γ-brass (Cu_9Al_4, $D8_3$) Structure: A4B9_cP52_215_ei_3efgi-001

This structure previously used the label(s) `A4B9_cP52_215_ei_3efgi`. Calls to these addresses will be redirected here.

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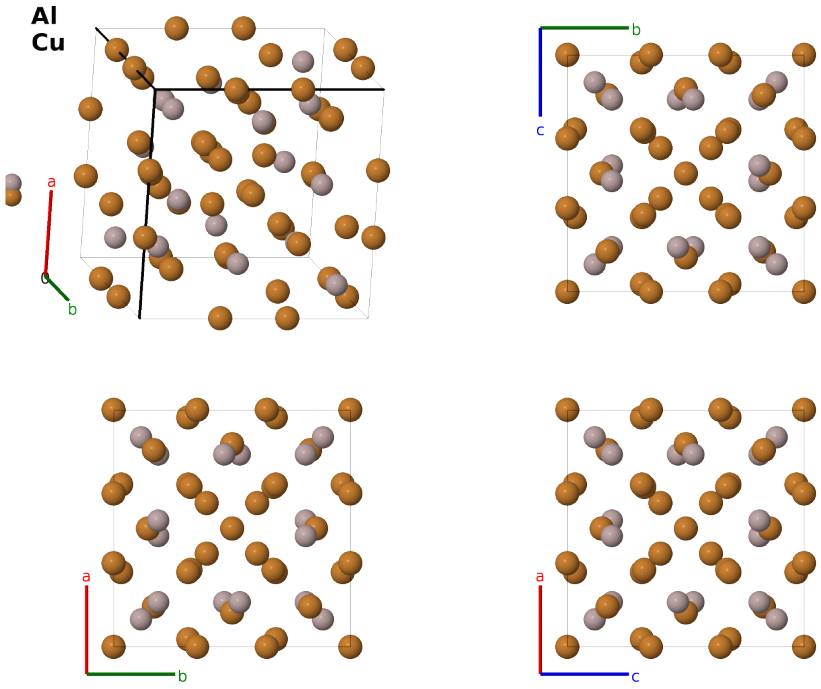
https://aflow.org/prototype-encyclopedia/TRNX

https://aflow.org/prototype-encyclopedia/A4B9_cP52_215_ei_3efgi-001



Prototype	Al_4Cu_9
AFLOW prototype label	A4B9_cP52_215_ei_3efgi-001
***Strukturbericht* designation**	$D8_3$
Mineral name	γ-brass
ICSD	1625
CCDC	1591705
Pearson symbol	cP52
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	`aflow --proto=A4B9_cP52_215_ei_3efgi-001 --params=`$a, x_1, x_2, x_3, x_4, x_5, x_6, x_7, z_7, x_8, z_8$

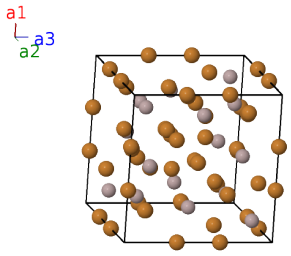
Other compounds with this structure
Cu_9Ga_4, $InMn_3$

- (Arnberg, 1978) give the Wyckoff positions of the Cu-IV and Cu-V atoms as (6g) $(x, 1/2, 1/2)$, but give the coordinates in the form $(x, 0, 0)$ corresponding to the (6f) site.
- (Stokhuyzen, 1974) used (6f) for both types of atoms in the isostructural system Ga_9Al_4.
- (Pearson, 1958) places the Cu-IV atoms on a (6f) site and Cu-V on (6g), but does not give explicit coordinates.
- Placing the Cu-V atoms on (6f) sites yields an interatomic distance of 1.8Å. This contradicts (Arnberg, 1978), who say that the minimum interatomic distance between the Cu-IV and Cu-V atoms is 2.48Å . Placing the Cu-V atoms on (6g) sites gives this distance, in agreement with (Pearson, 1958), so we make this choice for the crystal structure.
- This is a variety of γ-brass comparable to the $D8_2$ structure. In fact, if we
  - Replace the Al and Cu-III atoms by Zn, while setting $x_4 = x_1 + 1/2$,
  - Replace the Al II and Cu-VI atoms by Zn, with $x_8 = x_7 + 1/2$ and $z_8 = z_7 + 1/2$,
  - Set $x_3 = x_2 + 1/2$ and
  - Set $x_6 = x_5 + 1/2$,

  then this structure is identical to $D8_2$ γ-brass.
- (Pearson, 1958), pp. 252, gives a list of compounds which can take on the $D8_1$, $D8_2$, or $D8_3$ structure, depending on the exact composition.
- (Mizutani, 2010) classifies this as a "P-cell" γ-brass.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4e)	Cu I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4e)	Cu I

$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4e)	Cu II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4e)	Cu III
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1$	=	$ax_5\,\hat{\mathbf{x}}$	(6f)	Cu IV
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1$	=	$-ax_5\,\hat{\mathbf{x}}$	(6f)	Cu IV
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{y}}$	(6f)	Cu IV
$\mathbf{B_{20}}$	=	$-x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{y}}$	(6f)	Cu IV
$\mathbf{B_{21}}$	=	$x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{z}}$	(6f)	Cu IV
$\mathbf{B_{22}}$	=	$-x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{z}}$	(6f)	Cu IV
$\mathbf{B_{23}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B_{24}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B_{25}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B_{26}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B_{27}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B_{28}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(6g)	Cu V
$\mathbf{B_{29}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + az_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{30}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + az_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{31}}$	=	$-x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{32}}$	=	$x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{33}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{34}}$	=	$z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$az_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{35}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-az_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{36}}$	=	$-z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{37}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{38}}$	=	$-x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{39}}$	=	$x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{40}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Al II
$\mathbf{B_{41}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{42}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{43}}$	=	$-x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{44}}$	=	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{45}}$	=	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{46}}$	=	$z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{47}}$	=	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{48}}$	=	$-z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{49}}$	=	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI

$\mathbf{B_{50}}$	=	$-x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{51}}$	=	$x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI
$\mathbf{B_{52}}$	=	$-x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Cu VI

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