Ca_5Pb_3	*hP*48	(186) $P6_3mc$ – dc^6

Ca_5Pb_3 [1]
Structural features: $PbCa_8Ca$ monocapped square antiprisms ($PbCa_6Ca_3$ tricapped trigonal prisms) share atoms to form a 3D-framework with infinite columns of face-linked Ca_6 octahedra and infinite linear -Ca- chains parallel to [001]. Deformation derivative of Mn_5Si_3.

Helleis O. et al. (1963) [1]
Ca_5Pb_3
a = 1.623, c = 0.704 nm, c/a = 0.434, V = 1.6060 nm^3, Z = 6

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Ca1	12*d*	1	0.000	0.333	0.260		14-vertex Frank-Kasper Pb_6Ca_8
Ca2	6*c*	.*m*.	0.087	0.913	0.040		15-vertex polyhedron Pb_5Ca_{10}
Pb3	6*c*	.*m*.	0.203	0.797	0.010		pseudo Frank-Kasper Ca_9Pb_2
Ca4	6*c*	.*m*.	0.421	0.579	0.040		15-vertex polyhedron Pb_5Ca_{10}
Pb5	6*c*	.*m*.	0.537	0.463	0.008		pseudo Frank-Kasper Ca_9Pb_2
Ca6	6*c*	.*m*.	0.756	0.244	0.036		15-vertex polyhedron Pb_5Ca_{10}
Pb7	6*c*	.*m*.	0.870	0.130	0.000		pseudo Frank-Kasper Ca_9Pb_2

Transformation from published data: origin shift 0 0 0.240
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.180

Remarks: The presence of additional Ca in Wyckoff positions 2*a* and 2*b* was tested and rejected; partial occupation of these sites by B, C or O could not be excluded. Refinement in the Mn_5Si_3-type subcell gave R = 0.14. On page 93 of [1] the Hermann-Mauguin symbol for the space group is misprinted as $P6_3/cm$ instead of $P6_3cm$; on page 98 the Wyckoff position of the fourth Ca site is misprinted as 12*c* instead of 12*d*.

References: [1] Helleis O., Kandler H., Leicht E., Quiring W., Wölfel E. (1963), Z. Anorg. Allg. Chem. 320, 86-100.