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^{121}Sb-NMR studies of single crystal $PrOs_4Sb_{12}$

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^{121}Sb-NMR measurements were performed for a single crystal $PrOs_4Sb_{12}$ with typical dimensions of 2×2 × 3 mm^3 at fixed frequency of $f = 100.14$ MHz in the field range of 0-15 T.

Figure 1 shows the ^{121}Sb NMR spectrum for a fixed frequency $f_0 = 100.14$ MHz in the paramagnetic state at 5 K for Hk $< 001 >$ direction. Sb(1) NMR signals (Fig. 2) are explained by a nuclear quadrupole (eqQ) second order spectrum for Hk $< 001 >$ kV_{ZZ}, where V_{ZZ} is the principal axis of a maximum electric field gradient (EFG). Other extra lines come from the different Sb(2,3) sites.

In order to assign the observed ^{121}Sb NMR lines, the resonance fields were calculated by exact diagnalization of the 6×6 nuclear spin Hamiltonian matrix of ^{121}Sb, by using the values, the quadrupole frequency $\nu_Q = 44.143$ MHz, and asymmetry parameter $\eta = 0.46$ at $T = 5$ K [1]. The solid lines in Fig. 1 show calculated resonance fields for Hk $< 001 >$. The observed ^{121}Sb NMR spectrum is well reproduced assuming the three different Sb sites for H k$< 001 >$ with different angle sets, (θ, ϕ) ' $(0°, 0°)$ for Sb(1), $(90°, 47°)$ for Sb(2), and $(90°, 43°)$ for Sb(3), where θ and ϕ are the polar angles of the applied field direction with respect to the EFG principal axes, (X, Y, Z). The principal axes for the EFG are determined as indicated in Fig. 2. These results agree well with the calculated EFG of Sb site by a FLAPW method based on LDA.

We also measured the Knight shift (KS) in the superconducting state for $H// < 100 >$. The KS does not change below T_c. The KS for $H// < 110 >$ are now in progress.

[1] H. Kotegawa, et al, Phys. Rev. Lett.90, 027001, (2003).