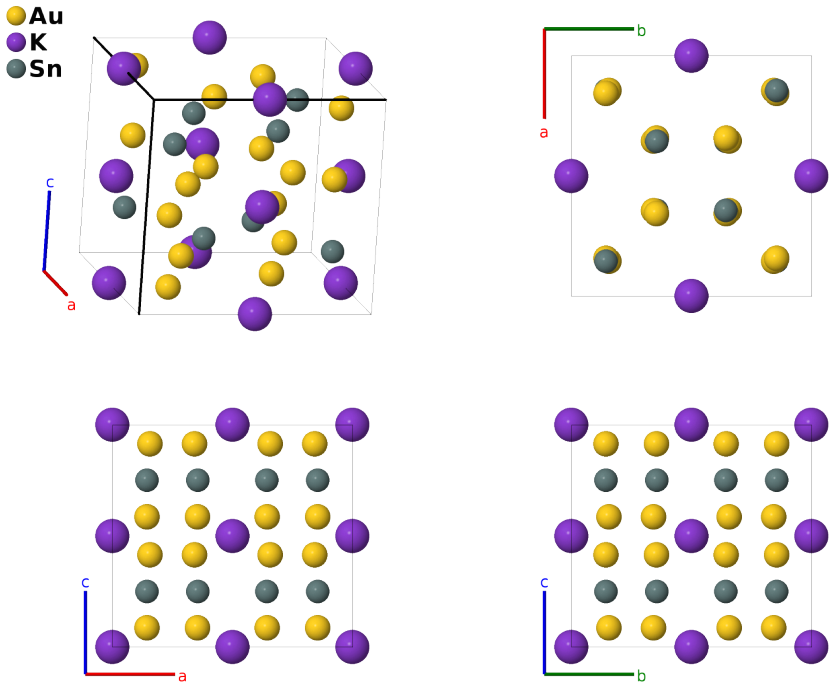
KAu_4Sn_2 Structure: A4BC2_tI28_120_i_a_h-001

This structure originally had the label `A4BC2_tI28_120_i_d_e`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/KAKD

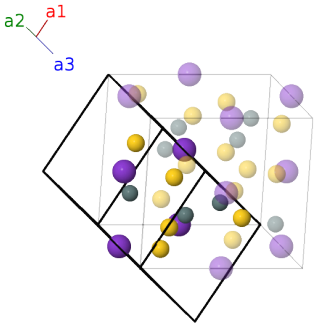
https://aflow.org/p/A4BC2_tI28_120_i_a_h-001



Prototype	Au_4KSn_4
AFLOW prototype label	A4BC2_tI28_120_i_a_h-001
ICSD	58522
Pearson symbol	tI28
Space group number	120
Space group symbol	$I\bar{4}c2$
AFLOW prototype command	`aflow --proto=A4BC2_tI28_120_i_a_h-001 --params=`$a, c/a, x_2, x_3, y_3, z_3$

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
$\mathbf{B_3}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Sn 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)	Sn 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)	Sn 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)	Sn I
$\mathbf{B_7}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_8}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_9}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_{10}}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_{11}}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_{12}}$	=	$\left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_{13}}$	=	$\left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B_{14}}$	=	$-\left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Au I

References

[1] H.-D. Sinnen and H. U. Schuster, *Darstellung und Struktur des KAu4Sn2*, Z. Naturforsch. B **33**, 1077–1079 (1978), doi:10.1515/znb-1978-1004.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.