Rare Earth-rich Magnesium Compounds RE_4RhMg (RE = Y, La–Nd, Sm, Gd–Tm, Lu)

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The series of magnesium compounds RE_4RhMg (RE = Y, La–Nd, Sm, Gd–Tm, Lu) was prepared by high-frequency melting of the elements in sealed tantalum tubes. All samples were investigated by powder X-ray diffraction. The structures with RE = Sm, Gd, Dy, Ho, and Er as rare earth metal components were refined from single crystal diffractometer data: Gd_4RhIn-type, $F\bar{4}3m$, Z = 16, a = 1392.1(1) pm, $wR2$ = 0.060, 616 F^2 values, 19 variables for Sm_4RhMg, a = 1380.8(2) pm, $wR2$ = 0.071, 530 F^2 values, 19 variables for Gd_4RhMg, a = 1366.9(1) pm, $wR2$ = 0.070, 594 F^2 values, 20 variables for Dy_4RhMg, a = 1355.7(2) pm, $wR2$ = 0.077, 578 F^2 values, 20 variables for $Ho_{3.52}RhMg_{1.48}$, and a = 1355.4(2) pm, $wR2$ = 0.075, 559 F^2 values, 20 variables for $Er_{3.94}RhMg_{1.06}$. The rhodium atoms have slightly distorted trigonal prismatic rare earth coordination. Condensation of the RhRE_6 prisms leads to a three-dimensional network which leaves large voids that are filled by regular Mg_4 tetrahedra with a Mg–Mg distance of 312 pm in Sm_4RhMg. The magnesium atoms have twelve nearest neighbors (3 Mg + 9 RE) in icosahedral coordination. In the structures with holmium and erbium, the RE1 positions which are not involved in the trigonal prismatic network exhibit RE1/Mg mixing. Shortest distances occur for Sm–Rh (286 pm) within the rigid three-dimensional network of condensed trigonal prisms.

Key words: Magnesium, Intermetallics, Crystal Chemistry