

Li₄Fe[C₂O₄]₃Cl[H₂O]₉

hP132

(188) *P*-6c2 – 1⁸k³jihg**Li₄[Fe(C₂O₄)₃]Cl·9H₂O [1]**

Structural features: Distorted Fe[C₂O₄]₃ octahedral units (a FeO₆ octahedron sharing edges with three planar O₂C-CO₂ (oxalate) units) and similar Li[C₂O₄]₃ units are interconnected to form infinite slabs with large rings centered by Cl; additional Li and H₂O between the slabs.

Declercq J.P. et al. (1993) [1]

C₆ClFeH₁₈Li₄O₂₁*a* = 0.9465, *c* = 2.672 nm, *c/a* = 2.823, *V* = 2.0730 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12l	1	0.01943	0.18697	0.0583		single atom C
C2	12l	1	0.11873	0.32957	0.0753		coplanar triangle O ₂ C
O3	12l	1	0.15223	0.46297	0.0559		single atom C
O4	12l	1	0.15913	0.18967	0.1428		single atom C
C5	12l	1	0.20093	0.33187	0.1259		non-coplanar triangle O ₂ C
O6	12l	1	0.29723	0.46247	0.1443		single atom C
(OH ₂)7	12l	1	0.40743	0.33117	0.0383		single atom Li
(OH ₂)8	12l	1	0.46083	0.06277	0.185		single atom Li
(OH ₂)9	6k	<i>m</i> ..	0.20793	0.44417	1/4		single atom Li
(OH ₂)10	6k	<i>m</i> ..	0.23003	0.13217	1/4		single atom Li
Li11	6k	<i>m</i> ..	0.35693	0.02817	1/4		tetrahedron (OH ₂) ₄
Li12	6j	..2	0.47093	0.52907	0		tetrahedron (OH ₂) ₂ O ₂
Cl13	4i	3..	2/3	1/3	0.11		octahedron (OH ₂) ₆
Li14	4h	3..	1/3	2/3	0.1011		octahedron O ₆
Fe15	4g	3..	0	0	0.10023		octahedron O ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 2/3 1/3 0Experimental: single crystal, diffractometer, X-rays, *R* = 0.046, *T* = 295 K

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

References: [1] Declercq J.P., Feneau Dupont J., Ladrière J. (1993), *Polyhedron* 12, 1031-1037.