Low Temperature KBD$_4$ Structure: AB4C_tP12_137_a_g_b-001
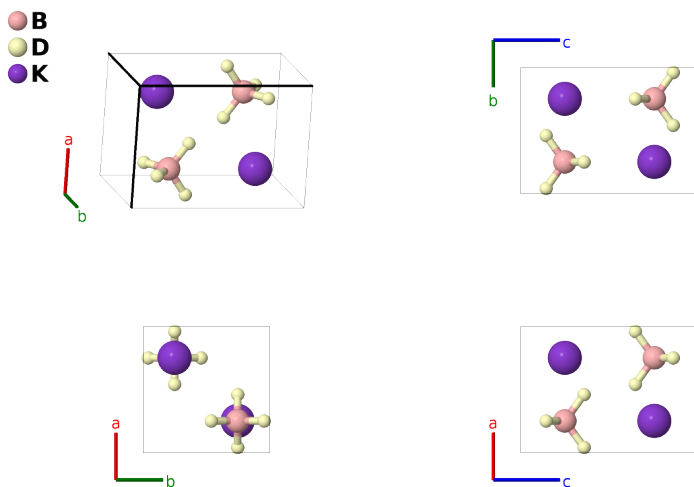
|	
Prototype	BD$_4$K
AFLOW prototype label	AB4C_tP12_137_a_g_b-001
ICSD	99264
Pearson symbol	tP12
Space group number	137
Space group symbol	$P4_2/nmc$
AFLOW prototype command	aflow --proto=AB4C_tP12_137_a_g_b-001 --params=$a, c/a, y_3, z_3$

- This is the low temperature structure of KBD$_4$, stable below 70K, with data taken at 1.5K. Above that it transforms into the cubic room temperature KBD$_4$ structure, also known as the NaBH$_4$ structure.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
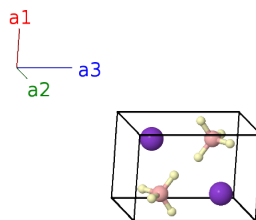
Basis vectors

		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
$\mathbf{B_6}$	$=$	$\frac{1}{4}\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B_7}$	$=$	$-\left(y_3 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B_8}$	$=$	$y_3\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B_9}$	$=$	$\frac{3}{4}\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{11}}$	$=$	$\left(y_3 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	D I
$\mathbf{B_{12}}$	$=$	$-y_3\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ay_3\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	D I

References

[1] G. Renaudin, S. Gomes, H. Hagemann, L. Keller, and K. Yvon, *Structural and spectroscopic studies on the alkali borohydrides MBH_4 (M = Na, K, Rb, Cs)*, J. Alloys Compd. **375**, 98–106 (2004), doi:10.1016/j.jallcom.2003.11.018.

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[1] S. D. Cataldo, C. Heil, W. von der Linden, and L. Boeri, *$LaBH_8$: the first high-T_c low-pressure superhydride*, Phys. Rev. B **104**, L020511 (2021), doi:10.1103/PhysRevB.104.L020511.