

β -Ga Structure (*Obsolete*):

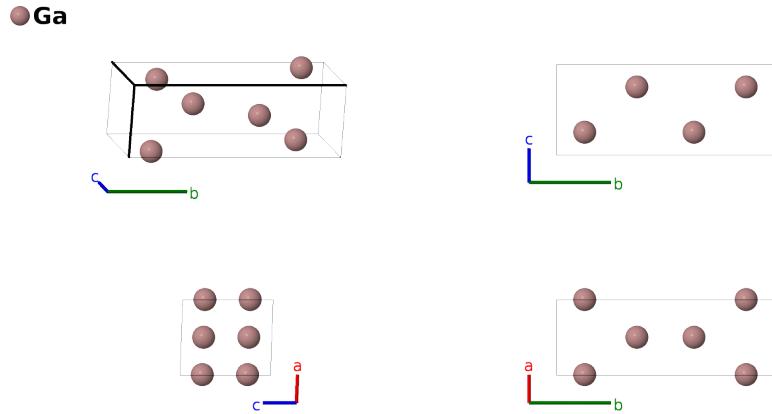
A_mC4_15_e-001

This structure originally had the label A_mC4_15_e. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/BRYB>

https://aflow.org/p/A_mC4_15_e-001



Prototype

Ga

AFLOW prototype label

A_mC4_15_e-001

ICSD

23247

Pearson symbol

mC4

Space group number

15

Space group symbol

$C2/c$

AFLOW prototype command

aflow --proto=A_mC4_15_e-001
--params=a, b/a, c/a, β , y_1

- This was proposed as a metastable structure of gallium, visible for short times at atmospheric pressure. The true structure is isostructural with indium (A6), and stabilized under pressure.

Base-centered Monoclinic primitive vectors

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

\mathbf{a}_1 \mathbf{a}_3 \mathbf{a}_2



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1 =$	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Ga I
$\mathbf{B}_2 =$	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Ga I

References

- [1] L. Bosio and A. Defrain, *Structure cristalline du gallium β* , Acta Crystallogr. Sect. B **25**, 995 (1969), doi:10.1107/S0567740869003360.

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).