YOF Structure: ABC_hR6_166_c_c_c-002

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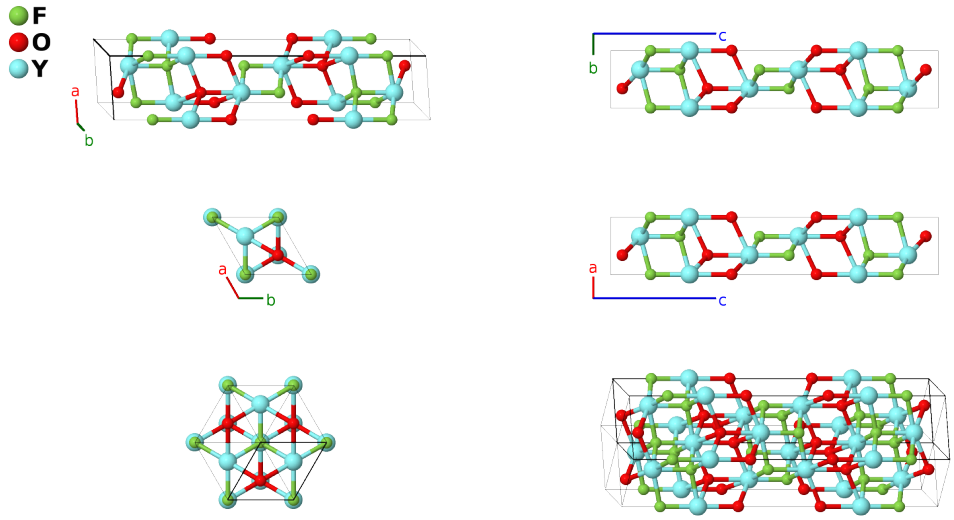
https://aflow.org/p/DGDK

https://aflow.org/p/ABC_hR6_166_c_c_c-002



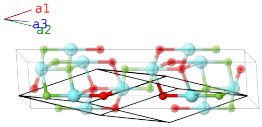
Prototype	FOY
AFLOW prototype label	ABC_hR6_166_c_c_c-002
ICSD	30623
Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC_hR6_166_c_c_c-002 --params=`$a, c/a, x_1, x_2, x_3$

Other compounds with this structure
DyOF, ErOF, EuOF, GdOF, HoOF, LaOF, NdOF, PrOF, SmOF, TbOF

- 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)
- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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

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[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.