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## Segregation of calcium and magnesium into different substructures. $\text{Ca}_4\text{Ag}_{0.948}\text{Mg}$ and other compounds with $\text{Gd}_4\text{RhIn}$ -type structure

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Structure

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**Segregation of Calcium and Magnesium into Different Substructures.**

**Ca<sub>4</sub>Ag<sub>0.948</sub>Mg and Other Compounds with Gd<sub>4</sub>RhIn-Type Structure.** — The compounds Ln<sub>4</sub>PdMg (Ln: Ca, Eu, Tb—Lu), Ln<sub>4</sub>AgMg (Ln: Ca, Yb), Ln<sub>4</sub>PtMg (Ln: Eu, Tb—Lu), and Ln<sub>4</sub>AuMg (Ln: Ca, Eu, Yb) are prepared by induction melting of the elements. The structures of Yb<sub>4</sub>PdMg and Ca<sub>4</sub>Ag<sub>0.948</sub>Mg are determined by single crystal XRD. They crystallize with the Gd<sub>4</sub>RhIn-type structure in the space group F43m with Z = 16. Ca<sub>4</sub>Ag<sub>0.948</sub>Mg exhibits segregation of Ca and Mg into different substructures. Calcium forms trigonal prisms around the silver atoms and magnesium forms covalently bonded tetrahedra, which are embedded in larger cavities of the adamantane-like three-dimensional network of edge- and corner-sharing AgCa<sub>6</sub> trigonal prisms. The electronic structure and chemical bonding in Ca<sub>4</sub>AgMg is analyzed by means of DFT calculations. Eu<sub>4</sub>PdMg and Eu<sub>4</sub>PtMg show Curie—Weiss behavior above 230 K. Ferromagnetic ordering occurs at 150.1 and 139.1 K for the Pd- and Pt-containing compound, respectively. — (KERSTING, M.; MATAR, S. F.; SCHWICKERT, C.; POETTGEN\*, R.; Z. Naturforsch., B: Chem. Sci. 67 (2012) 1, 61-69; Inst. Anorg. Anal. Chem., Westfael. Wilhelms-Univ., D-48149 Muenster, Germany; Eng.) — W. Pewestorf