ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE $Ce_2Co_7B_3$ COMPOUND

A. Szajek[a], M. Richter[b]

[a]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

[b]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

9.7 cm

The rare earth compounds $R_{n+1}Co_{3n+5}B_{2n}$ (R = rare earth atoms) are interesting as they allow systematic studies of dependence of magnetic moments on local environment, not to mention their relevance to the search for high performance permanent magnets. The compounds crystallize in hexagonal $CaCu_5$-type structure, belonging to the $P6/mmm$ space group. Their structure is generated from RCo_5 (n = 0) by replacing Co atoms by B atoms, until the saturation (n = ∞) is reached in RCo_3B_2 [1]. The electronic structure of the $R_{n+1}Co_{3n+5}B_{2n}$ ($R = Y, Gd, Tb$) was studied using TB-LMTO-ASA method [2, 3]. Here we present results for $R = Ce$ and n=3, $Ce_2Co_7B_3$ compound, based on the fully relativistic FPLO code [4]. The magnetic moments on Co atoms are sensitive to the number of cobalt ions in the local environment and are equal to 1.55, 0.56, and 0.06 $\mu_B/atom$ for Co(2c), Co($6i_1$) and Co($6i_2$), respectively. The density of electronic states is dominated by d-electrons.

[1] Y.B. Kuzma et al., Kristallografia 18 (1973) 710.

[2] A. Szajek, J. Magn. Magn. Mater. 185, 322 (1998).

[3] A. Szajek J.A. Morkowski, Materials Science-Poland 24 (2006) 839.

[4] FPLO-5.10-20 improved version of FPLO code by K. Kopernik and H. Eschrig, Phys. Rev. B 59 (1999) 1743; http:// www.fplo.de

13.4 cm

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Corresponding author :

A. Szajek

Address for correspondence :

Institute of Molecular Physics, Polish Academy of Sciences
ul. M. Smoluchowskiego 17, 60-179 Poznań, Poland

Email address :

szajek@ifmpan.poznan.pl