THE ELECTRONIC AND MAGNETIC PROPERTIES OF $Pr_3Co_{13}B_2$ AND $Pr_5Co_{19}B_6$ COMPOUNDS

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The $Pr_3Co_{13}B_2$ and $Pr_5Co_{19}B_6$ compounds were manufactured as promising systems suitable for fabrication of permanent magnets. They belong to the $R_{m+n}Co_{5m+3n}B_{2n}$ family with (m=2n, n=1), (m=2, n=3), and (m=3, n=2), respectively [1]. The band structure calculations are performed by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (TB-LMTO ASA) [2]. The calculated magnetic moments on Co atoms depend on their local environment and vary in the range of 0.22 to 1.70 $\mu_B/atom$. The calculated values of the total magnetic moments are equal to: 23.56 (20 [3]) and 29.62 (23.7[4]) $\mu_B/f.u.$ for $Pr_3Co_{13}B_2$ and $Pr_5Co_{19}B_6$ compounds, respectively, where the experimental values are given in the parenthesis. The main contributions to the total densities of electronic states at the Fermi level are provided by 3d electrons of the Co atoms.

[1] Y. Chen et al., J. Alloys Compd. **289** (1999) 96.
[2] O.K. Andersen, Phys. Rev. B **12** (1975) 3060.
[3] Y. Chen et al., Appl. Phys. Lett. **74** (1999) 856.
[4] Y. Chen et al., Phys. Rev. B **61** (2000) 3502

9.7 cm

13.4 cm

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