Khatyrkite (Al_2Cu, $C16$) Structure: A2B_tI12_140_h_a-001

This structure previously used the label(s) `A2B_tI12_140_h_a`. Calls to these addresses will be redirected here.

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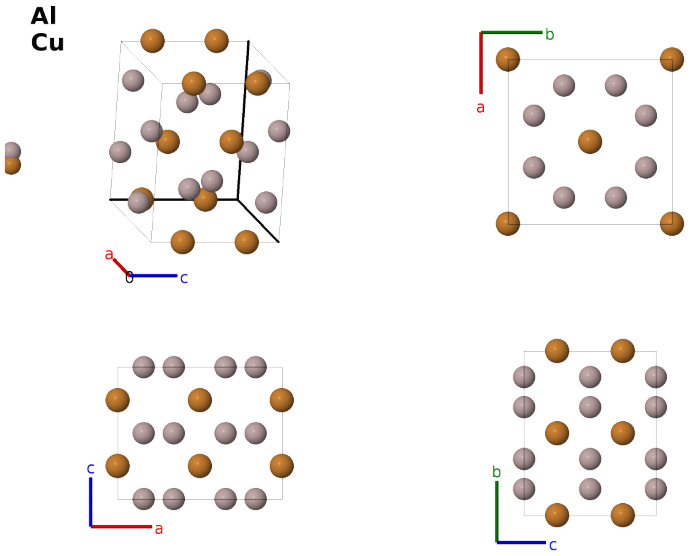
https://aflow.org/prototype-encyclopedia/PARL

https://aflow.org/prototype-encyclopedia/A2B_tI12_140_h_a-001



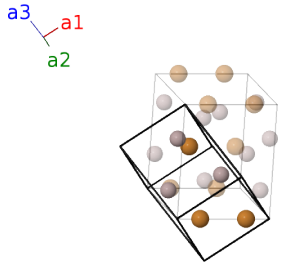
Prototype	Al_2Cu
AFLOW prototype label	A2B_tI12_140_h_a-001
***Strukturbericht* designation**	$C16$
Mineral name	khatyrkite
ICSD	198177
CCDC	1925080
Pearson symbol	tI12
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A2B_tI12_140_h_a-001 --params=`$a, c/a, x_2$

Other compounds with this structure

Co_2B, Cr_2B, Fe_2B, Fe_2Bi, Ge_2Fe, Hf_2Al, Hf_2Ga, Hf_2Ge, Hf_2Ni, Hf_2Si, Hf_2Th, Hf_2Zr, In_2Ag, Mn_2B, Mo_2B, Na_2Au, Ni_2B, Pb_2Au, Pb_2Pd, Pb_2Rh, Sb_2Ti, Sb_2V, Sc_2Co, Sn_2Co, Sn_2Fe, Sn_2Rh (HT), Ta_2B, Ta_2Ni, Ta_2Si, Ta_2Zr, Th_2Ag, Th_2Al, Th_2Au, Th_2Cu, Th_2Ga, Th_2Ge, Th_2Pd, Th_2Zn, Tl_2Au, Tl_2Pd, Tl_2Pt, W_2B, Zr_2Co, Zr_2Fe, Zr_2Ga, Zr_2Ni, Zr_2Rh

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)	Cu I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B_3}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Al I

References

[1] J. B. Friauf, *The Crystal Structures of Two Intermetallic Compounds*, J. Am. Chem. Soc. **49**, 3107–3114 (1927), doi:10.1021/ja01411a017.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017