

KAu₄Sn₂ Structure: A4BC2_tI28_120_i_a_h-001

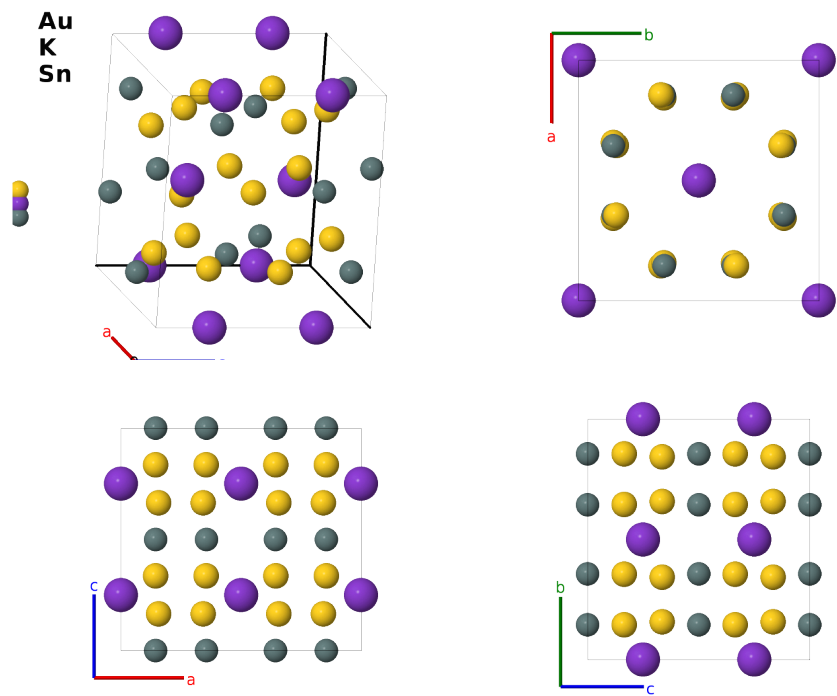
This structure previously used the label(s) **A4BC2_tI28_120_i_d_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/KAKD>

https://aflow.org/prototype-encyclopedia/A4BC2_tI28_120_i_a_h-001



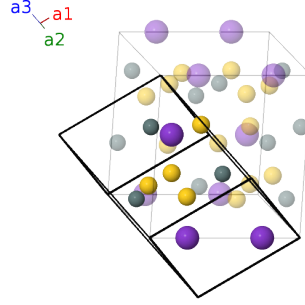
Prototype	Au ₄ KSn ₄
AFLOW prototype label	A4BC2_tI28_120_i_a_h-001
ICSD	58522
CCDC	1622533
Pearson symbol	tI28
Space group number	120
Space group symbol	$I\bar{4}c2$
AFLOW prototype command	<code>aflow --proto=A4BC2_tI28_120_i_a_h-001</code> <code>--params=a, c/a, x₂, x₃, y₃, z₃</code>

Other compounds with this structure

CeNi₄Sn₂, LaNi₄Sn₂, NdNi₄Sn₂, PrNi₄Sn₂, SmNi₄Sn₂

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_3$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (2x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Sn I
$\mathbf{B}_4$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 - (2x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Sn I
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8h)	Sn I
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(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
$\mathbf{B}_{11}$	$= (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B}_{12}$	$= (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B}_{13}$	$= (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16i)	Au I
$\mathbf{B}_{14}$	$= -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(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.

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