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Valence state and magnetism of $Yb_7Co_4InGe_{12}$. ZSOLT RAK, MARIA CHONDROUDI, S.D. MAHANTI, Michigan State University, M.G. KANATZIDIS, Northwestern University — Ytterbium (Yb) compounds exhibit unusual physical properties due to the Yb f-electrons, which play an active role in bonding, giving rise to intermediate valence, heavy-fermion or Kondo behavior. Many physical characteristics of the Yb systems are related to the fact that Yb can have two valence states: nonmagnetic divalent Yb^{2+} (f^{14}) and magnetic trivalent Yb^{3+} (f^{13}). We have synthesized a new Yb containing quaternary $Yb_7Co_4InGe_{12}$. XPS and magnetic susceptibility measurements indicate that all Yb are all trivalent. To understand the Yb valency in this compound, we have carried out *ab initio* electronic structure calculations within density functional theory using FP-LAPW method. The electronic structure is obtained using LSDA with on-site Coulomb correlation potential (LSDA+U) included for both 4f electrons of Yb and 3d electrons of Co. As a one "f-hole" analogue of many Ce compounds[1,2], we find that all the Yb atoms are trivalent, in agreement with XPS and magnetic susceptibility measurements. [1]A. I. Liechtenstein, V. P. Antropov, and B. N Harmon, Phys. Rev. B 49, 10770 (1994). [2]E. Bauer, Adv. Phys. 40, 417 (1991).

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