Calculated magnetic moments and electronic structure of the compounds $R_{n+1}Co_{3n+5}B_{2n}$, R = Gd, Tb, n = 0, 1, 2, 3 and ∞

A. Szajek and J.A. Morkowski

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

The lantanide compounds $R_{n+1}Co_{3n+5}B_{2n}$ 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 Pb/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 series $Y_{n+1}Co_{3n+5}B_{2n}$ was studied by one of us [2]. In the present paper results for R = Gd and Tb are given {together with special cases for Sn (n = 0 and ∞) and Tm (n = 2)}.The tight binding linear muffin tin orbitals method in the atomic spheres approximation (TB-LMTO-ASA) was employed [3]. The experimental value of the lattice constant was used. Results of calculations are summarized in plots of the total and partial densities of states and in the Table 1 of calculated magnetic moments for atoms in different inequivalent crystallographic positions. The conclusion is that in the series studied magnetic moments of the rare earth atoms are antiparallel to the magnetic moments in Co.

Compound	Atoms	The magnetic moments [μ_B]	
		R = Gd	R = Tb
n = 0	R (1a)	-7.580	-9.530
x = 0.0	Co(2c)	1.553	1.575
RCo_5	Co(3g)	1.585	1.545
n = 1	R(1a)	-7.442	-9.394
x = 0.2	R(1b)	-7.556	-9.508
RCo_4B	Co(2c)	1.649	1.619
	Co(6i)	0.877	0.863
	B(2d)	-0.035	-0.056
n = 2	R(1a)	-7.500	-9.439
x = 0.27	R(2e)	-7/377	-9.349
$R_3Co_{11}B_4$	Co(2c)	1.648	1.749
	Co(3g)	0.171	0.126
	Co(6i)	0.792	0.787
	B(4h)	-0.035	-0.032
n = 3	R(1a)	-7.457	-9.423
x = 0.30	R(1b)	-7.236	-9.219
$R_2Co_7B_3$	R(2e)	-7.366	-9.309
	Co(2c)	1.776	1.760
	Co($6i_1$)	0.795	0.744
	Co($6i_2$)	0.164	0.184
	B(2d)	-0.014	-0.016
	B(4h)	-0.034	-0.031
n = ∞		-7.227	-9.183
x = 0.4		0.106	0.086
RCo_3B_2		-0.005	-0.003

Table 1. The magnetic moments of $R_{n+1}Co_{3n+5}B_{2n}$ (n = 0, 1, 2, 3 and ∞) or $R(Co_{1-x}B_x)_5$

[1] Y.B. Kuz'ma *et al.*, Kristallografia **18,** 710 (1973).
[2] A. Szajek, J. Magn. Magn. Mater. **185,** 322 (1998).
[3] O.K. Andersen, O. Jepsen and M. Šob, in: M.S. Yussouff (Ed.), Electronic Structure and Its Applications, Springer, Berlin, 1987, p. 2.

Name of the presenting author (poster): J.A. Morkowski
e-mail address: jmorkows@ifmpan.poznan.pl
url's: http://www.ifmpan.poznan.pl