R_2 Au_3Zn Structure: A3B_oC32_64_def_d-001

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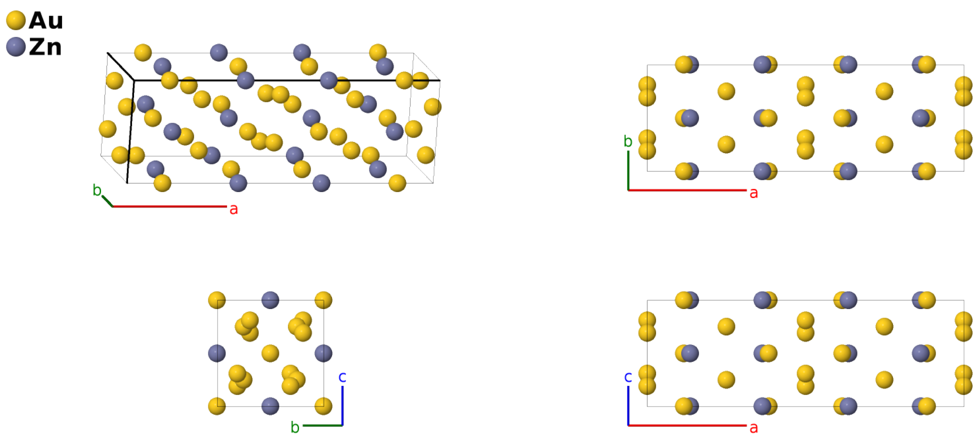
https://aflow.org/p/GVGD

https://aflow.org/p/A3B_oC32_64_def_d-001

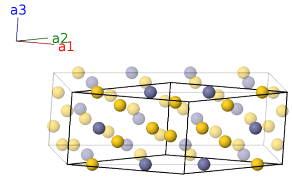


Prototype	Au_3Zn
AFLOW prototype label	A3B_oC32_64_def_d-001
ICSD	150693
Pearson symbol	oC32
Space group number	64
Space group symbol	$Cmce$
AFLOW prototype command	`aflow --proto=A3B_oC32_64_def_d-001` `--params=`$a, b/a, c/a, x_1, x_2, y_3, y_4, z_4$

- Au_3Zn is known to exist in three forms, depending upon the exact composition and temperature (Hisatsune, 1998):
  - The tetragonal R_1 phase is stable below ≈ 475K with a composition very nearly stoichiometric.
  - The orthorhombic R_2 phase (this structure) is stable below ≈ 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 ≈ 700K over a considerably wider range of stoichiometries than either the R_1 or R_2 phases.
- (Iwaskai, 1962) gave structure of the R_2 phase in the *Abam* of space group #64. We used FINDSYM to transform this to the *Cmca* setting.
- (Iwaskai, 1962) gave the lattice constants in kX units. We used the conversion factor 1 kX = 1.00202Å. (Wood, 1947)
- We use the orthorhombic lattice constants from (Wilkens, 1958) rather than the pseudo-tetragonal lattice constants of (Iwaskai, 1962).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(8d)	Au I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Au I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(8d)	Au I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Au I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}}$	(8d)	Zn I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Zn I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(8d)	Zn I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Zn I
$\mathbf{B_9}$	=	$-\left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Au II
$\mathbf{B_{10}}$	=	$\left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Au II
$\mathbf{B_{11}}$	=	$\left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Au II
$\mathbf{B_{12}}$	=	$-\left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Au II
$\mathbf{B_{13}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Au III
$\mathbf{B_{14}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Au III
$\mathbf{B_{15}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Au III
$\mathbf{B_{16}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	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.