

$(\text{Li}_{0.1}\text{Ca}_{0.9})(\text{Li}_{0.03}\text{Ge}_{0.97})_2$	$hP6$	$(186) P6_3mc - b^2a$
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Li_{0.13}Ca_{0.9}Ge_{1.97} [1]; "CaGe₂ 2H" [1]

Structural features: Infinite puckered hexagon-mesh Ge layers in h stacking; Ca in trigonal prismatic voids (partial substitution ignored).

Müller W. et al. (1970) [1]

Ca_{0.90}Ge_{1.97}Li_{0.13}

$a = 0.398$, $c = 1.019$ nm, $c/a = 2.560$, $V = 0.1398$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.292		16-vertex polyhedron Ge ₁₀ Ca ₆
M2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.604		monocapped trigonal prism Ge ₃ Ca ₄
M3	$2a$	$3m.$	0	0	0.0		trigonal prism Ge ₃ Ca ₃

M1 = 0.9Ca + 0.1Li; M2 = 0.985Ge + 0.015Li; M3 = 0.985Ge + 0.015Li

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.208

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.103$

Remarks: The phase is also referred to as 2H-CaGe₂ but is only observed with substitution by Li.

References: [1] Müller W., Schäfer H., Weiss A. (1970), Z. Naturforsch. B 25, 431-432.