Crystal-field states of the Sm^{2+} ion in topological Kondo insulator SmB_6: specific heat studies

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Topological Kondo insulator SmB_6 exhibits the hybridization gap of 20 meV, but experiments like temperature dependence of the magnetic susceptibity and of the specific heat with a very large extra specific heat with a large maximum (about 10 J/K mol) at 50 K point to the existence of in-gap localized states of the debated origin [1,2]. We have attributed [3] these states as originating from the the Sm^{2+} ion which can be theoretically revealed by calculations within the spin-orbital $|LSL_zS_z>$ space, with L=3 and S=3. The in-gap states originate from the 49-fold degenerated quasi-atomic term ^7F $(4f^6)$ which becomes split by the cubic crystal-field (CEF) and the finite spin-orbit interactions. These interactions competite with each other - the six-order cubic CEF interactions produce the 7-fold degenerated ground state whereas the spin-orbit interactions, even of the weakest one, produce a singlet (J=0) ground state. The derived CEF and spin-orbit parameters produce the lowest singlet state at 0 K with an excited triplet at 89 K and a next triplet at 215 K. Such states are within the 20-meV hybridization gap.
Our approach is very similar to the one used by us in description of 3d compounds (CoO, NiO) [4,5], where the spin-orbit coupling is taken relatively weak - it is in contrast to the standard approach used for rare-earth ions with the quantum number J as the good quantum number. This similarity is due to a fact that the orbital quantum number L=3 for the Sm^{2+} ion is the same as for the Co^{2+} or Ni^{2+} ions.

References:

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