Room Temperature KBD_4 Structure: AB8C_cF40_225_a_f_b-001

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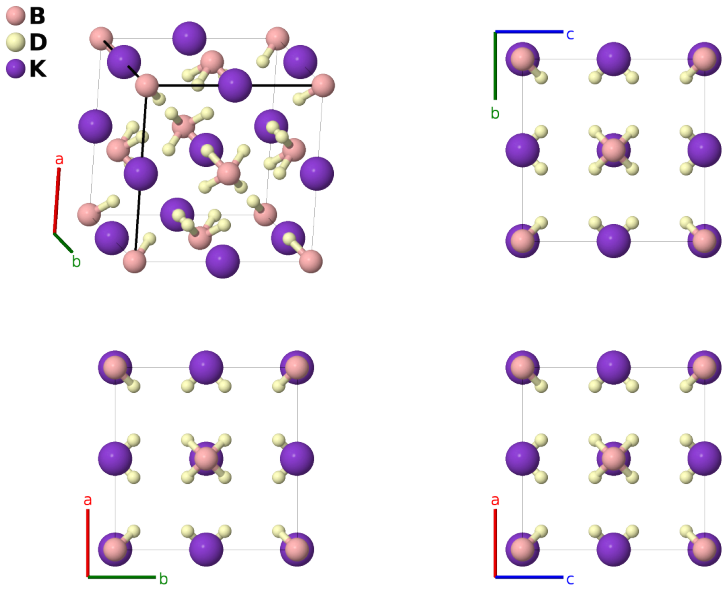
https://aflow.org/p/WSA1

https://aflow.org/p/AB8C_cF40_225_a_f_b-001



Prototype	BH_4K
AFLOW prototype label	AB8C_cF40_225_a_f_b-001
ICSD	99263
Pearson symbol	cF40
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB8C_cF40_225_a_f_b-001 --params=`a, x_3

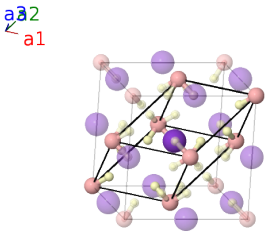
Other compounds with this structure
$CsBD_4$, $CsBH_4$, KBH_4, $LaBH_8$, $NaBD_4$, $NaBH_4$, $RbBD_4$, $RbBH_4$

- This is the room-temperature phase of all of these structures.
- Below 70K KBD_4 transforms into a tetragonal structure with the deuterium atoms forming a tetrahedron around the boron, but this is not seen for (Cs,Na,Rb)BD_4 or (Cs,Na,Rb)BH_4, where the system remains cubic (Renaudin, 2004).
- In all of the ABD_4 structures the deuterium atoms only occupy half of the (32f) sites. (Soldate, 1954) suggests that in the H_4 compounds the hydrogen atoms form a rotating tetrahedra around the boron atoms.
- (Di Cataldo, 2021) predict $LaBH_8$ forms in this structure at pressures around 50 GPa, where it would superconduct with $T_c = 126$K. In this case the (32f) sites are fully filled.

- Most authors use $NaBH_4$ as the prototype, but since (Renaudin, 2004) provide information on the location of the deuterium atoms we use KBD_4, with data taken at room temperature, we use this as the prototype.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\ \mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	B I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_6}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + 3x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 + 3x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	D I
$\mathbf{B_{10}}$	=	$3x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	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.

[2] A. M. Soldate, *Crystal Structure of Sodium Borohydride*, J. Am. Chem. Soc. **69**, 987–988 (1954), doi:10.1021/ja01197a002.

Found in

[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.