Ternary Gallides *RE*MgGa (*RE* = Y, La, Pr, Nd, Sm–Tm, Lu) – Synthesis and Crystal Chemistry

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The title compounds have been synthesized by reacting the elements in sealed niobium or tantalum tubes in a high-frequency furnace. They crystallize with the hexagonal ZrNiAl type structure, space group $P\delta 2m$. All gallides have been characterized through their X-ray powder diffractogram. The cell volume decreases from the lanthanum to the lutetium compound as expected from the lanthanoid contraction. The structures of LaMgGa, PrMgGa, NdMgGa, SmMgGa and TmMgGa have been refined from single crystal diffractometer data. The structures contain two crystallographically independent gallium sites which both have a trigonal prismatic coordination: Gal by six *RE* and Ga2 by six Mg atoms. These trigonal prisms are capped on the rectangular sites by three Mg (*RE*) atoms, leading to coordination number 9 for each gallium atom. Together, the gallium and magnesium atoms form a three-dimensional [MgGa] network in which the rare earth atoms fill distorted hexagonal channels. Within the network the magnesium atoms have short Mg–Mg contacts, *i. e.* 312 pm in SmMgGa. The Mg–Ga distances in that gallide range from 284 to 287 pm. Bonding in the network is thus governed by strong Mg–Ga and Mg–Mg bonding. EuMgGa crystallizes with the orthorhombic TiNiSi type: *Pnma*, *a* = 783.1(2), *b* = 472.8(1), *c* = 829.8(2) pm.

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