

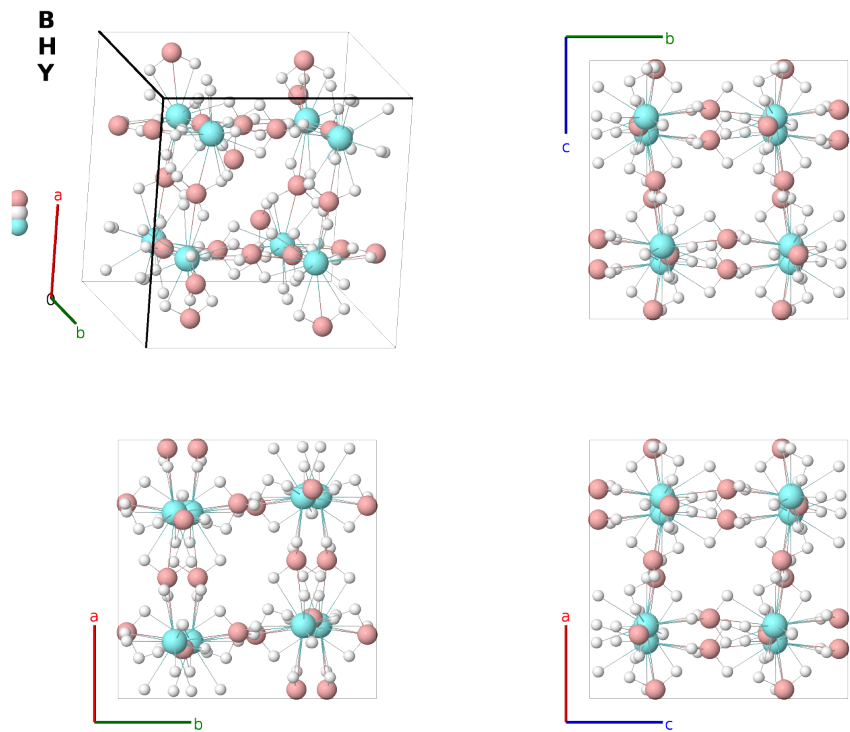
# Room-Temperature Y(BH<sub>4</sub>)<sub>3</sub> Structure: A3B12C\_cP128\_205\_d\_4d\_c-001

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<https://aflow.org/prototype-encyclopedia/71TL>

[https://aflow.org/prototype-encyclopedia/A3B12C\\_cP128\\_205\\_d\\_4d\\_c-001](https://aflow.org/prototype-encyclopedia/A3B12C_cP128_205_d_4d_c-001)



|                         |                                                                                                                                                                                                                                                                                                                 |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | B <sub>3</sub> H <sub>12</sub> Y                                                                                                                                                                                                                                                                                |
| AFLOW prototype label   | A3B12C_cP128_205_d_4d_c-001                                                                                                                                                                                                                                                                                     |
| ICSD                    | 167702                                                                                                                                                                                                                                                                                                          |
| CCDC                    | 1683595                                                                                                                                                                                                                                                                                                         |
| Pearson symbol          | cP128                                                                                                                                                                                                                                                                                                           |
| Space group number      | 205                                                                                                                                                                                                                                                                                                             |
| Space group symbol      | $Pa\bar{3}$                                                                                                                                                                                                                                                                                                     |
| AFLOW prototype command | <pre>aflow --proto=A3B12C_cP128_205_d_4d_c-001 --params=a, x<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></pre> |

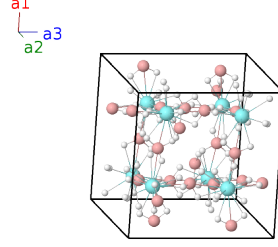
**Other compounds with this structure**  
Ce(BH<sub>4</sub>)<sub>3</sub>, Lu(BH<sub>4</sub>)<sub>3</sub>, Nd(BH<sub>4</sub>)<sub>3</sub>, Pr(BH<sub>4</sub>)<sub>3</sub>

- $\text{Y}(\text{BH}_4)_3$  has been observed in three phases (Frommen, 2010):
  - This 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
  - A high temperature cubic phase.
- This sample used deuterium, and the data was taken at 293K.

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### Simple Cubic primitive vectors

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




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### Basis vectors

|                   | Lattice<br>coordinates                                                                                            |     | Cartesian<br>coordinates                                                                                                       | Wyckoff<br>position | Atom<br>type |
|-------------------|-------------------------------------------------------------------------------------------------------------------|-----|--------------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$                                                        | $=$ | $ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$                                                        | (8c)                | Y I          |
| $\mathbf{B}_2$    | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8c)                | Y I          |
| $\mathbf{B}_3$    | $= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8c)                | Y I          |
| $\mathbf{B}_4$    | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$  | $=$ | $a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$  | (8c)                | Y I          |
| $\mathbf{B}_5$    | $= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$                                                       | $=$ | $-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$                                                       | (8c)                | Y I          |
| $\mathbf{B}_6$    | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (8c)                | Y I          |
| $\mathbf{B}_7$    | $= x_1 \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $ax_1 \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$  | (8c)                | Y I          |
| $\mathbf{B}_8$    | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + x_1 \mathbf{a}_3$ | $=$ | $-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$ | (8c)                | Y I          |
| $\mathbf{B}_9$    | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$                                                        | $=$ | $ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$                                                        | (24d)               | B I          |
| $\mathbf{B}_{10}$ | $= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (24d)               | B I          |
| $\mathbf{B}_{11}$ | $= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (24d)               | B I          |
| $\mathbf{B}_{12}$ | $= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$  | $=$ | $a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$  | (24d)               | B I          |
| $\mathbf{B}_{13}$ | $= z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$                                                        | $=$ | $az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$                                                        | (24d)               | B I          |
| $\mathbf{B}_{14}$ | $= \left(z_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - y_2 \mathbf{a}_3$  | $=$ | $a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$  | (24d)               | B I          |
| $\mathbf{B}_{15}$ | $= -\left(z_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (24d)               | B I          |
| $\mathbf{B}_{16}$ | $= -z_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-az_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (24d)               | B I          |
| $\mathbf{B}_{17}$ | $= y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$                                                        | $=$ | $ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$                                                        | (24d)               | B I          |

|                     |                                                                                          |     |                                                                                                          |       |     |
|---------------------|------------------------------------------------------------------------------------------|-----|----------------------------------------------------------------------------------------------------------|-------|-----|
| $\mathbf{B}_{18} =$ | $-y_2 \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_2 -$                                 | $=$ | $-ay_2 \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | B I |
|                     | $(x_2 - \frac{1}{2}) \mathbf{a}_3$                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{19} =$ | $(y_2 + \frac{1}{2}) \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$ | $=$ | $a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{20} =$ | $-(y_2 - \frac{1}{2}) \mathbf{a}_1 - z_2 \mathbf{a}_2 +$                                 | $=$ | $-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | B I |
|                     | $(x_2 + \frac{1}{2}) \mathbf{a}_3$                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{21} =$ | $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$                                | $=$ | $-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$                                 | (24d) | B I |
| $\mathbf{B}_{22} =$ | $(x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{23} =$ | $x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $ax_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{24} =$ | $-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 +$                 | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$ | (24d) | B I |
|                     | $z_2 \mathbf{a}_3$                                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{25} =$ | $-z_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$                                | $=$ | $-az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$                                 | (24d) | B I |
| $\mathbf{B}_{26} =$ | $-(z_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 +$                 | $=$ | $-a(z_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$ | (24d) | B I |
|                     | $y_2 \mathbf{a}_3$                                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{27} =$ | $(z_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (y_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(z_2 + \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{28} =$ | $z_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (y_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $az_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{29} =$ | $-y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$                                | $=$ | $-ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$                                 | (24d) | B I |
| $\mathbf{B}_{30} =$ | $y_2 \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $ay_2 \hat{\mathbf{x}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{31} =$ | $-(y_2 - \frac{1}{2}) \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_2 +$                 | $=$ | $-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$ | (24d) | B I |
|                     | $x_2 \mathbf{a}_3$                                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{32} =$ | $(y_2 + \frac{1}{2}) \mathbf{a}_1 + z_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{33} =$ | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                                 | $=$ | $ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$                                  | (24d) | H I |
| $\mathbf{B}_{34} =$ | $-(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 +$                                 | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | H I |
|                     | $(z_3 + \frac{1}{2}) \mathbf{a}_3$                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{35} =$ | $-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 -$                                 | $=$ | $-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | H I |
|                     | $(z_3 - \frac{1}{2}) \mathbf{a}_3$                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{36} =$ | $(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$  | (24d) | H I |
| $\mathbf{B}_{37} =$ | $z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$                                 | $=$ | $az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$                                  | (24d) | H I |
| $\mathbf{B}_{38} =$ | $(z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - y_3 \mathbf{a}_3$ | $=$ | $a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$  | (24d) | H I |
| $\mathbf{B}_{39} =$ | $-(z_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 +$                                 | $=$ | $-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | H I |
|                     | $(y_3 + \frac{1}{2}) \mathbf{a}_3$                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{40} =$ | $-z_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 -$                                 | $=$ | $-az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | H I |
|                     | $(y_3 - \frac{1}{2}) \mathbf{a}_3$                                                       |     |                                                                                                          |       |     |
| $\mathbf{B}_{41} =$ | $y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                                 | $=$ | $ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$                                  | (24d) | H I |
| $\mathbf{B}_{42} =$ | $-y_3 \mathbf$                                                                           |     |                                                                                                          |       |     |





$$\begin{aligned}
\mathbf{B}_{113} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 &= a y_6 \hat{\mathbf{x}} + a z_6 \hat{\mathbf{y}} + a x_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{114} &= -y_6 \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_3 &= -a y_6 \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{115} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_2 - x_6 \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{116} &= -\left(y_6 - \frac{1}{2}\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - a z_6 \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{117} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}} - a z_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{118} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}} - a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{119} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a x_6 \hat{\mathbf{x}} - a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{120} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a z_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{121} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= -a z_6 \hat{\mathbf{x}} - a x_6 \hat{\mathbf{y}} - a y_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{122} &= -\left(z_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + y_6 \mathbf{a}_3 &= -a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a y_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{123} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 + x_6 \mathbf{a}_2 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a x_6 \hat{\mathbf{y}} - a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{124} &= z_6 \mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a z_6 \hat{\mathbf{x}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{125} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= -a y_6 \hat{\mathbf{x}} - a z_6 \hat{\mathbf{y}} - a x_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{126} &= y_6 \mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a y_6 \hat{\mathbf{x}} - a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{127} &= -\left(y_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 + x_6 \mathbf{a}_3 &= -a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a x_6 \hat{\mathbf{z}} &(24d) & \text{H IV} \\
\mathbf{B}_{128} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 + z_6 \mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a z_6 \hat{\mathbf{y}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24d) & \text{H IV}
\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 167702 [ $Y(BH_4)_3$ ].

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