R_1 Au_3Zn Structure: A3B_tI64_142_def_d-001

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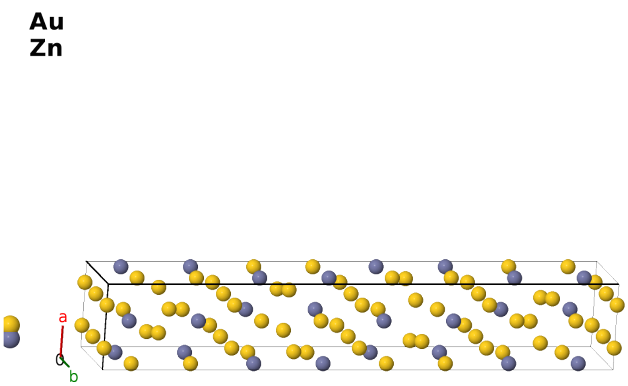
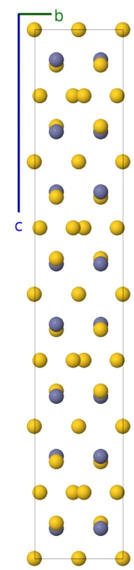
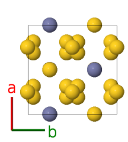
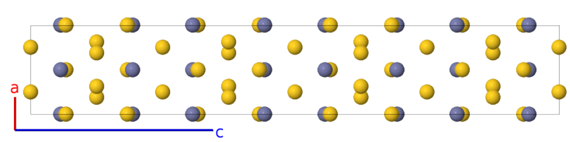
https://aflow.org/prototype-encyclopedia/A3B_tI64_142_def_d-001









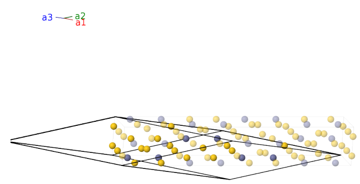
Prototype	Au_3Zn
AFLOW prototype label	A3B_tI64_142_def_d-001

ICSD	58628
CCDC	1622634
Pearson symbol	tI64
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	`aflow --proto=A3B_tI64_142_def_d-001` `--params=`$a, c/a, z_1, z_2, x_3, x_4$

- Au_3Zn is known to exist in three forms, depending upon the exact composition and temperature (Hisatsune, 1998):
  - The tetragonal R_1 phase (this structure) is stable below $\approx$ 475K with a composition very nearly stoichiometric.
  - The orthorhombic R_2 phase is stable below $\approx$ 550K with a composition range somewhat wider than the R_1 phase.
  - The tetragonal H phase has the $D0_{23}$ structure and is stable at temperatures up to $\approx$ 700K over a considerably wider range of stoichiometries than either the R_1 or R_2 phases.
- (Iwaskai, 1962) gave structure of the R_1 phase in setting 1 of space group $I4_1/acd$ #142. We used FINDSYM to transform this to the standard setting 2.
- (Iwaskai, 1962) gave the lattice constants in kX units. We used the conversion factor 1 kX = 1.00202Å. (Wood, 1947)

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
$\mathbf{B_1}$	=	$\left(z_1 + \frac{1}{4}\right)\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{4}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_3}$	=	$-\left(z_1 - \frac{1}{4}\right)\mathbf{a}_1 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_4}$	=	$-\left(z_1 - \frac{1}{2}\right)\mathbf{a}_1 - \left(z_1 - \frac{1}{4}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_5}$	=	$-\left(z_1 - \frac{3}{4}\right)\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_6}$	=	$-z_1\,\mathbf{a}_1 - \left(z_1 - \frac{3}{4}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_7}$	=	$\left(z_1 + \frac{3}{4}\right)\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_8}$	=	$\left(z_1 + \frac{1}{2}\right)\mathbf{a}_1 + \left(z_1 + \frac{3}{4}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Au I
$\mathbf{B_9}$	=	$\left(z_2 + \frac{1}{4}\right)\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16d)	Zn I

$\mathbf{B_{10}}$	$=$	$z_2\,\mathbf{a}_1 + \left(z_2+\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} + c\left(z_2-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{11}}$	$=$	$-\left(z_2-\frac{1}{4}\right)\,\mathbf{a}_1 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{12}}$	$=$	$-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_2-\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\mathbf{\hat{y}} - c\left(z_2-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{13}}$	$=$	$-\left(z_2-\frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{14}}$	$=$	$-z_2\,\mathbf{a}_1 - \left(z_2-\frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{1}{4}a\,\mathbf{\hat{y}} - c\left(z_2-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{15}}$	$=$	$\left(z_2+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\mathbf{\hat{y}} + c\left(z_2+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{16}}$	$=$	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_2+\frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} + c\left(z_2+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16d)	Zn I
$\mathbf{B_{17}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3+\frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	$=$	$ax_3\,\mathbf{\hat{x}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{18}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_3\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{19}}$	$=$	$\left(x_3+\frac{1}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\mathbf{\hat{x}} + a\left(x_3-\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{20}}$	$=$	$-\left(x_3-\frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\mathbf{\hat{x}} - a\left(x_3-\frac{1}{4}\right)\,\mathbf{\hat{y}}$	(16e)	Au II
$\mathbf{B_{21}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3-\frac{3}{4}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	$=$	$-ax_3\,\mathbf{\hat{x}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{22}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3+\frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{23}}$	$=$	$-\left(x_3-\frac{3}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	$=$	$-\frac{1}{4}a\,\mathbf{\hat{x}} - a\left(x_3-\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{24}}$	$=$	$\left(x_3+\frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\mathbf{\hat{x}} + a\left(x_3+\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(16e)	Au II
$\mathbf{B_{25}}$	$=$	$\left(x_4+\frac{3}{8}\right)\,\mathbf{a}_1 + \left(x_4+\frac{1}{8}\right)\,\mathbf{a}_2 + \left(2x_4+\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$ax_4\,\mathbf{\hat{x}} + a\left(x_4+\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{26}}$	$=$	$-\left(x_4-\frac{3}{8}\right)\,\mathbf{a}_1 - \left(x_4-\frac{1}{8}\right)\,\mathbf{a}_2 - \left(2x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$-ax_4\,\mathbf{\hat{x}} - a\left(x_4-\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{27}}$	$=$	$\left(x_4+\frac{1}{8}\right)\,\mathbf{a}_1 - \left(x_4-\frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-a\left(x_4-\frac{1}{2}\right)\,\mathbf{\hat{x}} + a\left(x_4+\frac{1}{4}\right)\,\mathbf{\hat{y}} - \frac{1}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{28}}$	$=$	$-\left(x_4-\frac{1}{8}\right)\,\mathbf{a}_1 + \left(x_4+\frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$a\left(x_4+\frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_4-\frac{1}{4}\right)\,\mathbf{\hat{y}} - \frac{1}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{29}}$	$=$	$-\left(x_4-\frac{5}{8}\right)\,\mathbf{a}_1 - \left(x_4-\frac{7}{8}\right)\,\mathbf{a}_2 - \left(2x_4-\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_4-\frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_4-\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{30}}$	$=$	$\left(x_4+\frac{5}{8}\right)\,\mathbf{a}_1 + \left(x_4+\frac{7}{8}\right)\,\mathbf{a}_2 + \left(2x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$a\left(x_4+\frac{1}{2}\right)\,\mathbf{\hat{x}} + a\left(x_4+\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{31}}$	$=$	$-\left(x_4-\frac{7}{8}\right)\,\mathbf{a}_1 + \left(x_4+\frac{5}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$ax_4\,\mathbf{\hat{x}} - a\left(x_4-\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{5}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III
$\mathbf{B_{32}}$	$=$	$\left(x_4+\frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_4-\frac{5}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-ax_4\,\mathbf{\hat{x}} + a\left(x_4+\frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{5}{8}c\,\mathbf{\hat{z}}$	(16f)	Au III

References

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[1] K. Hisatsune, Y. Takuma, Y. Tanaka, K. Udoh, T. Morimura, and M. Hasaka, *Martensite transformation in Au_3Zn alloy*, Solid State Commun. **106**, 509–512 (1998), doi:10.1016/S0038-1098(98)00077-5.

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