LiNb$_6$O$_{15}$F Structure: ABC6D15_oP46_51_f_b_2e2i_cef4i2j-001

This structure originally had the label `ABC6D15_oP46_51_f_d_2e2i_aef4i2j`. Calls to that address will be redirected here.

https://aflow.org/p/0JVV

https://aflow.org/p/ABC6D15_oP46_51_f_b_2e2i_cef4i2j-001
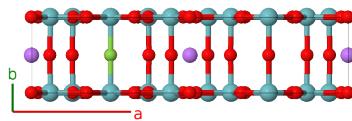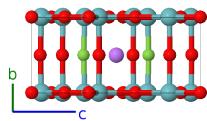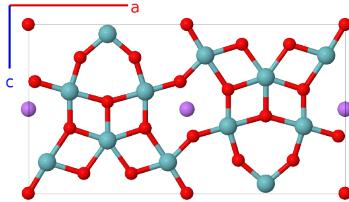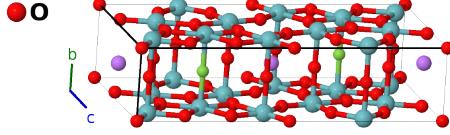
Prototype	FLiNb$_6$O$_{15}$
AFLOW prototype label	ABC6D15_oP46_51_f_b_2e2i_cef4i2j-001
ICSD	2910
Pearson symbol	oP46
Space group number	51
Space group symbol	$Pmma$
AFLOW prototype command	`aflow --proto=ABC6D15_oP46_51_f_b_2e2i_cef4i2j-001` `        --params=`$a, b/a, c/a, z_3, z_4, z_5, z_6, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13},$ $x_{14}, z_{14}, x_{15}, z_{15}$

- (Lundberg, 1965) suggests that the lithium atoms are either on the (2d) site or are statistically distributed on a (4f) site with approximate coordinates (0.08,1/2,0.10). For simplicity we place the atoms on the (2d) site.

- The X-ray scattering of an F$^-$ ion is almost identical to that of O^{-2}, and Lundberg was not able to distinguish between them. She arbitrarily designated the (2f) site she called O$_4$ as the location of the fluorine ion and we follow this, but in reality we have no idea if the F$^-$ ions are located on this site, are ordered on another site, or are statistically distributed on the oxygen sites.

- The ICSD entry does not place the lithium atoms.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
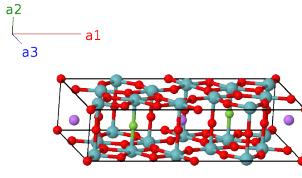
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\frac{1}{2}\,\mathbf{a_2}$	$=$	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Li I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Li I
$\mathbf{B_3}$	$=$	$\frac{1}{2}\,\mathbf{a_3}$	$=$	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_5}$	$=$	$\frac{1}{4}\,\mathbf{a_1} + z_3\,\mathbf{a_3}$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(2e)	Nb I
$\mathbf{B_6}$	$=$	$\frac{3}{4}\,\mathbf{a_1} - z_3\,\mathbf{a_3}$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(2e)	Nb I
$\mathbf{B_7}$	$=$	$\frac{1}{4}\,\mathbf{a_1} + z_4\,\mathbf{a_3}$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(2e)	Nb II
$\mathbf{B_8}$	$=$	$\frac{3}{4}\,\mathbf{a_1} - z_4\,\mathbf{a_3}$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(2e)	Nb II
$\mathbf{B_9}$	$=$	$\frac{1}{4}\,\mathbf{a_1} + z_5\,\mathbf{a_3}$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B_{10}}$	$=$	$\frac{3}{4}\,\mathbf{a_1} - z_5\,\mathbf{a_3}$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B_{11}}$	$=$	$\frac{1}{4}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2f)	F I
$\mathbf{B_{12}}$	$=$	$\frac{3}{4}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(2f)	F I
$\mathbf{B_{13}}$	$=$	$\frac{1}{4}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2f)	O III
$\mathbf{B_{14}}$	$=$	$\frac{3}{4}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(2f)	O III
$\mathbf{B_{15}}$	$=$	$x_8\,\mathbf{a_1} + z_8\,\mathbf{a_3}$	$=$	$ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(4i)	Nb III
$\mathbf{B_{16}}$	$=$	$-\left(x_8 - \frac{1}{2}\right)\mathbf{a_1} + z_8\,\mathbf{a_3}$	$=$	$-a\left(x_8 - \frac{1}{2}\right)\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(4i)	Nb III
$\mathbf{B_{17}}$	$=$	$-x_8\,\mathbf{a_1} - z_8\,\mathbf{a_3}$	$=$	$-ax_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(4i)	Nb III
$\mathbf{B_{18}}$	$=$	$\left(x_8 + \frac{1}{2}\right)\mathbf{a_1} - z_8\,\mathbf{a_3}$	$=$	$a\left(x_8 + \frac{1}{2}\right)\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(4i)	Nb III
$\mathbf{B_{19}}$	$=$	$x_9\,\mathbf{a_1} + z_9\,\mathbf{a_3}$	$=$	$ax_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(4i)	Nb IV
$\mathbf{B_{20}}$	$=$	$-\left(x_9 - \frac{1}{2}\right)\mathbf{a_1} + z_9\,\mathbf{a_3}$	$=$	$-a\left(x_9 - \frac{1}{2}\right)\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(4i)	Nb IV
$\mathbf{B_{21}}$	$=$	$-x_9\,\mathbf{a_1} - z_9\,\mathbf{a_3}$	$=$	$-ax_9\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}}$	(4i)	Nb IV
$\mathbf{B_{22}}$	$=$	$\left(x_9 + \frac{1}{2}\right)\mathbf{a_1} - z_9\,\mathbf{a_3}$	$=$	$a\left(x_9 + \frac{1}{2}\right)\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}}$	(4i)	Nb IV
$\mathbf{B_{23}}$	$=$	$x_{10}\,\mathbf{a_1} + z_{10}\,\mathbf{a_3}$	$=$	$ax_{10}\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{24}}$	$=$	$-\left(x_{10} - \frac{1}{2}\right)\mathbf{a_1} + z_{10}\,\mathbf{a_3}$	$=$	$-a\left(x_{10} - \frac{1}{2}\right)\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{25}}$	$=$	$-x_{10}\,\mathbf{a_1} - z_{10}\,\mathbf{a_3}$	$=$	$-ax_{10}\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{26}}$	$=$	$\left(x_{10} + \frac{1}{2}\right)\mathbf{a_1} - z_{10}\,\mathbf{a_3}$	$=$	$a\left(x_{10} + \frac{1}{2}\right)\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{27}}$	$=$	$x_{11}\,\mathbf{a_1} + z_{11}\,\mathbf{a_3}$	$=$	$ax_{11}\,\hat{\mathbf{x}} + cz_{11}\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{28}}$	$=$	$-\left(x_{11} - \frac{1}{2}\right)\mathbf{a_1} + z_{11}\,\mathbf{a_3}$	$=$	$-a\left(x_{11} - \frac{1}{2}\right)\hat{\mathbf{x}} + cz_{11}\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{29}}$	$=$	$-x_{11}\,\mathbf{a_1} - z_{11}\,\mathbf{a_3}$	$=$	$-ax_{11}\,\hat{\mathbf{x}} - cz_{11}\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{30}}$	$=$	$\left(x_{11} + \frac{1}{2}\right)\mathbf{a_1} - z_{11}\,\mathbf{a_3}$	$=$	$a\left(x_{11} + \frac{1}{2}\right)\hat{\mathbf{x}} - cz_{11}\,\hat{\mathbf{z}}$	(4i)	O V

$$\mathbf{B_{31}} = x_{12}\,\mathbf{a}_1 + z_{12}\,\mathbf{a}_3 = ax_{12}\,\hat{\mathbf{x}} + cz_{12}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VI}$$

$$\mathbf{B_{32}} = -\left(x_{12} - \tfrac{1}{2}\right)\mathbf{a}_1 + z_{12}\,\mathbf{a}_3 = -a\left(x_{12} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + cz_{12}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VI}$$

$$\mathbf{B_{33}} = -x_{12}\,\mathbf{a}_1 - z_{12}\,\mathbf{a}_3 = -ax_{12}\,\hat{\mathbf{x}} - cz_{12}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VI}$$

$$\mathbf{B_{34}} = \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a}_1 - z_{12}\,\mathbf{a}_3 = a\left(x_{12} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - cz_{12}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VI}$$

$$\mathbf{B_{35}} = x_{13}\,\mathbf{a}_1 + z_{13}\,\mathbf{a}_3 = ax_{13}\,\hat{\mathbf{x}} + cz_{13}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VII}$$

$$\mathbf{B_{36}} = -\left(x_{13} - \tfrac{1}{2}\right)\mathbf{a}_1 + z_{13}\,\mathbf{a}_3 = -a\left(x_{13} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + cz_{13}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VII}$$

$$\mathbf{B_{37}} = -x_{13}\,\mathbf{a}_1 - z_{13}\,\mathbf{a}_3 = -ax_{13}\,\hat{\mathbf{x}} - cz_{13}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VII}$$

$$\mathbf{B_{38}} = \left(x_{13} + \tfrac{1}{2}\right)\mathbf{a}_1 - z_{13}\,\mathbf{a}_3 = a\left(x_{13} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - cz_{13}\,\hat{\mathbf{z}} \qquad \text{(4i)} \qquad \text{O VII}$$

$$\mathbf{B_{39}} = x_{14}\,\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = ax_{14}\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O VIII}$$

$$\mathbf{B_{40}} = -\left(x_{14} - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = -a\left(x_{14} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O VIII}$$

$$\mathbf{B_{41}} = -x_{14}\,\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -ax_{14}\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - cz_{14}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O VIII}$$

$$\mathbf{B_{42}} = \left(x_{14} + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = a\left(x_{14} + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - cz_{14}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O VIII}$$

$$\mathbf{B_{43}} = x_{15}\,\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = ax_{15}\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O IX}$$

$$\mathbf{B_{44}} = -\left(x_{15} - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = -a\left(x_{15} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O IX}$$

$$\mathbf{B_{45}} = -x_{15}\,\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -ax_{15}\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O IX}$$

$$\mathbf{B_{46}} = \left(x_{15} + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = a\left(x_{15} + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}} \qquad \text{(4j)} \qquad \text{O IX}$$

References

[1] M. Lundberg, *The Crystal Structure of LiNb$_6$O$_{15}$F*, Acta Chem. Scand. **19**, 2274–2284 (1965), doi:10.3891/acta.chem.scand.19-2274.