

Ca₄Mg₃H₁₄*hP21*(189) *P-62m – igf²edc***Ca₄Mg₃H₁₄** [1]

Structural features: Filled-up derivative of Zr_4Al_3 with H in tetrahedral (Ca₄, Ca₃Mg), trigonal bipyramidal (Ca₂Mg₃) and trigonal (Mg₃) voids.

Gingl F. et al. (1992) [1]

Ca₄D₁₄Mg₃ $a = 0.62902$, $c = 0.6854$ nm, $c/a = 1.090$, $V = 0.2349$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	6i	..m	0.6103	0	0.2748		single atom Mg
D2	3g	<i>m2m</i>	0.2619	0	$\frac{1}{2}$		tetrahedron Ca ₄
D3	3f	<i>m2m</i>	0.2296	0	0		single atom Mg
Mg4	3f	<i>m2m</i>	0.5519	0	0		pentagonal bipyramid D ₇
Ca5	2e	3.m	0	0	0.2684		tricapped trigonal prism D ₉
Ca6	2d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism D ₉
D7	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle Mg ₃

Experimental: powder, diffractometer, neutrons, $R_p = 0.023$, $T = 293$ KRemarks: Identical to the phase called CaMgH_{3.72} in [2].

References: [1] Gingl F., Bonhomme F., Yvon K., Fischer P. (1992), J. Alloys Compd. 185, 273-278. [2] Nomura K., Ishido Y., Ono S. (1978), Yogyo Kyokaishi 86, 67-72.