KHF_2 ($F5_2$) Structure: A2BC_tI16_140_h_d_a-001

This structure originally had the label `A2BC_tI16_140_h_d_a`. Calls to that address will be redirected here.

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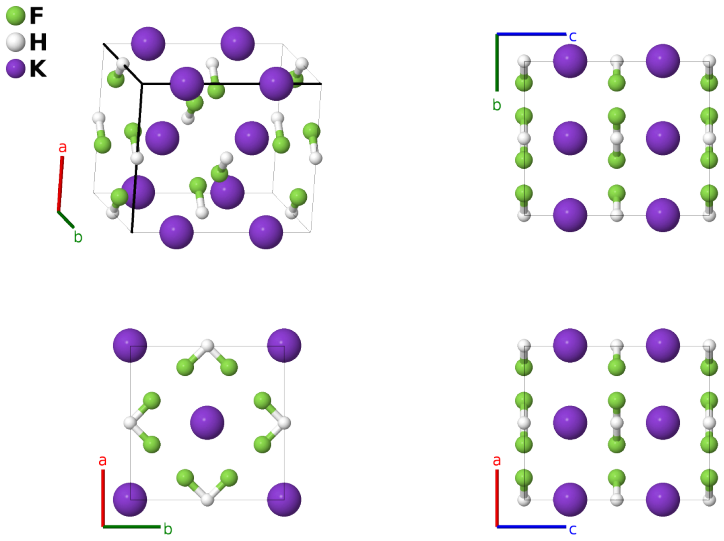
https://aflow.org/p/B7FR

https://aflow.org/p/A2BC_tI16_140_h_d_a-001



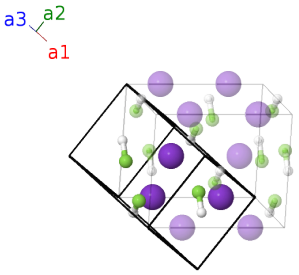
Prototype	F_2HK
AFLOW prototype label	A2BC_tI16_140_h_d_a-001
***Strukturbericht* designation**	$F5_2$
ICSD	18094
Pearson symbol	tI16
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A2BC_tI16_140_h_d_a-001 --params=`$a, c/a, x_3$

Other compounds with this structure
KN_3, CsN_3

- (Bozorth, 1923) originally determined the lattice constants of KHF_2 along with the positions of the potassium and fluorine atoms. He also assumed that the hydrogen atoms were on the (4d) Wyckoff sites. Both (Peterson, 1952) and (Ibers, 1964) confirmed his data. All three papers point out that it is possible that the hydrogen atoms are on half-filled (8h) sites, which would reduce to the (4d) site as the x coordinate approached zero. In KN_3 and CsN_3 the nitrogen atoms occupy the (4d) and (8h) Wyckoff sites, while the cation occupies the (4a) site.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	K I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	K I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4d)	H I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4d)	H I
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	F I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	F I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	F I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	F I

References

[1] J. A. Ibers, *Refinement of Peterson and Levy's Neutron Diffraction Data on KHF_2*, J. Chem. Phys. **40**, 402–404 (1964), doi:10.1063/1.1725126.

[2] S. W. Peterson and H. A. Levy, *A Single Crystal Neutron Diffraction Determination of the Hydrogen Position in Potassium Bifluoride*, J. Chem. Phys. **20**, 704–707 (1952), doi:10.1063/1.1700520.

[3] R. M. Bozorth, *The crystal structure of potassium hydrogen fluoride*, J. Am. Chem. Soc. **45**, 2128–2132 (1923), doi:10.1021/ja01662a013.