

LiCd[BO₃]*hP*18(174) *P*-6 – k²j³eda**LiCdBO₃ form I** [1]

Structural features: Infinite chains of edge-linked CdO₅ square pyramids are interconnected via BO₃ trigonal units (perpendicular to [001]) to form a 3D-framework; Li in tetrahedral voids.

Sokolova E.V. et al. (1980) [1]

BCdLiO₃ $a = 0.8324$, $c = 0.32638$ nm, $c/a = 0.392$, $V = 0.1958$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	3 <i>k</i>	<i>m</i> ..	0.14433	0.54067	$\frac{1}{2}$		single atom B
Cd2	3 <i>k</i>	<i>m</i> ..	0.32673	0.29717	$\frac{1}{2}$		square pyramid O ₅
Li3	3 <i>j</i>	<i>m</i> ..	0.05233	0.37767	0		tetrahedron O ₄
O4	3 <i>j</i>	<i>m</i> ..	0.10733	0.19267	0		single atom B
O5	3 <i>j</i>	<i>m</i> ..	0.47433	0.23167	0		single atom B
B6	1 <i>e</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	0		coplanar triangle O ₃
B7	1 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		coplanar triangle O ₃
B8	1 <i>a</i>	-6..	0	0	0		coplanar triangle O ₃

Transformation from published data: *y*,*x*,*z*; origin shift $\frac{2}{3}$ $\frac{1}{3}$ $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.037

References: [1] Sokolova E.V., Simonov M.A., Belov N.V. (1980), Sov. Phys. Crystallogr. 25, 733-734 (Kristallografiya 25, 1285-1286).