$LiClO_4 \cdot 3H_2O$ ($H4_{18}$) Structure: AB6CD7_hP30_186_b_d_a_b2c-001

This structure originally had the label `AB6CD7_hP30_186_b_d_a_b2c`. Calls to that address will be redirected here.

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https://aflow.org/p/TXNW

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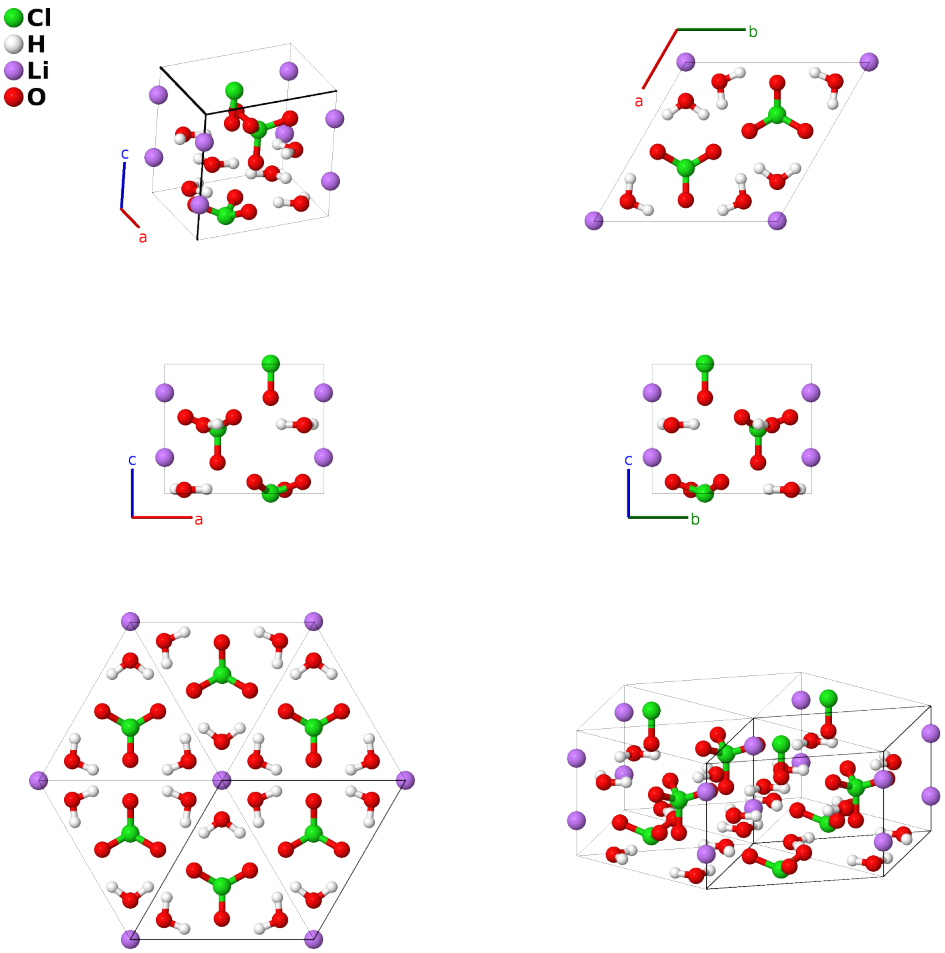


Prototype	ClH_6LiO_7
AFLOW prototype label	AB6CD7_hP30_186_b_d_a_b2c-001
***Strukturbericht* designation**	$H4_{18}$
ICSD	32534
Pearson symbol	hP30
Space group number	186
Space group symbol	$P6_3mc$

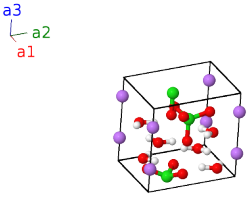
AFLOW prototype command `aflow --proto=AB6CD7_hP30_186_b_d_a_b2c-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6$

Other compounds with this structure

$LiTcO_4{\cdot}3H_2O$

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	Cl I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Cl I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1+2x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_9}$	=	$-2x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1-2x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{12}}$	=	$2x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1+2x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{15}}$	=	$-2x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{17}}$	=	$-x_5\,\mathbf{a}_1-2x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{18}}$	=	$2x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_6+y_6\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_6-y_6\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{20}}$	=	$-y_6\,\mathbf{a}_1+\left(x_6-y_6\right)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_6-2y_6\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{21}}$	=	$-\left(x_6-y_6\right)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_6-y_6\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_6+y_6\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\left(x_6-y_6\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{23}}$	=	$y_6\,\mathbf{a}_1-\left(x_6-y_6\right)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_6+2y_6\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{24}}$	=	$\left(x_6-y_6\right)\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_6-y_6\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{25}}$	=	$-y_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_6+y_6\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_6-y_6\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(12d)	H I

$\mathbf{B_{26}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{27}}$	=	$x_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{28}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{29}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	H I
$\mathbf{B_{30}}$	=	$-x_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	H I

References

[1] J.-O. Lundgren, R. Liminga, and R. Tellgren, *Neutron diffraction refinement of pyroelectric lithium perchlorate trihydrate*, Acta Crystallogr. Sect. B **38**, 15–20 (1982), doi:10.1107/S0567740882001940.

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