

$\text{Li}[\text{ClO}_4][\text{H}_2\text{O}]_3$	$hP18$	$(186) P6_3mc - c^2b^2a$
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$\text{LiClO}_4 \cdot 3\text{H}_2\text{O}$ [2], Strukturbericht notation $\text{H}4_{18}$

Structural features: Single ClO_4 tetrahedra and infinite chains of face-linked $\text{Li}(\text{OH}_2)_6$ octahedra. Li and Cl form a NiAs-type sublattice. See Fig. IV.22.

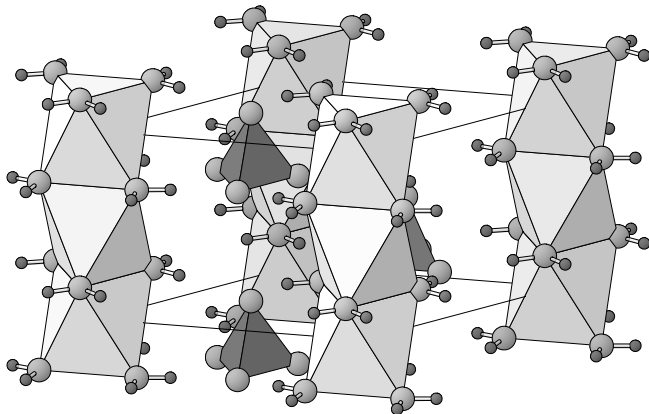


Fig. IV.22. **$\text{LiClO}_4 \cdot 3\text{H}_2\text{O}$**

Arrangement of ClO_4 tetrahedra (dark) and $\text{Li}(\text{OH}_2)_6$ octahedra (light) (O atoms large, H atoms small).

Lundgren J.O. et al. (1982) [1]

ClH_6LiO_7

$a = 0.77192$, $c = 0.54531$ nm, $c/a = 0.706$, $V = 0.2814$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$6c$	$.m.$	0.43466	0.56534	0.18769		single atom Cl
O2	$6c$	$.m.$	0.87768	0.12232	0.24884		non-colinear Li_2
Cl3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.27671		tetrahedron O_4
O4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.53861		single atom Cl
Li5	$2a$	$3m.$	0	0	0.0		8-vertex polyhedron O_6Li_2
H6	$12d$	1	0.32988	0.06662	0.24289		

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.72329

Experimental: single crystal, diffractometer, neutrons, $R = 0.047$, $T = 294$ K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lundgren J.O., Liminga R., Tellgren R. (1982), Acta Crystallogr. B 38, 15-20. [2] West C.D. (1934), Z. Kristallogr. 88, 198-204.