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Valence transitions and nanoscale Kondo-like behavior in Yb organometallic molecules C.H. BOOTH, W.W. LUKENS, Lawrence Berkeley National Laboratory (LBNL), D. KAZHDAN, Y.-J. HU, R.A. ANDERSEN, LBNL and University of California, Berkeley, E.D. BAUER, Los Alamos National Laboratory, L. MARON, INSA Toulouse, O. EISENSTEIN, Universite Montpellier —
When a material exhibiting Kondo behavior is reduced in size to the nanoscale, quantum confinement effects are dramatic, but still poorly understood. If the system is small enough, complex many-body calculations should no longer be necessary to describe the physics, and an understanding of the Kondo effect at the nanoscale can be attacked from a different direction. We present experimental and calculational results on Me-substituted complexes of $Cp^*_2Yb(bipy)$ that demonstrate the efficacy of this approach. In particular, these molecules exhibit temperature-independent paramagnetism and intermediate valence of the Yb. Moreover, the first excited state can be lowered below room temperature, generating temperature-dependent Yb valence behavior, and even first-order valence transitions. CASSCF calculations demonstrate the importance of π^* orbitals in obtaining appropriate ground states, and are able to reproduce trends in the excited state energies and the Yb valence. These results have direct implications for understanding not only nanoscale Kondo behavior, but also the general concept of valence tautomerism, and the importance of f-orbitals in bonding for lanthanide organometallics.

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