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The Preparation and Crystal Structure of Ternary Rare Earth Borides, RCo_3B_2 *

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Abstract

In the ternary system of rare earth-cobalt-boron, RCo_3B_2 compounds (R=rare earth elements) were prepared by arc-melting methods. Their crystal structure was investigated by X-ray diffraction methods. These ternary borides, RCo_3B_2 , crystallize in a hexagonal lattice. The lattice parameters are $a=5.020\pm 0.002\text{ \AA}$ and $c=3.027\pm 0.002\text{ \AA}$ for YCo_3B_2 and $a=5.066\pm 0.003\text{ \AA}$ and $c=3.022\pm 0.002\text{ \AA}$ for GdCo_3B_2 . The good agreement between the X-ray diffraction intensities observed and calculated shows that the ternary borides, YCo_3B_2 and GdCo_3B_2 , crystallize in the CaZn_5 -type structure. The space group and atomic positions are as follows: $\text{P6}/\text{mmm}$ (D_{6h}^{1h}), 1R in 1(a), 3Co in 3(g), and 2B in 2(c). It can be seen from these results that the ternary borides, RCo_3B_2 , have a superstructure in which two Co atoms in the 2(c) site of intermetallic compounds, RCo_5 , with the CaZn_5 -type structure are replaced by two B atoms. The B atoms in this structure are situated at the center of a trigonal prism formed by six Co atoms. The interatomic distances between B and the six Co atoms are 2.11–2.10 \AA and are fairly constant, although the radii of the rare earth atoms are changed according to the lanthanide contraction. We have also found RCo_3B_2 compounds to be isostructural with YCo_3B_2 and GdCo_3B_2 , where R=Ce, Sm, Tb, Dy, Ho, and Er. Efforts to prepare LaCo_3B_2 , PrCo_3B_2 , and NdCo_3B_2 by arc-melting were unsuccessful.

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