

Th₇S₁₂ (D_{8k}) Structure: A3B2_hP20_176_2h_ah-001

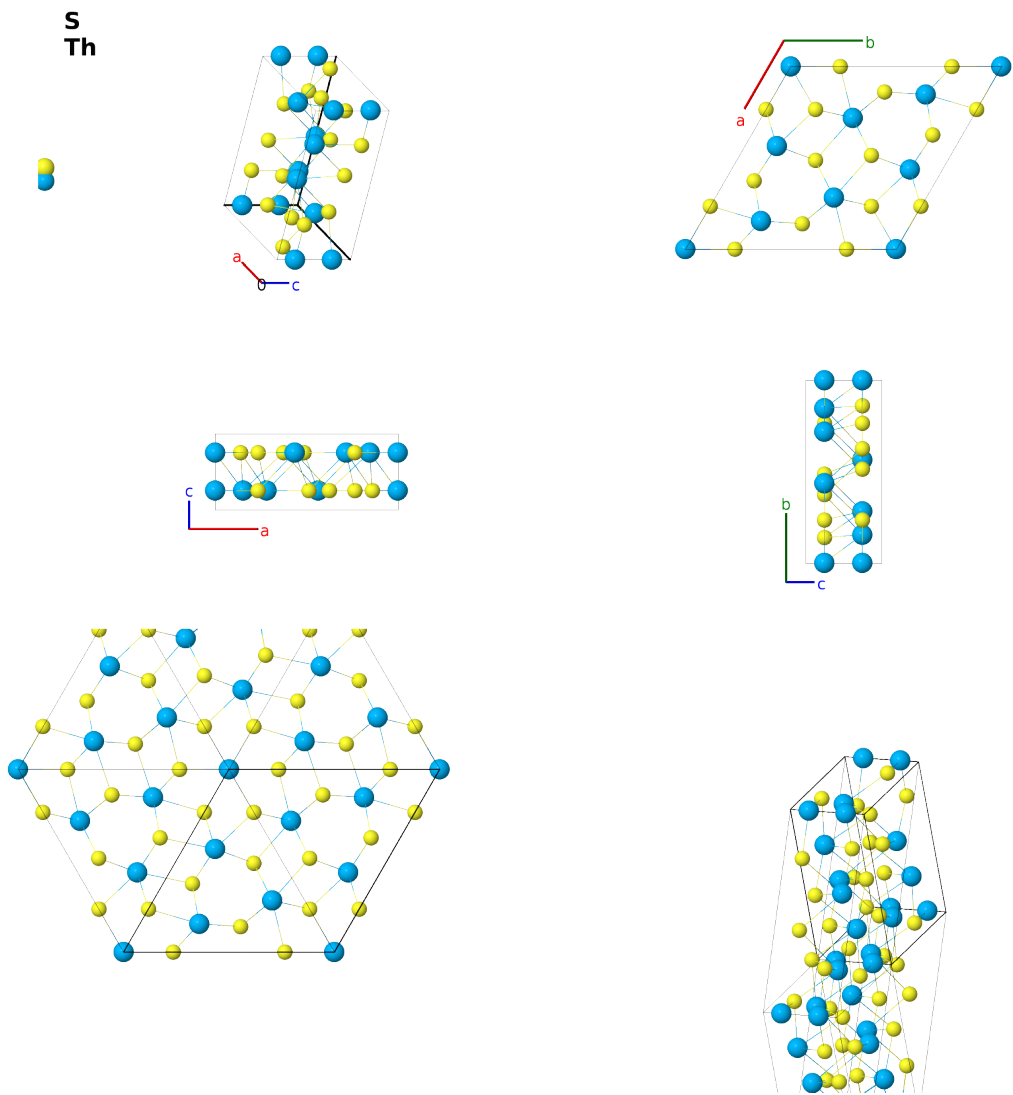
This structure previously used the label(s) **A3B2_hP20_176_2h_ah**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/X9DF>

https://aflow.org/prototype-encyclopedia/A3B2_hP20_176_2h_ah-001



Prototype	S ₁₂ Th ₇
AFLOW prototype label	A3B2_hP20_176_2h_ah-001
Strukturbericht designation	D _{8k}

ICSD	30644
CCDC	1604889
Pearson symbol	hP20
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	<code>aflow --proto=A3B2_hP20_176_2h_ah-001</code> <code>--params=a, c/a, x2, y2, x3, y3, x4, y4</code>

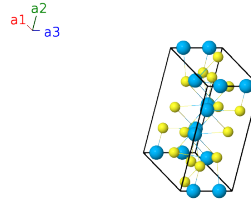
Other compounds with this structure

Th₇Se₁₂, (Ga, As)₇Pd₁₂

- The Th (2a) site is half-filled.
- (Zachariasen, 1949) gives the lattice constants in kX units. We used the conversion factor of 1.00202 from (Woods, 1947) to convert this to Ångströms. The ICSD entry uses kX units.

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)	Th I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2a)	Th I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	S I
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	S I
$\mathbf{B}_5$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	S I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	S I
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	S I
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	S I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	S II
$\mathbf{B}_{10}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	S II
$\mathbf{B}_{11}$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	S II
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	S II
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	S II
$\mathbf{B}_{14}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	S II
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Th II
$\mathbf{B}_{16}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Th II

$$\begin{aligned}
\mathbf{B}_{17} &= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(6h) &\quad \text{Th II} \\
\mathbf{B}_{18} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6h) &\quad \text{Th II} \\
\mathbf{B}_{19} &= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6h) &\quad \text{Th II} \\
\mathbf{B}_{20} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(6h) &\quad \text{Th II}
\end{aligned}$$

References

- [1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. IX. The crystal structure of Th₇S₁₂*, Acta Crystallogr. Sect. B **2**, 288–291 (1949), doi:10.1107/S0365110X49000746.
- [2] E. A. Wood, *The Conversion Factor for kX Units to Angström Units*, J. App. Phys. **18**, 929–930 (1947), doi:10.1063/1.1697570.

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