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Crystalline electric fields and the ground state of $YbRh_2Si_2$ and $YbIr_2Si_2$

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Abstract

We have constructed the crystalline electric field (CEF) splitting of the energy levels of Yb^{3+} ($4f^{13}$) in the clean intermetallic compounds $YbRh_2Si_2$ and $YbIr_2Si_2$. The data of measurements using methods of inelastic neutron scattering, electron spin resonance, and Mössbauer spectroscopy, together with relevant structural, thermodynamic, and magnetic properties, were used as input to calculations of the CEF level schemes in these non-Fermi-liquid systems. The experimental data of both compounds are found to be well explained on the basis of the CEF 4f-schemes with the $\Gamma_{t6}^{-(1)}$ ground state symmetry.

Keywords: Heavy fermion; Yb-based intermetallics; Crystalline electric field

$YbRh_2Si_2$ and $YbIr_2Si_2$ are the dense heavy fermion (HF) Kondo systems which are close to a quantum critical point, where magnetic ordering via RKKY interactions is balanced by Kondo screening [1,2]. The magnetic properties of these compounds are determined by the rare-earth moments, by their conduction-electron mediated exchange interaction, and by the effects of crystalline electric fields (CEF) acting on the 4f electrons. The strongly anisotropic electron spin resonance (ESR) spectra ascribed to the Yb^{3+}-ions ($4f^{13}$, $J=7/2$) have been detected in both compounds below a Kondo temperature T_K [3–5]. The CEF of tetragonal symmetry

$$H = B_2^0 V_2^0 + B_4^0 V_4^0 + B_4^4 V_4^4 + B_6^0 V_6^0 + B_6^4 V_6^4 \quad (1)$$

splits the ground multiplet $^2F_{7/2}$ of the Yb^{3+} into four Kramers doublets, two Γ_6 and two Γ_7. Here, B_k^q are the CEF parameters, and V_k^q are the Stevens operators. The first excited CEF states of 9.91 meV ($YbRh_2Si_2$) [3] and 5.17 meV ($YbIr_2Si_2$) [5] which contribute to the ESR relaxation with increasing temperature have been determined from the temperature dependence of the ESR linewidth and effective ESR g-factor. These values are essentially smaller than the corresponding quantities derived from the CEF schemes of the Yb^{3+} as a result of inelastic neutron scattering (INS) measurements in $YbRh_2Si_2$ (0–17–25–43 meV) [6] and in $YbIr_2Si_2$ (0–18–25–36 meV) [7]. However, the lowest CEF transition was visible as a weak broad shoulder in the INS spectra of both intermetallics because of a strongly broadened CEF levels due to Kondo hybridization of the localized f-moments with conduction electrons [8]. Moreover, naturally occurring random strains can be responsible for large discrepancies between the excited-state energy levels measured by optical, INS and ESR techniques [9].

The theoretical energy levels and wave functions were determined by diagonalizing the energy matrix of Hamiltonian (1) according to the least-squares fitting procedure as described in details earlier [10]. In general, the roles played by exchange interactions and by CEF effects cannot be separated easily. Several suggestions will allow us to solve this problem and to minimize a number of possible solutions.

First of all, we have taken into account that in metals with a Pauli-like susceptibility the g-shift contains a positive local ferromagnetic moment due to conduction electrons $\Delta g/g = -8\%$. On this reason, the values of the effective g-factors which were used as input for calculations (Table 1) deviate exactly to this difference from the quantities which were derived from the ESR experiments in $YbRh_2Si_2$ [4] and in $YbIr_2Si_2$ [5]. In addition, the value and the sign of the leading CEF parameter B_2^0 has been deduced from the quantity A_2^0 obtained as a result of the Mössbauer spectroscopy studies of ternary silicides

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