Chemical Bonding and Physical Properties of Yb_5Bi_3

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The binary compound Yb_5Bi_3 was synthesized by reaction of the elements in a sealed Ta container. Its crystal structure was determined from single-crystal X-ray diffraction data: β-Yb_5Sb_3-type, space group *Pnma*, Pearson code *oP*32, $a = 12.6375(6)$, $b = 9.7243(4)$, $c = 8.4117(5)$ Å, $V = 1033.72(9)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.028$, $wR_{ref}(F^2) = 0.069$, $T = 290$ K. Band structure calculations and analysis of the chemical bonding suggest mainly ionic interactions in the crystal structure and a possible presence of ytterbium in two valence states Yb^{2+} and Yb^{3+}. The magnetization measurements showed that at low temperatures Yb_5Bi_3 contains ytterbium exclusively in the $4f^{14}$ configuration without fluctuations to the Yb $4f^{13}$ configuration up to 400 K. From the Yb-L_{III} X-ray absorption spectroscopy data the effective valence of ytterbium was found to be 2.11 (89 % of Yb in $4f^{14}$ configuration).

Key words: Ytterbium, Bismuth, Intermetallic Compound, Chemical Bonding, Magnetism, Electrical Resistivity, X-Ray Absorption Spectroscopy