Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Constructing the effective spin model of Mn_6R_6 from ab initio calculations SHUN TONOOKA, KOICHI KUSAKABE, Osaka University, HIROKI NAKANO, University of Hyogo, NAOSHI SUZUKI, Osaka University — Determination of the effective spin model is an important issue for molecular magnetism. Generally, the effective spin model is determined so that the model reproduces the structure of the excitation spectrum. Only this strategy sometimes could not determine which model is the most suitable among several candidates. An example showing this difficulty is seen in $[Mn(hfac)_2NITPh]_6$ abbreviated as Mn_6R_6. Two different models are proposed for Mn_6R_6 by reproducing the magnetization process. One is the Heisenberg model with three-spin interactions. The other is the Heisenberg model with frustration. In this work, in order to examine the validity of each model, we calculate the spin density by the *ab- initio* calculation based on the unrestricted Hartree-Fock method and the density functional theory. We also calculate the spin density of the ground state in each model by numerical diagonalization. Each model shows the different spin density. The spin density of the ground state should give essential knowledge so as to constructing the effective spin model. We discuss the method to connect the effective spin model with the first principle calculation by calculating the spin density.

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Date submitted: 15 Jan 2006 Electronic form version 1.4