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

This structure originally had the label `A4B9_cP52_215_ei_3efgi`. Calls to that address will be redirected here.

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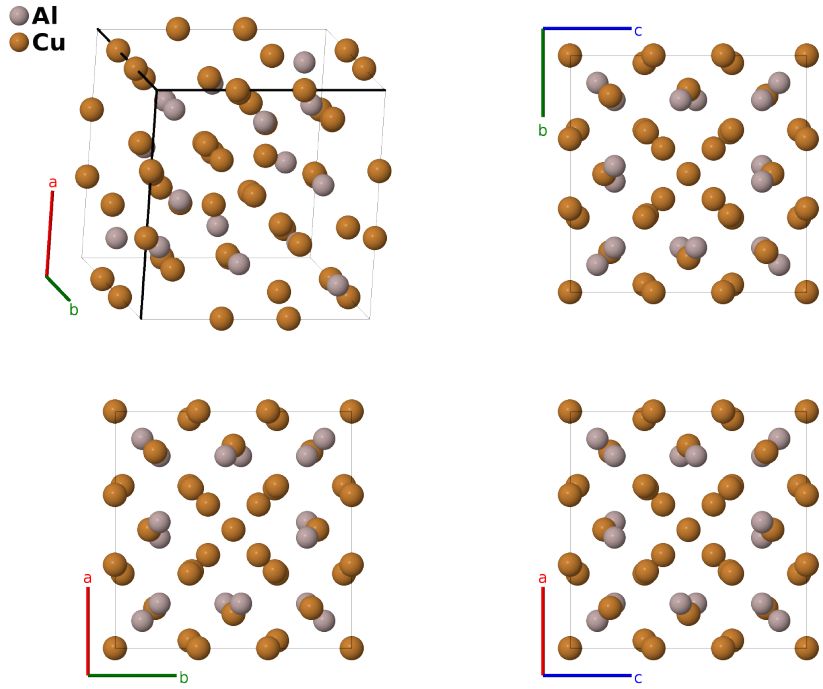
https://aflow.org/p/TRNX

https://aflow.org/p/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
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=`$a, x_1, x_2, x_3, x_4, x_5, x_6, x_7, z_7, x_8, z_8$

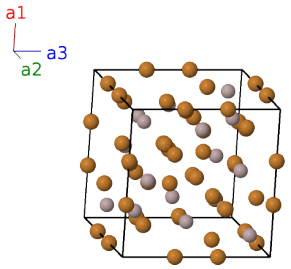
Other compounds with this structure
Cu_9Ga_4, $InMn_3$

- (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

$$\mathbf{B_{13}} = x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Cu III}$$
$$\mathbf{B_{14}} = -x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Cu III}$$
$$\mathbf{B_{15}} = -x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Cu III}$$
$$\mathbf{B_{16}} = x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Cu III}$$
$$\mathbf{B_{17}} = x_5\,\mathbf{a}_1 = ax_5\,\hat{\mathbf{x}} \quad \text{(6f)} \quad \text{Cu IV}$$
$$\mathbf{B_{18}} = -x_5\,\mathbf{a}_1 = -ax_5\,\hat{\mathbf{x}} \quad \text{(6f)} \quad \text{Cu IV}$$
$$\mathbf{B_{19}} = x_5\,\mathbf{a}_2 = ax_5\,\hat{\mathbf{y}} \quad \text{(6f)} \quad \text{Cu IV}$$
$$\mathbf{B_{20}} = -x_5\,\mathbf{a}_2 = -ax_5\,\hat{\mathbf{y}} \quad \text{(6f)} \quad \text{Cu IV}$$
$$\mathbf{B_{21}} = x_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Cu IV}$$
$$\mathbf{B_{22}} = -x_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Cu IV}$$
$$\mathbf{B_{23}} = x_6\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{Cu V}$$
$$\mathbf{B_{24}} = -x_6\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{Cu V}$$
$$\mathbf{B_{25}} = \tfrac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{Cu V}$$
$$\mathbf{B_{26}} = \tfrac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{Cu V}$$
$$\mathbf{B_{27}} = \tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + x_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{Cu V}$$
$$\mathbf{B_{28}} = \tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 - x_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{Cu V}$$
$$\mathbf{B_{29}} = x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + az_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{30}} = -x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + az_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{31}} = -x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{32}} = x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{33}} = z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{34}} = z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = az_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{35}} = -z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -az_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{36}} = -z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = -az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{37}} = x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{38}} = -x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{39}} = x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{40}} = -x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Al II}$$
$$\mathbf{B_{41}} = x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{42}} = -x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{43}} = -x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{44}} = x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{45}} = z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{46}} = z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3 = az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{47}} = -z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = -az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{48}} = -z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3 = -az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{49}} = x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{50}} = -x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{51}} = x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$
$$\mathbf{B_{52}} = -x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Cu VI}$$

References

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[3] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.

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