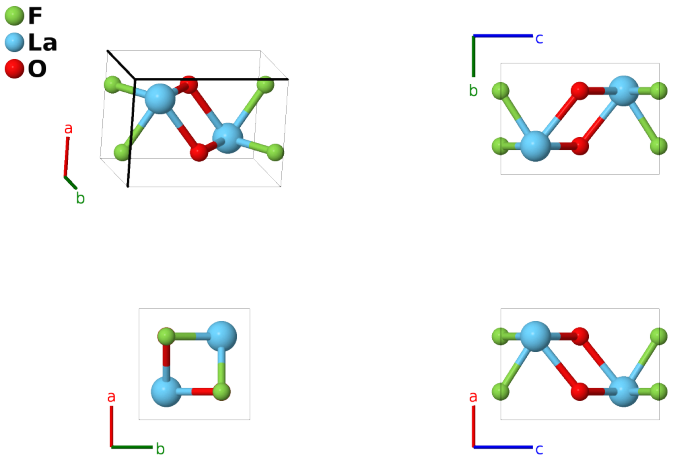
# LaOF Structure: ABC_tP6_129_a_c_b-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/JX34

https://aflow.org/p/ABC_tP6_129_a_c_b-001



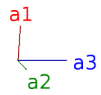

| | |
|---|---|
| **Prototype** | FLaO |
| **AFLOW prototype label** | ABC_tP6_129_a_c_b-001 |
| **ICSD** | 76427 |
| **Pearson symbol** | tP6 |
| **Space group number** | 129 |
| **Space group symbol** | $P4/nmm$ |
| **AFLOW prototype command** | `aflow --proto=ABC_tP6_129_a_c_b-001 --params=`$a, c/a, z_3$ |

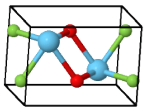
**Other compounds with this structure**
DyOF, ErOF, EuOF, GdOF, HoOF, NdOF, PuOF, PrOF, SmOF, TbOF, YOF

- The general formula for this compound is $XO_xF_{3-2x}$. For $x \leq 1$ the structure is tetragonal (LaOF prototype), and when $x > 1$ it is rhombohedral (YOF prototype). At high temperatures these structures transform into the cubic fluorite ($C1$) structure, with the anions statistically distributed over the (2c) sites. (Zachariasen, 1951; Petzel, 1993)

**Simple Tetragonal primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$ | (2a) | F I |
| $\mathbf{B_2}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$ | (2a) | F I |
| $\mathbf{B_3}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2b) | O I |
| $\mathbf{B_4}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2b) | O I |
| $\mathbf{B_5}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2c) | La I |
| $\mathbf{B_6}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2c) | La I |

**References**


[1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. XIV. Oxyfluorides, XOF*, Acta Cryst. **4**, 231–236 (1951), doi:10.1107/S0365110X51000787.

[2] T. Petzel, V. Marx, and B. Hormann, *Thermodynamics of the rhombohedral-cubic phase transition of ROF with R ≡ Y, La, Pr, Nd, Sm-Er*, J. Alloys Compd. **200**, 27–31 (1993), doi:10.1016/0925-8388(93)90466-Z.


**Found in**


[1] J. W. Fergus, *Crystal structure of lanthanum oxyfluoride*, J. Mater. Sci. Lett. **16**, 267–269 (1997), doi:10.1023/A:1018584614532.