(PS 4)

Crystalline electric field of Pr-based filled skutterudite with T_h point symmetry

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The point symmetry of Pr site of the cubic filled skutterudite compound is T_h, which has not four-fold rotation axis. The CEF Hamiltonian with the T_h symmetry is written as,[1]

$$H_{CEF} = B_{40}\left(C_{40} + \sqrt{\frac{5}{14}}(C_{4-4} + C_{44})\right) + B_{60}\left(C_{60} - \sqrt{\frac{7}{2}}(C_{6-4} + C_{64})\right)$$

$$+B_{62}\left((C_{6-2} + C_{62}) - \sqrt{\frac{5}{11}}(C_{6-6} + C_{66})\right).$$

If only the fourth-order terms of CEF Hamiltonian are considered, the energy scheme in the T_h symmetry is the same as in the O_h symmetry, and the non-Kramers' doublet $\Gamma_{2,3}$ does not become the ground state. To make the $\Gamma_{2,3}$ state to be the ground state, we have to consider the higher order terms, B_{60} and B_{62}, We have examined the effect of the sixth-order terms of CEF, and calculated the eigen values and eigen functions of Pr ($4f^2$) ion splitted by this CEF in two cases, assuming that $B_{40} = 100$ K in one case and $B_{40} = -100$ K in the other case. It is noted that the absolute values of B_{60} and B_{62} are less than $|B_{40}|$, in general.

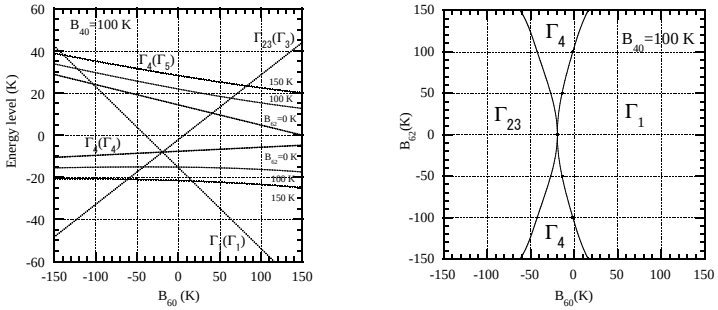

Figure 1: CEF energy scheme (left), and the phase diagram of the ground state (right) of Pr^{3+} of T_h point symmetry, assuming that $B_{40} = 100$ K.

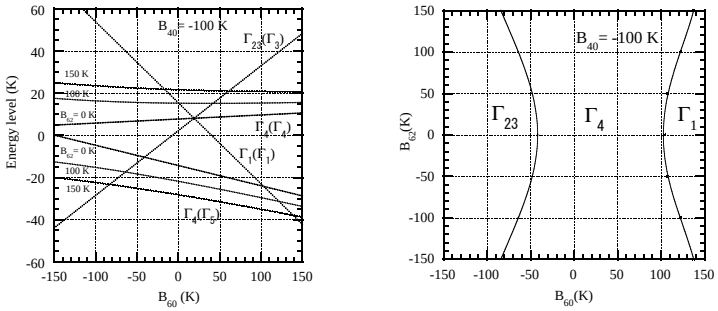

Figure 2: CEF energy scheme (left), and the phase diagram of the ground state (right) of Pr^{3+} of T_h point symmetry, assuming that $B_{40} = -100$ K.

[1] K. Takegahara et al, J. Phys. Soc. Jpn. **70** (2001) 1190.