LiKSO$_4$ ($H1_4$) Structure: ABC4D_hP14_173_a_b_bc_b-001
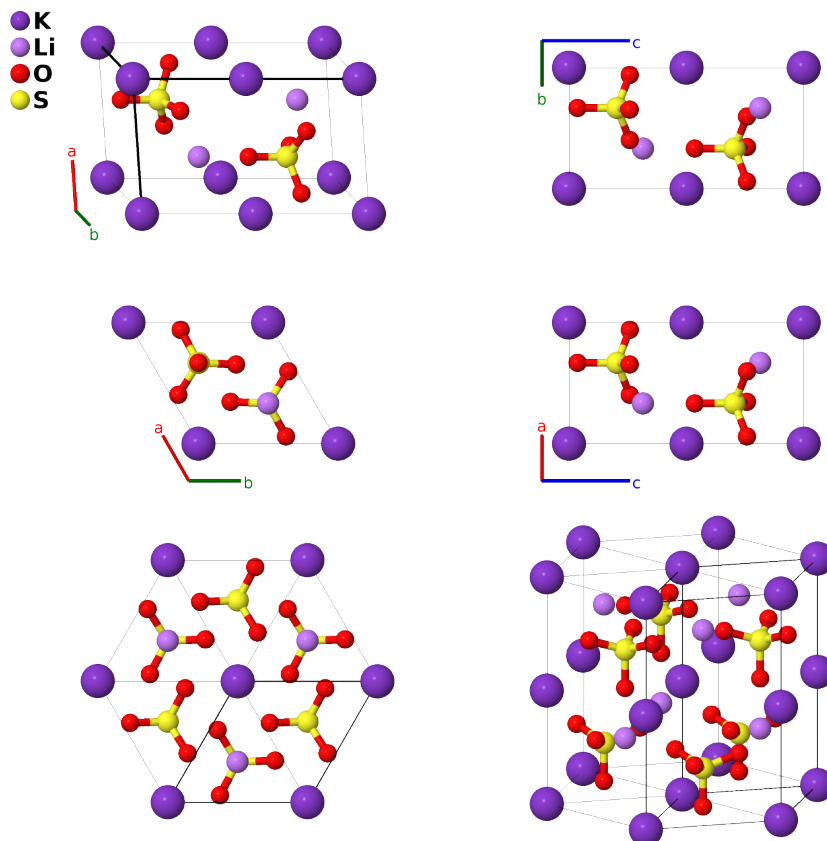
This structure originally had the label `ABC4D_hP14_173_a_b_bc_b`. Calls to that address will be redirected here.

https://aflow.org/p/F86C

https://aflow.org/p/ABC4D_hP14_173_a_b_bc_b-001

Prototype	KLiO$_4$S
AFLOW prototype label	ABC4D_hP14_173_a_b_bc_b-001
***Strukturbericht* designation**	$H1_4$
ICSD	48136
Pearson symbol	hP14
Space group number	173
Space group symbol	$P6_3$
AFLOW prototype command	aflow --proto=ABC4D_hP14_173_a_b_bc_b-001 --params=$a, c/a, z_1, z_2, z_3, z_4, x_5, y_5, z_5$

- As there is no center of symmetry in the structure, the point $z = 0$ can be set arbitrarily. Following (Bhakay-Tamhane, 1984) we set $z_1 = 0$.

- While *Strukturbericht* symbols $H1_1$, $H1_2$ and $H1_5$ are identical with $S1_1$, $S1_2$ and $S1_5$, respectively, there is no connection between this structure and $S1_4$, garnet (A2B3C12D3_cI160_230_a_c_h_d).

Hexagonal primitive vectors

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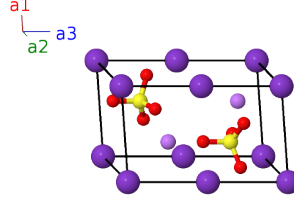
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a_3}$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	K I
$\mathbf{B_2}$	=	$\left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$c\left(z_1 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2a)	K I
$\mathbf{B_3}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Li I
$\mathbf{B_4}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2b)	Li I
$\mathbf{B_5}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_6}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_7}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2b)	S I
$\mathbf{B_8}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2b)	S I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{10}}$	=	$-y_5\,\mathbf{a_1} + \left(x_5 - y_5\right)\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{11}}$	=	$-\left(x_5 - y_5\right)\mathbf{a_1} - x_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$-\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{13}}$	=	$y_5\,\mathbf{a_1} - \left(x_5 - y_5\right)\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(-x_5 + 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{14}}$	=	$\left(x_5 - y_5\right)\mathbf{a_1} + x_5\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(6c)	O II

References

[1] S. Bhakay-Tamhane, A. Sequiera, and R. Chidambaram, *Structure of lithium potassium sulphate, LiKSO₄: a neutron diffraction study*, Acta Crystallogr. Sect. C **40**, 1648–1651 (1984), doi:10.1107/S0108270184009045.