

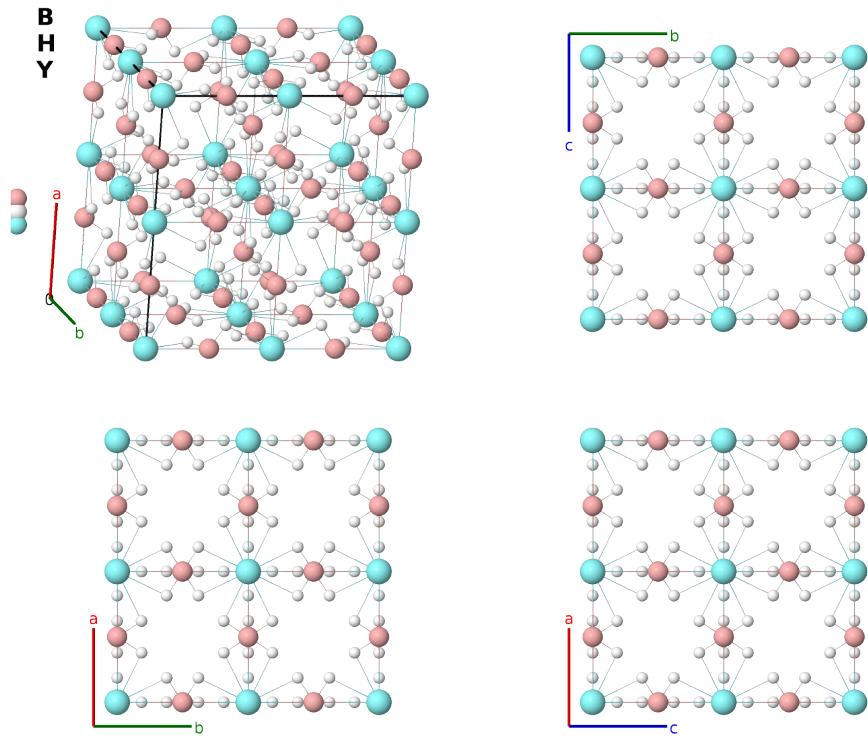
High-Temperature $\text{Y}(\text{BH}_4)_3$ Structure: A3B12C_cF128_226_c_i_b-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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. Osos, 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/T0MK>

https://aflow.org/prototype-encyclopedia/A3B12C_cF128_226_c_i_b-001



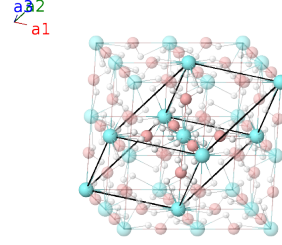
Prototype	$\text{B}_3\text{H}_{12}\text{Y}$
AFLOW prototype label	A3B12C_cF128_226_c_i_b-001
ICSD	167703
CCDC	1683596
Pearson symbol	cF128
Space group number	226
Space group symbol	$Fm\bar{3}c$
AFLOW prototype command	<code>aflow --proto=A3B12C_cF128_226_c_i_b-001 --params=a, y3, z3</code>

Other compounds with this structure
 $\text{Ce}(\text{BH}_4)_3$, $\text{Lu}(\text{BH}_4)_3$, $\text{Nd}(\text{BH}_4)_3$, $\text{Pr}(\text{BH}_4)_3$

- $\text{Y}(\text{BH}_4)_3$ has been observed in three phases (Frommen, 2010):
 - A room temperature cubic phase, stable up to 473K,
 - A (metastable?) orthorhombic phase, found in the 473-520K range, whose structure has not been determined, and
 - This high temperature cubic phase.
- This sample used deuterium, and was prepared at 475K and 10MPa and then cooled to room temperature.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(8b) Y I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(8b) Y I
$\mathbf{B}_3$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24c) B I
$\mathbf{B}_4$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24c) B I
$\mathbf{B}_5$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24c) B I
$\mathbf{B}_6$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24c) B I
$\mathbf{B}_7$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24c) B I
$\mathbf{B}_8$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(24c) B I
$\mathbf{B}_9$	$=$	$(y_3 + z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{10}$	$=$	$-(y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{11}$	$=$	$(y_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{12}$	$=$	$-(y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{13}$	$=$	$(y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{14}$	$=$	$-(y_3 + z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{15}$	$=$	$(y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{z}}$	(96i) H I
$\mathbf{B}_{16}$	$=$	$-(y_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{z}}$	(96i) H I

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{matrix} -(y_3 - z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + \\ (y_3 + z_3) \mathbf{a}_3 \end{matrix} = ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} & (96i) & \text{H I} \\
\mathbf{B}_{18} &= \begin{matrix} (y_3 + z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - \\ (y_3 - z_3) \mathbf{a}_3 \end{matrix} = -ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} & (96i) & \text{H I} \\
\mathbf{B}_{19} &= \begin{matrix} -(y_3 + z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + \\ (y_3 - z_3) \mathbf{a}_3 \end{matrix} = ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} & (96i) & \text{H I} \\
\mathbf{B}_{20} &= \begin{matrix} (y_3 - z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 - \\ (y_3 + z_3) \mathbf{a}_3 \end{matrix} = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} & (96i) & \text{H I} \\
\mathbf{B}_{21} &= \begin{matrix} -(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{22} &= \begin{matrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{23} &= \begin{matrix} (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{24} &= \begin{matrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{25} &= \begin{matrix} (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{26} &= \begin{matrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{27} &= \begin{matrix} -(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{28} &= \begin{matrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{29} &= \begin{matrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{30} &= \begin{matrix} -(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{31} &= \begin{matrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} & (96i) & \text{H I} \\
\mathbf{B}_{32} &= \begin{matrix} (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} & (96i) & \text{H I}
\end{aligned}$$

References

- [1] C. Frommen, N. Aliouane, S. Deledda, J. E. Fonnelløp, H. Grove, K. Lieutenant, I. Llamas-Jansa, S. Sartori, M. H. Sørby, and B. C. Hauback, *Crystal structure, polymorphism, and thermal properties of yttrium borohydride $Y(BH_4)_3$* , J. Alloys Compd.

496, 710–716 (2010), doi:10.1016/j.jallcom.2010.02.180.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 167703 [Y(BH₄)₃].

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).