHI MOTOUME, RIKEN — Spinel AlV$_2$O$_4$ is a mixed-valent system, where V ions construct a pyrochlore lattice with an average valence of 2.5+. This compound shows a phase transition at $T_c \sim 700$K, and a doubling of the unit cell along the [111] direction is observed below $T_c$. A 3-1 type “valence-skipping” charge-ordering (CO) due to the strong correlation has been proposed to describe this transition.[1] Recently, a more careful analysis reported a trimer formation on [111] Kagomé layers.[2] It is also pointed out that the temperature dependence of the magnetic susceptibility can be decomposed into the Curie-Weiss contribution from $S = 1$ local moments on 1/8 of V sites and a spin-gap contribution from the rest V sites.[2] In the present study, instead of the CO scenario, we focus on the pairing of the Kagomé layers which leads to seven V-sites clusters (heptamers) by two trimers and a V site between the trimers. On the basis of the exact diagonalization study, we found that this model explains well the magnetic susceptibility in experiments. Hence, the heptamer formation appears to be the origin of the phase transition in this compound rather than the CO due to the electron correlation. [1] K. Matsuno et al., J. Phys. Soc. Jpn. 70, 1456(2001) [2] Y. Horibe, et al., unpublished

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Date submitted: 11 Jan 2006