

α -Ga (A11) Structure: A_oC8_64_f-001

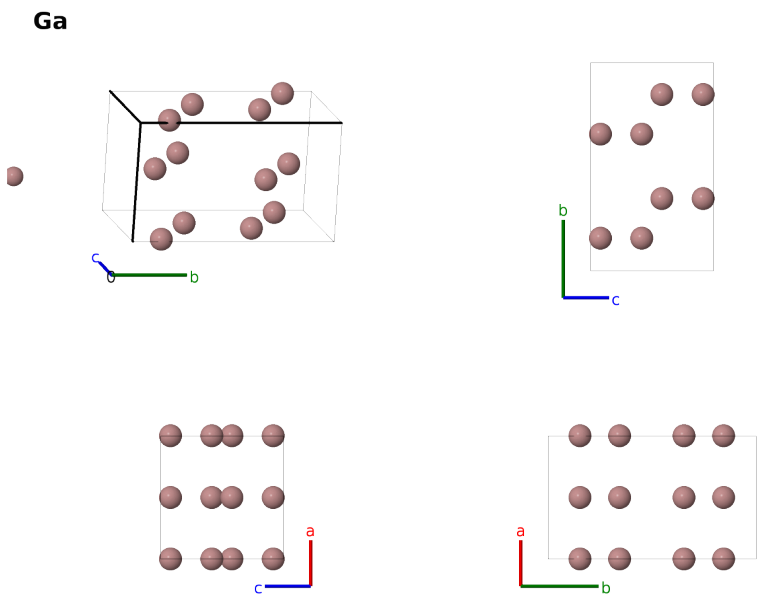
This structure previously used the label(s) **A_oC8_64_f.alpha-Ga**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/JS9R>

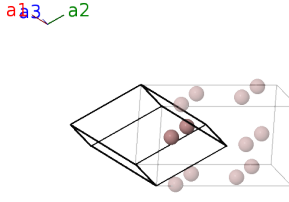
https://aflow.org/prototype-encyclopedia/A_oC8_64_f-001



Prototype	Ga
AFLOW prototype label	A_oC8_64_f-001
<i>Strukturbericht</i> designation	A11
ICSD	43388
CCDC	1612893
Pearson symbol	oC8
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=A_oC8_64_f-001 --params=a, b/a, c/a, y₁, z₁</code>

- α -gallium (A11), molecular iodine (A14), and black phosphorous (A17) all share the same AFLOW label, A_oC8_64_f. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8f)	Ga I
$\mathbf{B}_2$	$= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Ga I
$\mathbf{B}_3$	$= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Ga I
$\mathbf{B}_4$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8f)	Ga I

References

- [1] B. D. Sharma and J. Donohue, *A refinement of the crystal structure of gallium*, Z. Kristallogr. **117**, 293–300 (1962), doi:10.1524/zkri.1962.117.4.293.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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