R_1 Au_3Zn Structure: A3B_tI64_142_def_d-001

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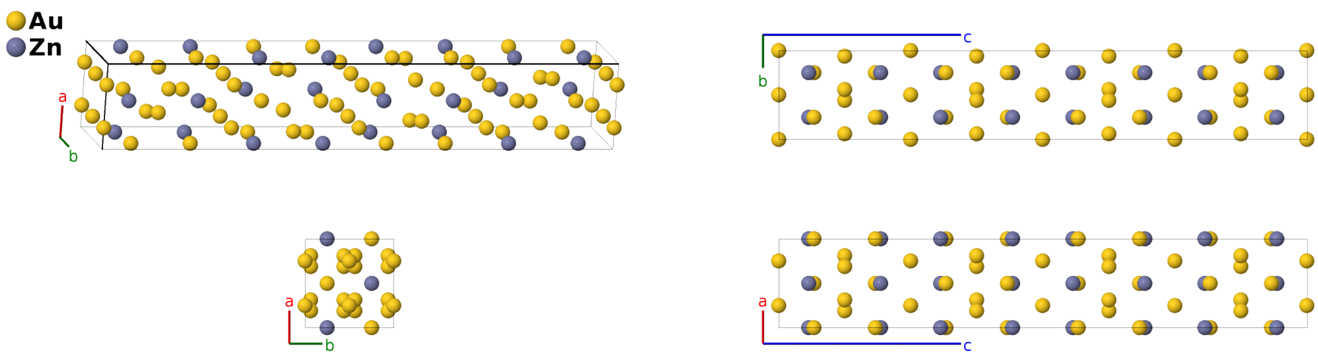
https://aflow.org/p/A3B_tI64_142_def_d-001

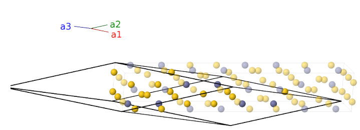


Prototype	Au_3Zn
AFLOW prototype label	A3B_tI64_142_def_d-001
ICSD	58628
Pearson symbol	tI64
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	`aflow --proto=A3B_tI64_142_def_d-001` `--params=`$a, c/a, z_1, z_2, x_3, x_4$

- 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

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_{10}}$	=	$z_{2}\,\mathbf{a}_{1}+\left(z_{2}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_{2}-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{11}}$	=	$-\left(z_{2}-\frac{1}{4}\right)\,\mathbf{a}_{1}-\left(z_{2}-\frac{1}{2}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-cz_{2}\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{12}}$	=	$-\left(z_{2}-\frac{1}{2}\right)\,\mathbf{a}_{1}-\left(z_{2}-\frac{1}{4}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_{2}-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{13}}$	=	$-\left(z_{2}-\frac{3}{4}\right)\,\mathbf{a}_{1}-z_{2}\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{3}{4}a\,\hat{\mathbf{y}}-cz_{2}\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{14}}$	=	$-z_{2}\,\mathbf{a}_{1}-\left(z_{2}-\frac{3}{4}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_{2}-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{15}}$	=	$\left(z_{2}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(z_{2}+\frac{1}{2}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_{2}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{16}}$	=	$\left(z_{2}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(z_{2}+\frac{3}{4}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_{2}+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Zn I
$\mathbf{B_{17}}$	=	$\frac{1}{4}\,\mathbf{a}_{1}+\left(x_{3}+\frac{1}{4}\right)\,\mathbf{a}_{2}+x_{3}\,\mathbf{a}_{3}$	=	$ax_{3}\,\hat{\mathbf{x}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{18}}$	=	$\frac{3}{4}\,\mathbf{a}_{1}-\left(x_{3}-\frac{1}{4}\right)\,\mathbf{a}_{2}-\left(x_{3}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{3}\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{19}}$	=	$\left(x_{3}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\frac{3}{4}\,\mathbf{a}_{2}+x_{3}\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+a\left(x_{3}-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{20}}$	=	$-\left(x_{3}-\frac{1}{4}\right)\,\mathbf{a}_{1}+\frac{1}{4}\,\mathbf{a}_{2}-\left(x_{3}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-a\left(x_{3}-\frac{1}{4}\right)\,\hat{\mathbf{y}}$	(16e)	Au II
$\mathbf{B_{21}}$	=	$\frac{3}{4}\,\mathbf{a}_{1}-\left(x_{3}-\frac{3}{4}\right)\,\mathbf{a}_{2}-x_{3}\,\mathbf{a}_{3}$	=	$-ax_{3}\,\hat{\mathbf{x}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{22}}$	=	$\frac{1}{4}\,\mathbf{a}_{1}+\left(x_{3}+\frac{3}{4}\right)\,\mathbf{a}_{2}+\left(x_{3}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(x_{3}+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{23}}$	=	$-\left(x_{3}-\frac{3}{4}\right)\,\mathbf{a}_{1}+\frac{1}{4}\,\mathbf{a}_{2}-x_{3}\,\mathbf{a}_{3}$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}}-a\left(x_{3}-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{24}}$	=	$\left(x_{3}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\frac{3}{4}\,\mathbf{a}_{2}+\left(x_{3}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+a\left(x_{3}+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Au II
$\mathbf{B_{25}}$	=	$\left(x_{4}+\frac{3}{8}\right)\,\mathbf{a}_{1}+\left(x_{4}+\frac{1}{8}\right)\,\mathbf{a}_{2}+\left(2x_{4}+\frac{1}{4}\right)\,\mathbf{a}_{3}$	=	$ax_{4}\,\hat{\mathbf{x}}+a\left(x_{4}+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III
$\mathbf{B_{26}}$	=	$-\left(x_{4}-\frac{3}{8}\right)\,\mathbf{a}_{1}-\left(x_{4}-\frac{1}{8}\right)\,\mathbf{a}_{2}-\left(2x_{4}-\frac{1}{4}\right)\,\mathbf{a}_{3}$	=	$-ax_{4}\,\hat{\mathbf{x}}-a\left(x_{4}-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III
$\mathbf{B_{27}}$	=	$\left(x_{4}+\frac{1}{8}\right)\,\mathbf{a}_{1}-\left(x_{4}-\frac{3}{8}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$-a\left(x_{4}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_{4}+\frac{1}{4}\right)\,\hat{\mathbf{y}}-\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III
$\mathbf{B_{28}}$	=	$-\left(x_{4}-\frac{1}{8}\right)\,\mathbf{a}_{1}+\left(x_{4}+\frac{3}{8}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$a\left(x_{4}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_{4}-\frac{1}{4}\right)\,\hat{\mathbf{y}}-\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III
$\mathbf{B_{29}}$	=	$-\left(x_{4}-\frac{5}{8}\right)\,\mathbf{a}_{1}-\left(x_{4}-\frac{7}{8}\right)\,\mathbf{a}_{2}-\left(2x_{4}-\frac{3}{4}\right)\,\mathbf{a}_{3}$	=	$-a\left(x_{4}-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_{4}-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III
$\mathbf{B_{30}}$	=	$\left(x_{4}+\frac{5}{8}\right)\,\mathbf{a}_{1}+\left(x_{4}+\frac{7}{8}\right)\,\mathbf{a}_{2}+\left(2x_{4}+\frac{3}{4}\right)\,\mathbf{a}_{3}$	=	$a\left(x_{4}+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_{4}+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III
$\mathbf{B_{31}}$	=	$-\left(x_{4}-\frac{7}{8}\right)\,\mathbf{a}_{1}+\left(x_{4}+\frac{5}{8}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$ax_{4}\,\hat{\mathbf{x}}-a\left(x_{4}-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	Au III

$$\mathbf{B_{32}} = \left(x_4 + \frac{7}{8}\right) \mathbf{a}_1 - \left(x_4 - \frac{5}{8}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 = -a x_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{5}{8} c \hat{\mathbf{z}} \quad (16f) \quad \text{Au III}$$

References

[1] H. Iwaskai, *Study on the Ordered Phases with Long Period in the Gold-Zinc Alloy System II. Structure Analysis of $Au_3Zn[R_1]$, $Au_3Zn[R_2]$ and Au_3+Zn*, J. Phys. Soc. Jpn. **17**, 1620–1633 (1962), doi:10.1143/JPSJ.17.1620.

[2] E. A. Wood, *The Conversion Factor for kX Units to Angström Units*, J. Appl. Phys. **18**, 929–930 (1947), doi:10.1063/1.1697570.

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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.