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s-f Mixing and Effective Hamiltonian for Pr Skutterudites

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The Pr skutterudites PrT_4X_{12} (T=Fe, Ru, Os; X=P, As, Sb), in which the Pr ions are in the f^2 configuration, have many properties, which need to be clarified. They include the origin of heavy-fermion behavior and the metal-insulator transtion, nature of quadrupolar order or mechanism of superconductivity. To understand those points from a microscopic viewpoint, one has to derive the interaction Hamiltonian of conduction electrons with f-orbitals of Pr ions. The purpose of this contribution is to present a progress report of our study along this direction.

The Pr skutterudites have a unique structure: each Pr ion is surrounded by 12 X atoms and the point group symmetry is T_h[1]. One promising crystal-level scheme appropriate for $PrOs_4Sb_{12}$ is the ground state Γ_1 and the first excited state $\Gamma_4^{(2)}$ forming a quasi-quartet[2, 3]. According to Harima and Takegahara[4], the conduction electrons consist mainly of the pnictogen p orbitals surrounding each Pr. The f states in the T_h field are classified into one Γ_1^- (a_u) and two Γ_4^- (t_u) orbitals; the sf mixing occurs with conduction electrons with the same symmetry.

Using our previous approach to U compounds[5] and CeB_6[6], we have derived an effective interaction $\mathcal{H}_{eff}$ due to the sf mixing within the second order. Some of the conclusions obtained so far are as follows:
(1) If one restricts conduction electrons to the a_u symmetry, no matrix element is present between the Γ_1 and $\Gamma_4^{(2)}$ crystal-field levels.
(2) $\mathcal{H}_{eff}$ originating from the mixing of conduction electrons with the t_u symmetry gives finite matrix elements between Γ_1 and $\Gamma_4^{(2)}$ and has both magnetic and quadrupolar contributions.
(3) Because of the result of (2) it is very likely that magnetic fluctuations corresponding the transition between Γ_1 and $\Gamma_4^{(2)}$ may be equally important, although the importance of quadrupolar fluctuations is often emphasized in the literature.

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