

Ca₅Ga₂As₆ Structure:

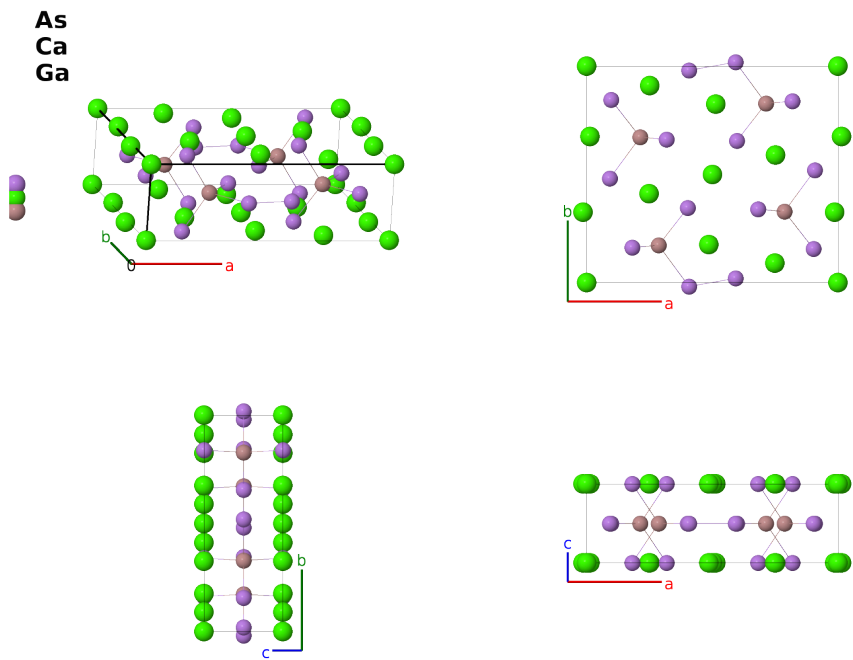
A6B5C2_oP26_55_g2h_a2g_h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/prototype-encyclopedia/JZ3U>

https://aflow.org/prototype-encyclopedia/A6B5C2_oP26_55_g2h_a2g_h-001



Prototype	Ca ₅ Ga ₂ As ₆
AFLOW prototype label	A6B5C2_oP26_55_g2h_a2g_h-001
ICSD	27
CCDC	1590662
Pearson symbol	oP26
Space group number	55
Space group symbol	<i>Pbam</i>
AFLOW prototype command	<code>aflow --proto=A6B5C2_oP26_55_g2h_a2g_h-001</code> <code>--params=a,b/a,c/a,x₂,y₂,x₃,y₃,x₄,y₄,x₅,y₅,x₆,y₆,x₇,y₇</code>

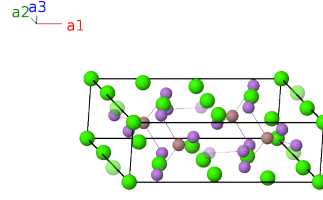
Other compounds with this structure

Ca₅Al₂Bi₆, Ca₅Al₂Sb₆, Ca₅Ga₂Sb₆, Ca₅In₂Sb₆, Eu₅In₂Sb₆, Sr₅In₂Sb₆

- (Verdier, 1976) place the origin so that the Ca-I atoms are at the (2d) Wyckoff position. We shifted the origin to place them on the (2a) Wyckoff sites.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Ca I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2a) Ca I
$\mathbf{B}_3$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g) As I
$\mathbf{B}_4$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g) As I
$\mathbf{B}_5$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) As I
$\mathbf{B}_6$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) As I
$\mathbf{B}_7$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g) Ca II
$\mathbf{B}_8$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g) Ca II
$\mathbf{B}_9$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Ca II
$\mathbf{B}_{10}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Ca II
$\mathbf{B}_{11}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g) Ca III
$\mathbf{B}_{12}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g) Ca III
$\mathbf{B}_{13}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Ca III
$\mathbf{B}_{14}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Ca III
$\mathbf{B}_{15}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As II
$\mathbf{B}_{16}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As II
$\mathbf{B}_{17}$	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As II
$\mathbf{B}_{18}$	$=$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As II
$\mathbf{B}_{19}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As III
$\mathbf{B}_{20}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As III
$\mathbf{B}_{21}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As III
$\mathbf{B}_{22}$	$=$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) As III
$\mathbf{B}_{23}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Ga I
$\mathbf{B}_{24}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Ga I
$\mathbf{B}_{25}$	$=$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Ga I

$$\mathbf{B}_{26} = \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} \quad (4h) \quad \text{Ga I}$$

References

- [1] P. Verdier, P. L’Haridon, M. Maunaye, and Y. Laurent, *Etude Structural de $\text{Ca}_5\text{Ga}_2\text{As}_6$* , Acta Crystallogr. Sect. B **32**, 726–728 (1976), doi:10.1107/S0567740876003889.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.