

YOF Structure:

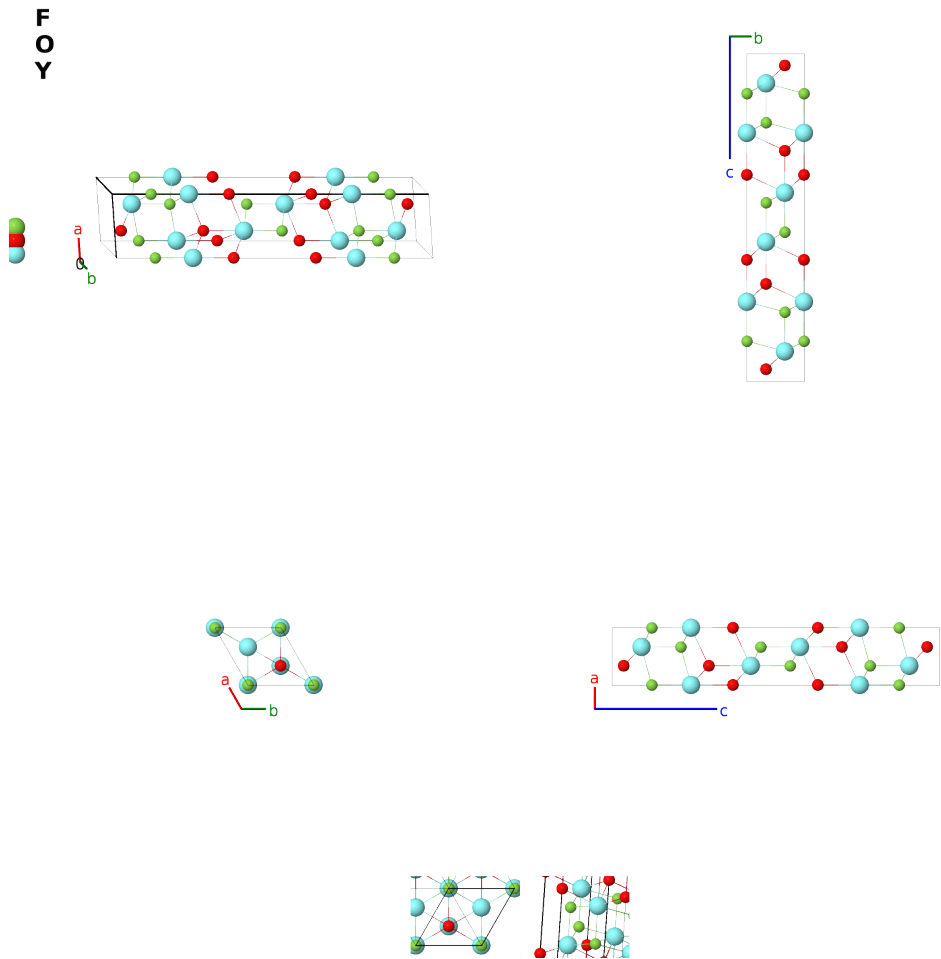
ABC_hR6_166_c_c_c-002

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/DGDK>

https://aflow.org/prototype-encyclopedia/ABC_hR6_166_c_c_c-002



Prototype	FOY
AFLOW prototype label	ABC_hR6_166_c_c_c-002
ICSD	30623
CCDC	1604870
Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$

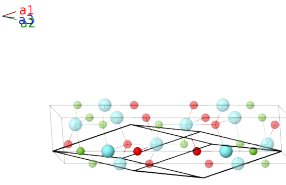
AFLOW prototype command `aflow --proto=ABC_hR6_166_c_c_c-002`
 `--params=a, c/a, x1, x2, x3`

Other compounds with this structure

DyOF, ErOF, EuOF, GdOF, HoOF, LaOF, NdOF, PrOF, SmOF, TbOF

- The general formula for this compound is $\text{XO}_x\text{F}_{3-2x}$. 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)
- SmSI and YOF have the same AFLOW prototype label, ABC_hR6_166_c_c_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c)	F I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c)	F I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Y I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Y 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 $R \equiv Y, La, Pr, Nd, Sm-Er$* , 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.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.