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Evidence for molecular Kondo effect in rare-earth metallocenes from f-occupancy and magnetic susceptibility C.H. BOOTH, M. DANIEL, W.W. LUKENS, Lawrence Berkeley National Laboratory, M.D. WALTER, R.A. ANDERSEN, Lawrence Berkeley National Laboratory and Department of Chemistry, University of California, Berkeley — The Kondo effect describes a quasibound singlet state formed by the interaction between a local magnetic moment on a lattice site and states at the Fermi level. In theory, a similar interaction should occur in the single molecule cerium bis-cyclooctatetraene (cerocene), where the configuration interaction between the f-orbitals and the carbon p(π)-orbitals create an intermediate valence state with a very high Kondo temperature, T_K [Dolg et al., J. Chem. Phys. **94**, 3011 (1991)]. Very little experimental evidence exists for such a state, however. We report Ce L_3-edge x-ray absorption near-edge structure (XANES) measurements of the f-occupation that demonstrate intermediate valence, with an f-occupancy of $n_f \sim 0.8$. Moreover, magnetic susceptibility $\chi(T)$ measurements demonstrate that the cerium in cerocene is paramagnetic, with a temperature-independent $\chi(T < 300K) = 1.5 \times 10^{-4}$ emu/mol. These data are consistent with a T_K of about 5000 K. A similar set of data on a series of ytterbium bis-cyclopentadienyl molecules supports this claim, except with a range of T_K's from 800 K to greater than 1500 K. Taken together, these data are strong evidence of a molecular Kondo effect in these insulating systems and give the first indication of how to tune such Kondo interactions.

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