

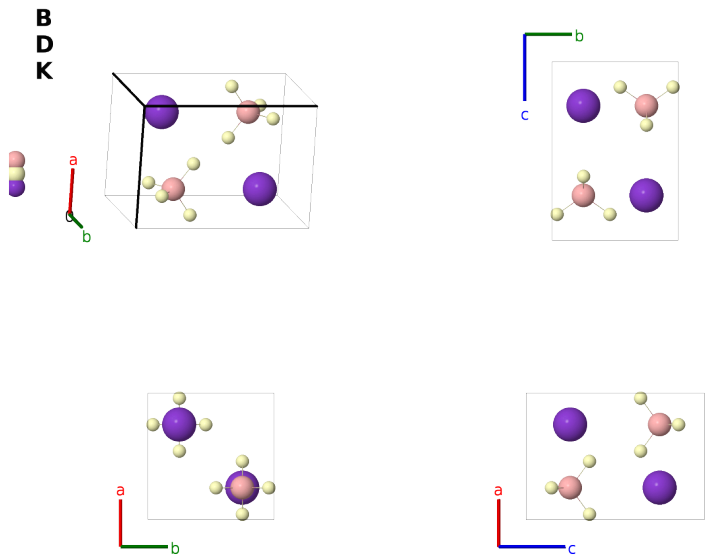
Low Temperature KBD₄ Structure: AB4C_tP12_137_a_g_b-001

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<https://aflow.org/prototype-encyclopedia/Q06Z>

https://aflow.org/prototype-encyclopedia/AB4C_tP12_137_a_g_b-001



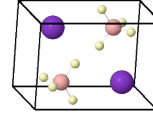
Prototype	BD ₄ K
AFLOW prototype label	AB4C_tP12_137_a_g_b-001
ICSD	99264
CCDC	1658491
Pearson symbol	tP12
Space group number	137
Space group symbol	$P4_2/nmc$
AFLOW prototype command	<pre>aflow --proto=AB4C_tP12_137_a_g_b-001 --params=a, c/a, y₃, z₃</pre>

- This is the low temperature structure of KBD₄, stable below 70K, with data taken at 1.5K. Above that it transforms into the cubic room temperature KBD₄ structure, also known as the NaBH₄ structure.

Simple Tetragonal primitive vectors



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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2a)	B I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2a)	B I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2b)	K I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2b)	K I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_7$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_{11}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B}_{12}$	$= -y_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	D I

References

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