

$\text{Ba}_{0.5}\text{CaIn}_3\text{O}_6$	$hP24$	$(176) P6_3/m - h^3ec$
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BaCa₂In₆O₁₂ [1]; (K,Na)_{0.9}(Mg,Fe)₂(Mg,Fe,Al,Si)₆O₁₂ [3]

Structural features: Double infinite chains of edge-linked InO₆ octahedra share vertices to form a 3D-framework; Ca in trigonal prismatic voids, Ba in channels of hexagonal cross-section parallel to [001] (partial disorder). Variant of Sr_{0.5}CaSc₃O₆.

Lalla A., Müller Buschbaum H. (1988) [1]

$\text{Ba}_{0.50}\text{CaIn}_3\text{O}_6$

$a = 0.988$, $c = 0.3211$ nm, $c/a = 0.325$, $V = 0.2714$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	$6h$	$m..$	0.0032	0.3501	$\frac{1}{4}$		octahedron O ₆
O2	$6h$	$m..$	0.1958	0.3051	$\frac{1}{4}$		non-coplanar triangle In ₃
O3	$6h$	$m..$	0.6012	0.1339	$\frac{1}{4}$		square pyramid In ₃ Ca ₂
Ba4	$4e$	$3..$	0	0	0.143	0.25	
Ca5	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O ₆

Experimental: single crystal, diffractometer, X-rays, $R = 0.077$

Remarks: Short interatomic distances for partly occupied site(s). An incommensurate structure is reported for off-stoichiometric Ba_{0.85}Ca_{2.15}In₆O₁₂ in [2], modulation vector $a^*/3+b^*/3+0.1385(1)c^*$.

References: [1] Lalla A., Müller Buschbaum H. (1988), Z. Anorg. Allg. Chem. 563, 11-15. [2] Baldinozzi G., Goutenoire F., Hervieu M., Suard E., Grebille D. (1996), Acta Crystallogr. B 52, 780-789. [3] Gasparik T., Tripathi A., Parise J.B. (2000), Am. Mineral. 85, 613-618.