Tetragonal Perovskite $KCuF_3$ Structure: AB3C_tI20_140_d_bh_a-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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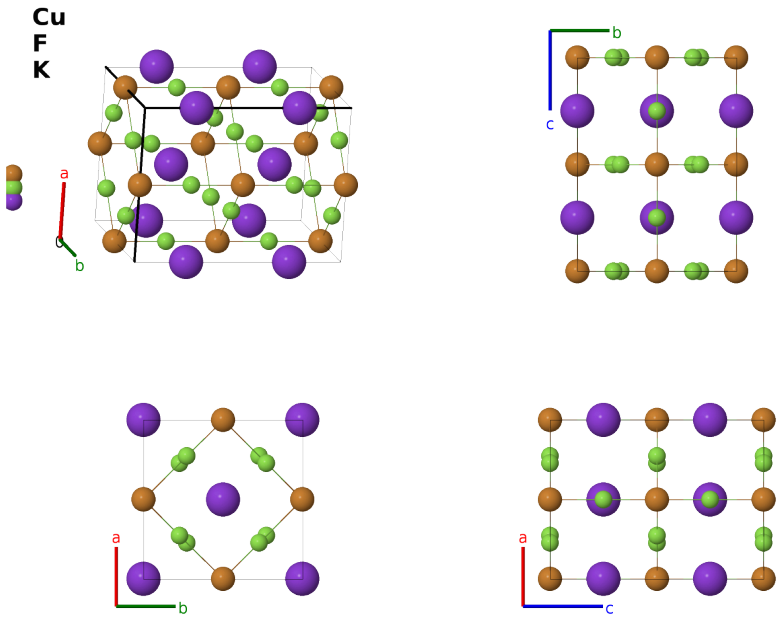
https://aflow.org/prototype-encyclopedia/ALM7

https://aflow.org/prototype-encyclopedia/AB3C_tI20_140_d_bh_a-001



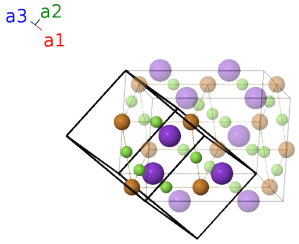
Prototype	CuF_3K
AFLOW prototype label	AB3C_tI20_140_d_bh_a-001
ICSD	17011
CCDC	1597511
Pearson symbol	tI20
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=AB3C_tI20_140_d_bh_a-001 --params=`$a, c/a, x_4$

Other compounds with this structure
$CsAgF_3$, $KCrF_3$, $RbCuF_3$, $RbAgF_3$

- This is a tetragonal distortion of the cubic perovskite ($E2_1$) structure. The pseudo-cubic cell has dimensions a/$\sqrt{2}$, c/2.

Body-centered Tetragonal primitive vectors

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



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
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	F I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	F I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4d)	Cu I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4d)	Cu I
$\mathbf{B_7}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_8}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	F II

References

[1] A. Okazaki and Y. Suemune, *The Crystal Structure $KCuF_3$*, J. Phys. Soc. Japan **16**, 176–183 (1961), doi:10.1143/JPSJ.16.176.

Found in

[1] A. Okazaki and Y. Suemune, *The Crystal Structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$ and $KCuF_3$ above and below their Néel Temperatures*, J. Phys. Soc. Japan **16**, 671–675 (1961), doi:10.1143/JPSJ.16.671.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).