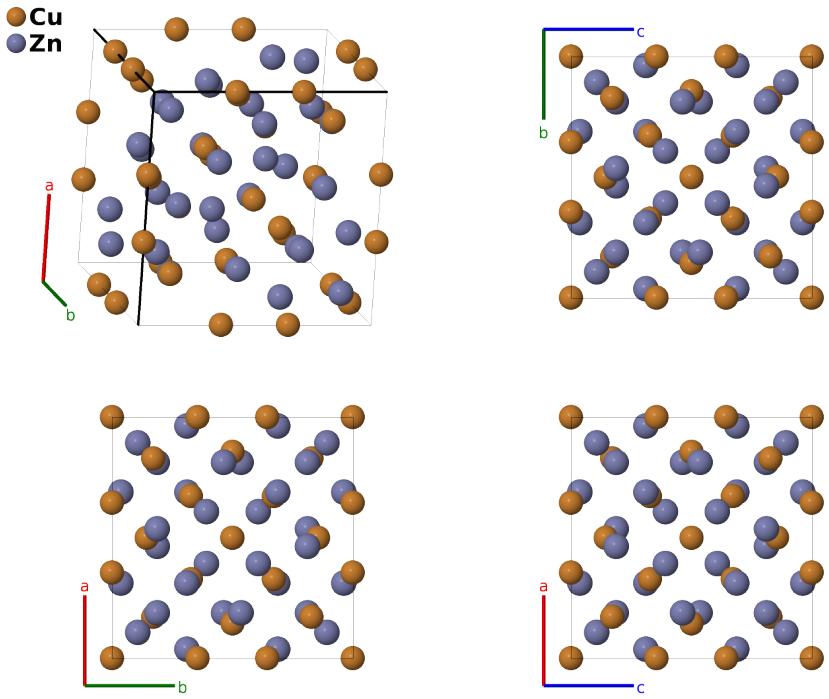
γ-Brass (Cu_5Zn_8, $D8_2$) Structure: A5B8_cI52_217_ce_cg-001

This structure originally had the label `A5B8_cI52_217_ce_cg`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/AYKC

https://aflow.org/p/A5B8_cI52_217_ce_cg-001



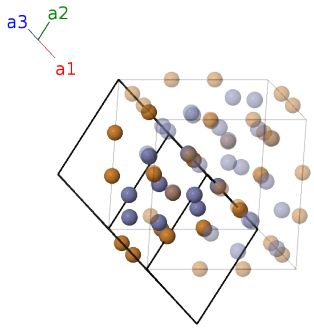
Prototype	Cu_5Zn_8
AFLOW prototype label	A5B8_cI52_217_ce_cg-001
***Strukturbericht* designation**	$D8_2$
Mineral name	γ-brass
ICSD	240667
Pearson symbol	cI52
Space group number	217
Space group symbol	$I\bar{4}3m$
AFLOW prototype command	`aflow --proto=A5B8_cI52_217_ce_cg-001 --params=`$a, x_1, x_2, x_3, x_4, z_4$

Other compounds with this structure
Cu_xZn_{1-x}, Cu_xCd_{1-x}, Fe_xZn_{1-x}

- γ-brass comes in a variety of compositions. See the $D8_1$ and $D8_3$ structure pages for more information.
- We use the data from (Gourdon, 2007) for $Cu_{5.00}Zn_{8.00}$. At this composition the authors state that the sites are fully occupied.
- (Mizutani, 2010) classifies this as a "I-cell" γ-brass.

Body-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$2x_1\,\mathbf{a}_1 + 2x_1\,\mathbf{a}_2 + 2x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_2}$	=	$-2x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_3}$	=	$-2x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_4}$	=	$-2x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_5}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B_6}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B_7}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B_8}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Zn I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(12e)	Cu II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(12e)	Cu II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(12e)	Cu II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(12e)	Cu II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{z}}$	(12e)	Cu II
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{z}}$	(12e)	Cu II
$\mathbf{B_{15}}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{16}}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{17}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{18}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{19}}$	=	$2x_4\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{20}}$	=	$-2x_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 - z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{21}}$	=	$(x_4 - z_4)\,\mathbf{a}_2 - (x_4 + z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II

$\mathbf{B_{22}}$	=	$-(x_4+z_4)\,\mathbf{a}_2+(x_4-z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{23}}$	=	$(x_4+z_4)\,\mathbf{a}_1+2x_4\,\mathbf{a}_2+(x_4+z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+az_4\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{24}}$	=	$-(x_4-z_4)\,\mathbf{a}_1-2x_4\,\mathbf{a}_2-(x_4-z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+az_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{25}}$	=	$-(x_4+z_4)\,\mathbf{a}_1+(x_4-z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II
$\mathbf{B_{26}}$	=	$(x_4-z_4)\,\mathbf{a}_1-(x_4+z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(24g)	Zn II

References

[1] O. Gourdon, D. Gout, D. J. Williams, T. Proffen, S. Hobbs, and G. J. Miller, *Atomic Distributions in the γ-Brass Structure of the Cu-Zn System: A Structural and Theoretical Study*, Inorg. Chem. **46**, 251–260 (2007), doi:10.1021/ic0616380.

[2] U. Mizutani, *Hume-Rothery Rules for Structurally Complex Alloy Phases* (CRC Press, Boca Raton, London, New York, 2010).