Tetracalcium Trimagnesium Tetradekahydride, $Ca_4Mg_3H_{14}$: The First Ternary Alkaline Earth Hydride*

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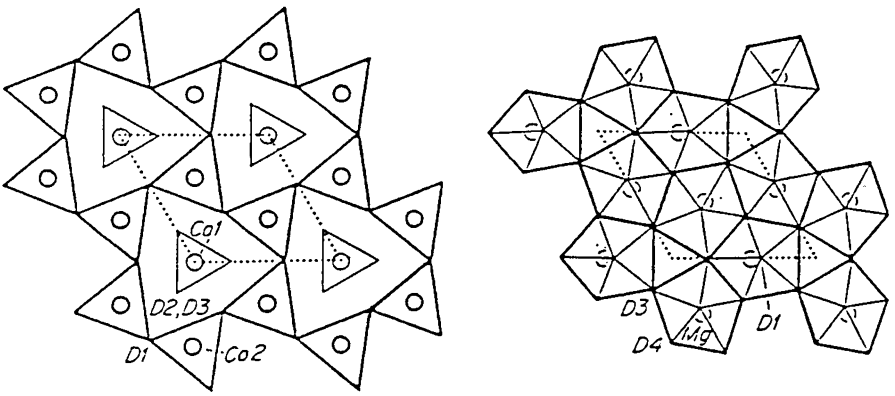
The title compound and its deuteride, $Ca_4Mg_3D_{14}$, were prepared from CaMg alloy at 410(10)°C (deuteride: 458(8)°C) under 53(3) bar hydrogen (95(5) bar deuterium) pressure, and characterized by X-ray and neutron powder diffraction. The compound crystallizes with a new hexagonal



a b

Deuterium coordination polyhedra around the metal atoms in hexagonal $Ca_4Mg_3D_{14}$, projected along [0001]. (a) tricapped trigonal prisms around Ca1 (thin lines) and Ca2 (thick lines); (b) pentagonal bipyramids around Mg. Ca1 in $z = 0.27$, Ca2 in $z = 1/2$, Mg in $z = 0$, D1 in $z = 0.27$, D2 in $z = 1/2$, D3 and D4 in $z = 0$.

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structure type (space group $P\bar{6}2m$ (189); lattice parameters at 20°C: a = 6.3056(2) Å, c = 6.8820(2) Å (hydride), a = 6.2902(2) Å, c = 6.8540(3) Å (deuteride), Z = 1) that contains an ordered array of four symmetry independent deuterium atoms having respectively tetrahedral (D1: [3Ca, Mg], D2: [4Ca]), trigonal bipyramidal (D3: [2Ca, 3Mg]) and triangular (D4: [3Mg]) metal coordinations. The metal–deuterium bond distances range from 1.85 to 2.44 Å (Mg–D) and from 2.29 to 2.48 Å (Ca–D).