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Intermediate valence, local antiferromagnetic coupling and the Kondo effect in ytterbium organometallic molecules C.H. BOOTH, W.W. LUKENS, Lawrence Berkeley National Laboratory (LBNL), M.D. WALTER, D. KAZHDAN, R.A. ANDERSEN, LBNL and University of California, Berkeley, E.D. BAUER, Los Alamos National Laboratory, L. MARON, INSA Toulouse, O. EISENSTEIN, Universite Montpellier — Studying magnetic ions coupling to aromatic rings in organometallic molecules provides an analogous route to studying the Kondo effect in nanoscale systems. We extend the number of molecules displaying such effects in their magnetism and x-ray absorption spectroscopy from cerocene [$Ce(C_8H_8)_2$] and $Cp^*{}_2Yb$(bipy) [Cp*=pentamethylcyclopentadienyl, bipy=bipyridine) to a collection of $Cp^*{}_2Yb(L)$ molecules, where L is one of various bipyridyl or diazadiene ligands. Clear trends are observed in both the magnetic susceptibility and the Yb valence that indicate changes in the fundamental temperature scale. CASSCF calculations indicate the intermediate valence is primarily due to a configuration interaction between the open-shell $f^{13}\pi^{*1}$ and the closed-shell $f^{14}\pi^{*0}$ spin-singlet states, in direct analogy to the Kondo effect in intermetallic systems. These studies increase the range of molecular species where such properties are observed, and point toward understanding the ubiquity of such effects and their involvement in fundamental bonding and magnetism in organometallic molecules.

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