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The Electronic structure and rattling motion in La-based skutterudites proved by NMR/NQR

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NMR/NQR are useful probes for detecting microscopic motion of an observed nucleus as well as for studying electronic structure. In order to clarify the rattling motion of rare-earth ions, we performed La-NMR and P-NMR/Sb-NQR measurements on LaT_4X_{12}(T= Fe, Ru, Os; X= P, Sb). The spin-lattice relaxation rate at the La site and X site exhibits different temperature dependence in $LaOs_4Sb_{12}$, $LaFe_4Sb_{12}$, and $LaOs_4P_{12}$. We consider that rattling phonon contributes to additional $1/T_1$ at the La site, resulting in the different temperature dependence in $1/T_1$ at the La and X site. However, absence of the site-dependent behavior of $1/T_1$ is observed in $LaRu_4Sb_{12}$, $LaRu_4P_{12}$, and $LaFe_4P_{12}$ although the size of the cage in $LaRu_4Sb_{12}$ is nearly the same as that in $LaOs_4Sb_{12}$. These results indicate that the size of the cage does not necessarily determine whether the rattling phonon contributes to $1/T_1$ at the La site, but there exist other important factors for the rattling phonon.

To investigate the coupling between La-nucleus spin and electronic structure, we plotted Knight shift at the La site against its susceptibility as shown in Fig.1. Hyperfine coupling constant (which corresponds to the slope in Fig. 1) at the La site of $LaFe_4P_{12}$, $LaRu_4P_{12}$, and $LaRu_4Sb_{12}$ have positive sign, which is the case when s-electron Fermi-contact interaction dominates at the La site. Contrastingly, hyperfine coupling constant at the La site of $LaOs_4Sb_{12}$, $LaFe_4Sb_{12}$, and $LaOs_4P_{12}$ have negative sign. This negative sign indicates that d-electrons of transition metal element affect hyperfine-field at the La site mediated by core-polarization effect. Our results suggest intimate relation between the d-bands of transition metal and the rattling motion through electron-phonon coupling in the filled skutterudites.

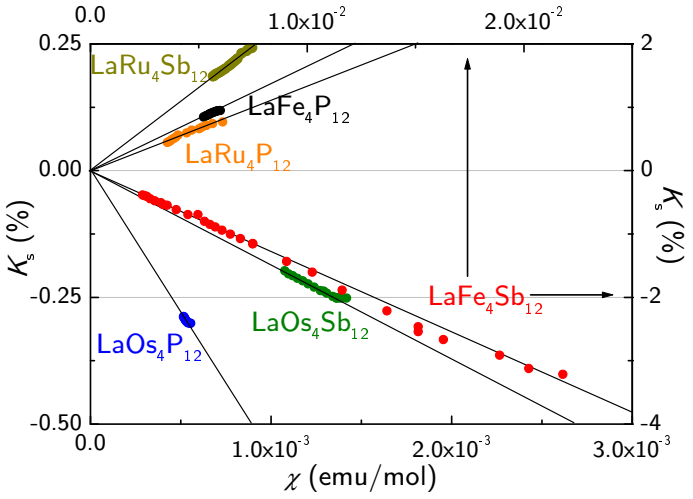

Figure 1: Knight shift vs susceptibility (K-χ plot) for various La-based skutterudite obtained with La-NMR.