

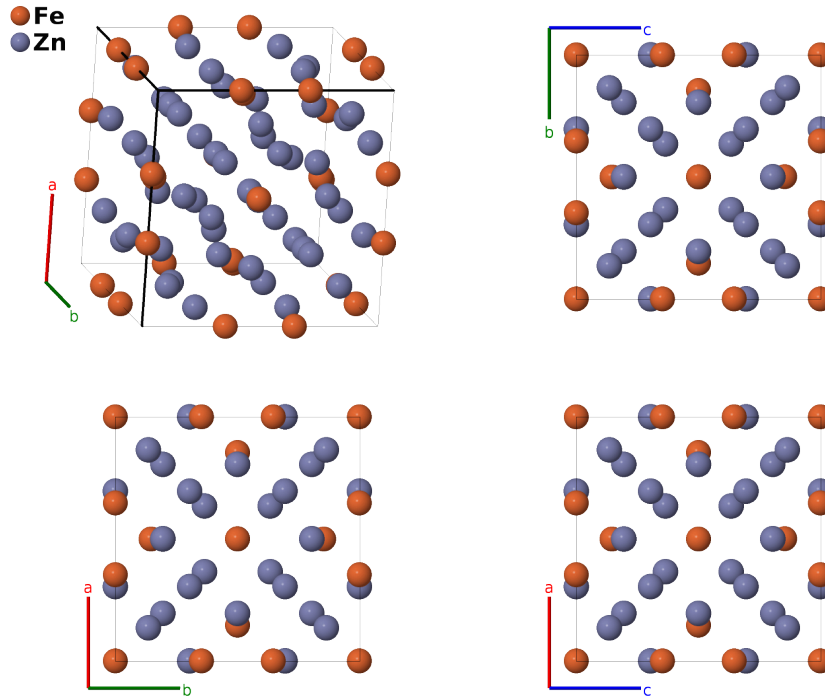
γ -brass ($\text{Fe}_3\text{Zn}_{10}$, $D8_1$) Structure: A3B10_cI52_229_e_fh-001

This structure originally had the label A3B10_cI52.229_e_fh. Calls to that address will be redirected here.

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<https://aflow.org/p/TJ2T>

https://aflow.org/p/A3B10_cI52_229_e_fh-001



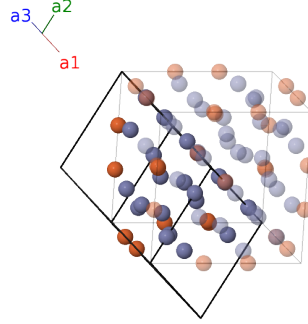
Prototype	$\text{Fe}_3\text{Zn}_{10}$
AFLOW prototype label	A3B10_cI52_229_e_fh-001
<i>Strukturbericht</i> designation	$D8_1$
Mineral name	brass
ICSD	none
Pearson symbol	cI52
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B10_cI52_229_e_fh-001 --params=a, x1, x2, y3</code>

- Adding another atom at the origin changes this to the $L2_2$ structure.

- The $D8_1$ structure is defined in (Pearson, 1958) quoting (Schramm, 1938). More recent investigations such as (Johansson, 1968), (Brandon, 1974) and (Yu, 2005) find that γ -Fe₃Zn₁₀ forms in the $D8_2$ structure, with Fe atoms on one (8c) site, Zn atoms on the other (8e) site and the (24g) sites, and a 50-50 alloy of Fe and Zn on the other (8e) site.
- We use Brandon's data, mapping (12g) \rightarrow (12e), (24g) \rightarrow (24h), and averaging the two (8e) sites to produce the (12e) coordinate here.
- (Mizutani, 2010) classifies this as an "I-cell" γ -brass.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}}$	(12e)	Fe I
\mathbf{B}_2	$-x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}}$	(12e)	Fe I
\mathbf{B}_3	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{y}}$	(12e)	Fe I
\mathbf{B}_4	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{y}}$	(12e)	Fe I
\mathbf{B}_5	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	=	$ax_1 \hat{\mathbf{z}}$	(12e)	Fe I
\mathbf{B}_6	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	=	$-ax_1 \hat{\mathbf{z}}$	(12e)	Fe I
\mathbf{B}_7	$2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_8	$-2x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_9	$-2x_2 \mathbf{a}_2$	=	$-ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_{10}	$-2x_2 \mathbf{a}_1$	=	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_{11}	$2x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_{12}	$-2x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 - 2x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_{13}	$2x_2 \mathbf{a}_2$	=	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_{14}	$2x_2 \mathbf{a}_1$	=	$-ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(16f)	Zn I
\mathbf{B}_{15}	$2y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{16}	$y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{17}	$-y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{18}	$-2y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{19}	$y_3 \mathbf{a}_1 + 2y_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{20}	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{21}	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{22}	$-y_3 \mathbf{a}_1 - 2y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{z}}$	(24h)	Zn II
\mathbf{B}_{23}	$y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + 2y_3 \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(24h)	Zn II

$$\mathbf{B}_{24} = y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 = -ay_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} \quad (24h) \quad \text{Zn II}$$

$$\mathbf{B}_{25} = -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 = ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} \quad (24h) \quad \text{Zn II}$$

$$\mathbf{B}_{26} = -y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - 2y_3 \mathbf{a}_3 = -ay_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} \quad (24h) \quad \text{Zn II}$$

References

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Found in

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