

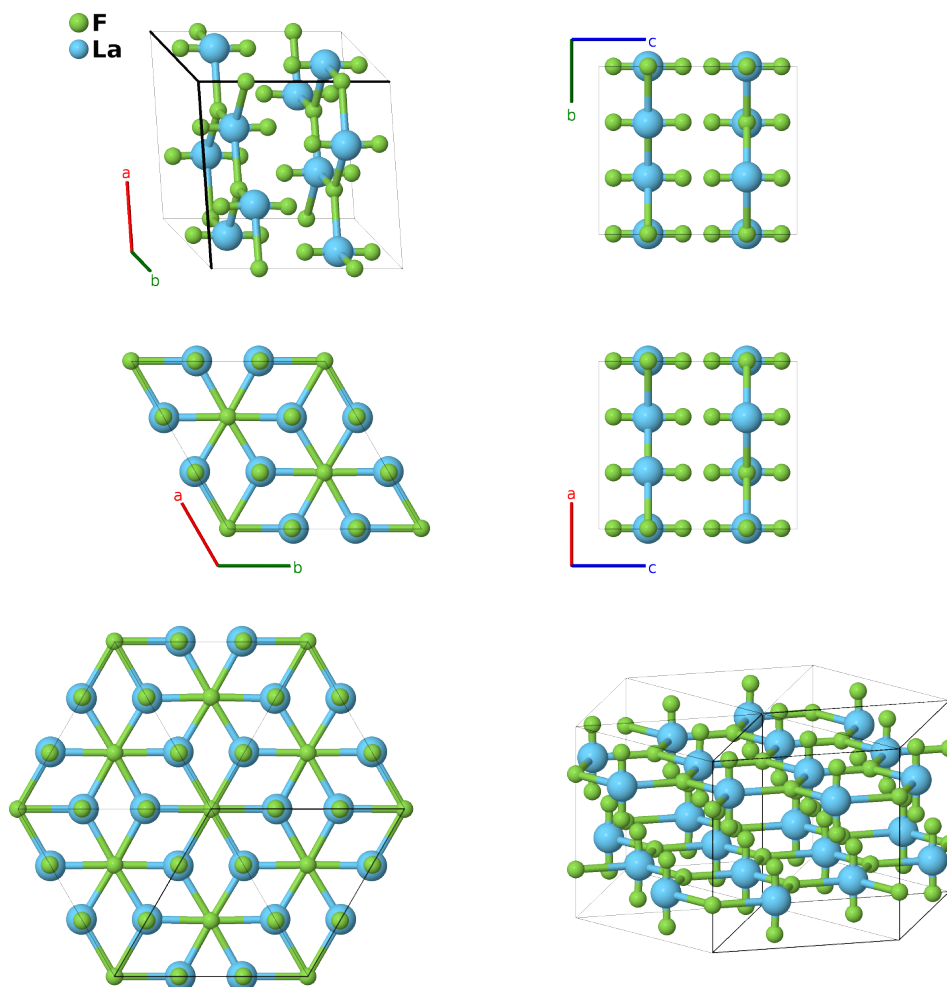
# $D0_6$ (Tysonite, $\text{LaF}_3$ ) Structure (*Obsolete*): A3B\_hP24\_193\_ack\_g-001

This structure originally had the label A3B\_hP24\_193\_ack\_g. Calls to that address will be redirected here.

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<https://aflow.org/p/JJ07>

[https://aflow.org/p/A3B\\_hP24\\_193\\_ack\\_g-001](https://aflow.org/p/A3B_hP24_193_ack_g-001)



Prototype	$\text{F}_3\text{La}$
AFLOW prototype label	A3B_hP24_193_ack_g-001
<i>Strukturbericht</i> designation	$D0_6$
Mineral name	tysonite
ICSD	none
Pearson symbol	hP24
Space group number	193

Space group symbol

$P6_3/mcm$

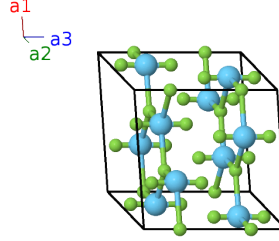
AFLOW prototype command

aflow --proto=A3B\_hP24\_193\_ack\_g-001  
--params= $a, c/a, x_3, x_4, z_4$

- This structure was one of several considered by (Hermann, 1937) as a candidate structure for tysonite, and was chosen because it gave the best positioning of the fluorine atoms. Later, (Zalkin, 1985) showed that the structure was trigonal rather than hexagonal, and isostructural with  $\text{Cu}_3\text{P}$  ( $D0_{21}$ ). We keep the original structure as part of the historical record.

### Hexagonal primitive vectors

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



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2a)	F I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2a)	F I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	F II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	F II
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	F II
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	F II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{16}$	$= -x_4 \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{18}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{20}$	$= x_4 \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	F III
$\mathbf{B}_{21}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	F III

$$\mathbf{B}_{22} = -x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = -\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} \quad (12k) \quad \text{F III}$$

$$\mathbf{B}_{23} = -x_4 \mathbf{a}_1 - z_4 \mathbf{a}_3 = -\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} \quad (12k) \quad \text{F III}$$

$$\mathbf{B}_{24} = x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - cz_4 \hat{\mathbf{z}} \quad (12k) \quad \text{F III}$$

## References

- [1] I. Oftedal, *Zur Kristallstruktur von Tysonit (Ce, La, ...)F<sub>3</sub>*, Z. Physik. Chem. B **13**, 190–200 (1931), doi:10.1515/zpch-1931-1315.
- [2] A. Zalkin and D. H. Templeton, *Refinement of the trigonal crystal structure of lanthanum trifluoride with neutron diffraction data*, Acta Crystallogr. Sect. B **41**, 91–93 (1985), doi:10.1107/S0108768185001689.

## Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).