

New Intermetallic Compounds $RE_4Co_2Mg_3$ ($RE = Pr, Gd, Tb, Dy$) – Syntheses, Structure, and Chemical Bonding

Selcan Tuncel^a, Ute Ch. Rodewald^a, Samir F. Matar^b, Bernard Chevalier^b, and Rainer Pöttgen^a

^a Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 30, 48149 Münster, Germany

^b Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB), CNRS [UPR 9048], Université Bordeaux 1, 87 avenue du Docteur Albert Schweitzer, 33608 Pessac Cedex, France

Reprint requests to Prof. Dr. R. Pöttgen. E-mail: pottgen@uni-muenster.de

Z. Naturforsch. **2007**, 62b, 162 – 168; received October 20, 2006

The magnesium compounds $RE_4Co_2Mg_3$ ($RE = Pr, Gd, Tb, Dy$) were prepared by induction melting of the elements in sealed tantalum tubes. The samples were studied by powder X-ray diffraction. The structures of the gadolinium and of the terbium compound were refined from single crystal diffractometer data: $Nd_4Co_2Mg_3$ -type, $P2/m$, $Z = 1$, $a = 754.0(4)$, $b = 374.1(1)$, $c = 822.5(3)$ pm, $\beta = 109.65(4)^\circ$, $wR2 = 0.0649$, 730 F^2 values for $Gd_4Co_2Mg_3$ and $a = 750.4(2)$, $b = 372.86(6)$, $c = 819.5(2)$ pm, $\beta = 109.48(3)^\circ$, $wR2 = 0.0398$, 888 F^2 values for $Tb_4Co_2Mg_3$ with 30 variables each. The $RE_4Co_2Mg_3$ structures are 3 : 1 intergrowth variants of distorted CsCl and AlB_2 related slabs of compositions $RE Mg$ and $RE Co_2$. Characteristic structural features (exemplary for $Tb_4Co_2Mg_3$) are relatively short Tb–Co (271 pm), Co–Co (232 pm) and Mg–Mg (314 pm) distances. The latter are a geometrical constraint of the distortion of the $RE Mg$ and $RE Co_2$ slabs. Chemical bonding analysis (ELF and ECOV data) for $Gd_4Co_2Mg_3$ reveals strong Gd–Co bonding followed by Mg–Co, while the Mg–Mg interactions can be considered as weak. The Co–Co contacts are only weakly bonding. The bonding and antibonding states are almost filled.

Key words: Magnesium, Intermetallics, Crystal Chemistry, Chemical Bonding