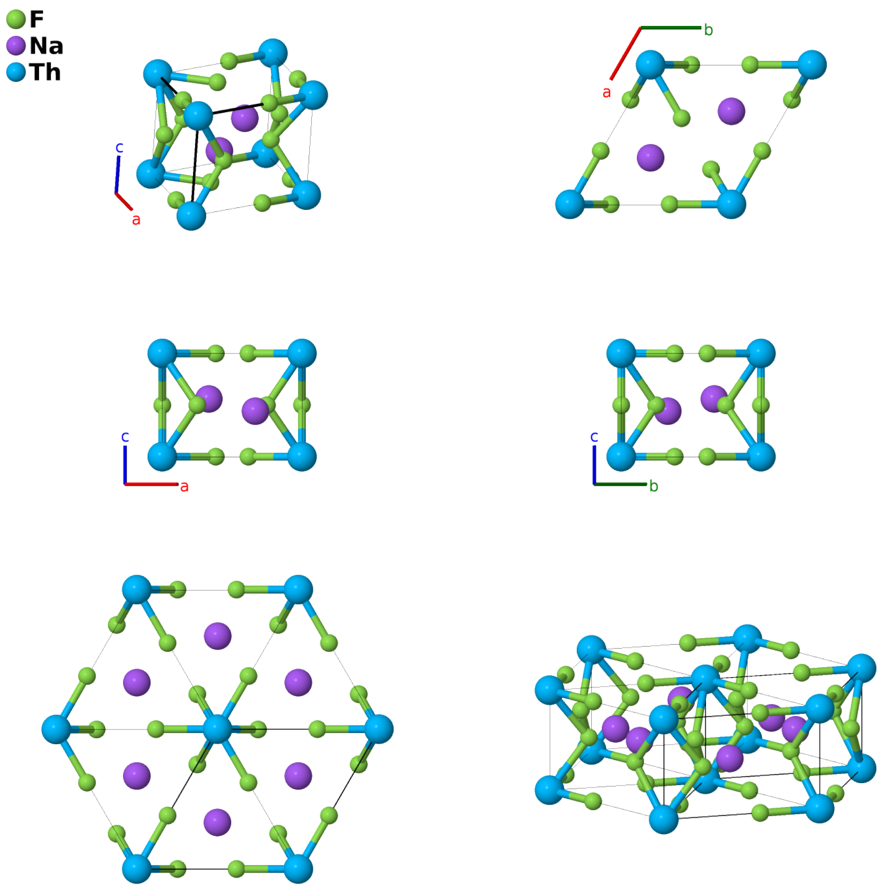
β-Na_2ThF_6 Structure: A6B2C_hP9_150_ef_d_a-001

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/R3Z7

https://aflow.org/p/A6B2C_hP9_150_ef_d_a-001



Prototype	F_6Na_2Th
AFLOW prototype label	A6B2C_hP9_150_ef_d_a-001
ICSD	418148
Pearson symbol	hP9
Space group number	150
Space group symbol	$P321$
AFLOW prototype command	`aflow --proto=A6B2C_hP9_150_ef_d_a-001` `--params=`$a, c/a, z_2, x_3, x_4$

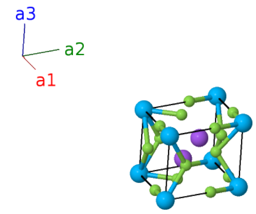
Other compounds with this structure

β_2-K_2UF_6

- When $z_2 = 1/2$ this transforms into δ-Na_2ThF_6 which has the hexagonal β_1-K_2UF_6 structure.
- We use the data from (Grzechnik, 2007) taken at 100K and ambient pressure.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Th I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	Na I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	Na I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3e)	F I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3e)	F I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3e)	F I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	F II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	F II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	F II

References

[1] A. Grzechnik, M. Fechtelkord, W. Morgenroth, J. M. Posse, and K. Friese, *Crystal structure and stability of β-Na_2ThF_6 at non-ambient conditions*, J. Phys.: Condens. Matter **19**, 266219 (2007), doi:10.1088/0953-8984/19/26/266219.

Found in

[1] A. Grzechnik, C. C. Underwood, J. W. Kolis, and K. Friese, *Crystal structures and stability of K_2ThF_6 and $K_7Th_6F_{31}$ on compression*, J. Fluor. Chem. **150**, 8–13 (2013), doi:10.1016/j.jfluchem.2013.02.024.