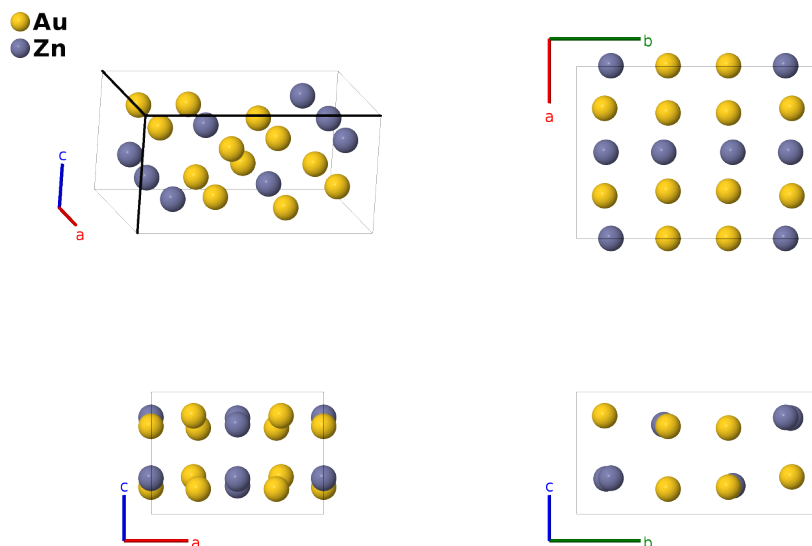


Metastable Au₅Zn₃ Structure: A5B3_oP16_26_a2c_a2b-001

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<https://aflow.org/p/PD7K>

https://aflow.org/p/A5B3_oP16_26_a2c_a2b-001



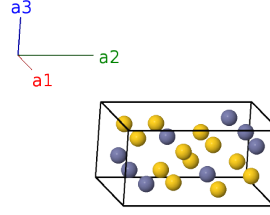
Prototype	Au ₅ Zn ₃
AFLOW prototype label	A5B3_oP16_26_a2c_a2b-001
ICSD	58629
Pearson symbol	oP16
Space group number	26
Space group symbol	<i>Pmc</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=A5B3_oP16_26_a2c_a2b-001 --params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

- (Iwasaki, 1965) found this structure to form metastably between 300° and 600°. Below 300° it transforms into the ordered Au₅Zn₃ structure.
- There is considerable disorder on most of the sites in this system, to wit:
 - Site Au-I (2a) is 60% gold and 40 % zinc,
 - Site Zn-I (2c) is 20% gold and 80 % zinc,
 - Site Zn-II (2b) is 10% gold and 90 % zinc,
 - Site Zn-III (2b) is 40% gold and 60 % zinc,
 - Site Au-II (4c) is 85% gold and 15 % zinc, and
 - Site Au-III (4c) is 100% gold with no zinc.

- We label each site by its dominant component.
- (Iwaskai, 1965) gave the lattice constants in kX units. We used the conversion factor $1 \text{ kX} = 1.00202 \text{ \AA}$. (Wood, 1947).
- The ICSD entry is from (Iwasaki, 1962).

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	Au I
\mathbf{B}_2	$= -y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Au I
\mathbf{B}_3	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	Zn I
\mathbf{B}_4	$= -y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Zn I
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2b)	Zn II
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Zn II
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	Zn III
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Zn III
\mathbf{B}_9	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Au II
\mathbf{B}_{10}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Au II
\mathbf{B}_{11}	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Au II
\mathbf{B}_{12}	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Au II
\mathbf{B}_{13}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Au III
\mathbf{B}_{14}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Au III
\mathbf{B}_{15}	$= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Au III
\mathbf{B}_{16}	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Au III

References

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