

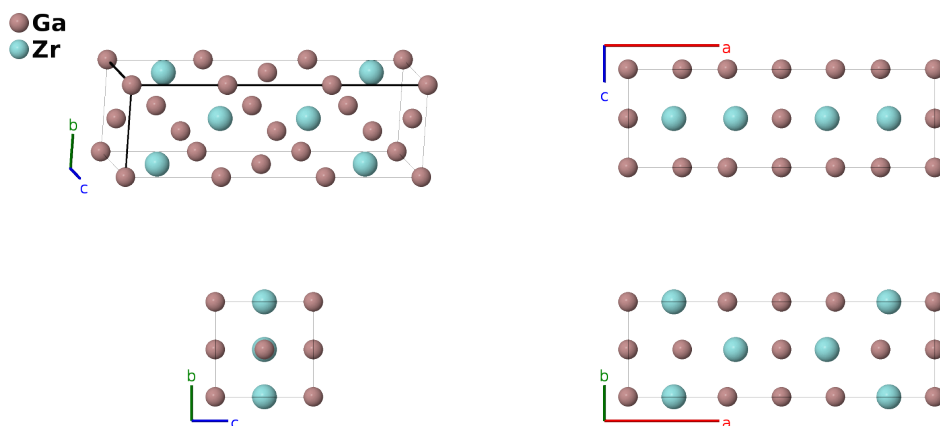
# Ga<sub>2</sub>Zr Structure:

## A2B\_oC12\_65\_acg\_h-001

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<https://afLOW.org/p/V3JJ>

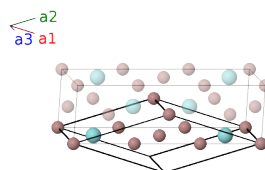
[https://afLOW.org/p/A2B\\_oC12\\_65\\_acg\\_h-001](https://afLOW.org/p/A2B_oC12_65_acg_h-001)



Prototype	Ga <sub>2</sub> Zr
AFLOW prototype label	A2B_oC12_65_acg_h-001
ICSD	104041
Pearson symbol	oC12
Space group number	65
Space group symbol	<i>Cmmm</i>
AFLOW prototype command	<code>afLOW --proto=A2B_oC12_65_acg_h-001 --params=a, b/a, c/a, x<sub>3</sub>, x<sub>4</sub></code>

### Base-centered Orthorhombic primitive vectors

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



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Ga I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{x} + \frac{1}{2}c \hat{z}$	(2c) Ga II

$$\begin{array}{llllll}
\mathbf{B}_3 & = & x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 & = & ax_3 \hat{\mathbf{x}} & (4g) \quad \text{Ga III} \\
\mathbf{B}_4 & = & -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 & = & -ax_3 \hat{\mathbf{x}} & (4g) \quad \text{Ga III} \\
\mathbf{B}_5 & = & x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) \quad \text{Zr I} \\
\mathbf{B}_6 & = & -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 & = & -ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) \quad \text{Zr I}
\end{array}$$

## References

- [1] M. Pötzschke and K. Schubert, *Zum Aufbau einiger zu  $T^4$ - $B^3$  homologer und quasihomologer Systeme: I. Die Systeme Titan-Gallium, Zirkonium-Gallium und Hafnium-Gallium*, Z. Metallkd. **54**, 474–488 (1962), doi:10.1515/ijmr-1962-530708.