

Low Temperature GaMo₄S₈ Structure: AB4C8_hR13_160_a_ab_2a2b-001

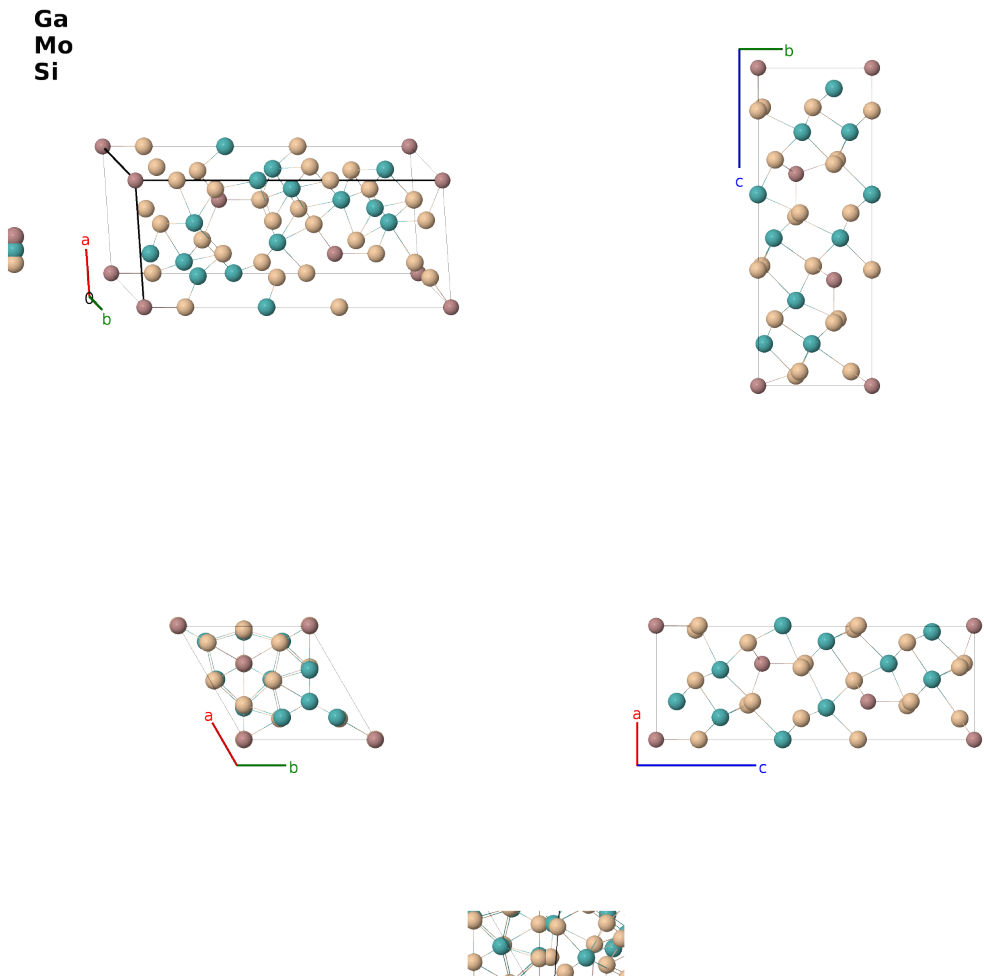
This structure previously used the label(s) **AB4C8_hR13_160_a_ab_2a2b**. Calls to these addresses will be redirected here.

Cite this page as:

- 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.
- 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/5V5H>

https://aflow.org/prototype-encyclopedia/AB4C8_hR13_160_a_ab_2a2b-001



Prototype	GaMo ₄ S ₈
AFLOW prototype label	AB4C8_hR13_160_a_ab_2a2b-001
ICSD	33995
CCDC	1606728
Pearson symbol	hR13
Space group number	160

Space group symbol $R3m$

AFLOW prototype command `aflow --proto=AB4C8_hR13_160_a_ab_2a2b-001`
`--params=a, c/a, x1, x2, x3, x4, x5, z5, x6, z6, x7, z7`

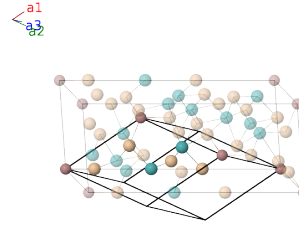
Other compounds with this structure

GaV₄S₈

- At temperatures below 45K GaMo₄S₈ transforms from its high-temperature cubic structure to this rhombohedral structure.
- We use the data from (François, 1991) at 8K.
- Space group $R3m$ #160 allows a arbitrary choice of the zero of the z -axis. Here we use this freedom to place the gallium atom at the origin ($z_1 = 0$).

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a)	Ga I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a)	Mo I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(1a)	Si I
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(1a)	Si II
$\mathbf{B}_5$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Mo II
$\mathbf{B}_6$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Mo II
$\mathbf{B}_7$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	Mo II
$\mathbf{B}_8$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Si III
$\mathbf{B}_9$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Si III
$\mathbf{B}_{10}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(3b)	Si III
$\mathbf{B}_{11}$	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Si IV
$\mathbf{B}_{12}$	$= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(3b)	Si IV

$$\mathbf{B}_{13} = x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 = -\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}} \quad (3b) \quad \text{Si IV}$$

References

- [1] M. François, W. Lengauer, K. Yvon, M. Sergent, M. Potel, P. Gougeon, and H. B. Yaich-Aerrache, *Structural phase transition in GaMo_4S_8 by X-ray powder diffraction*, Z. Kristallogr. **196**, 111–120 (1991), doi:10.1524/zkri.1991.196.14.111.

First cited in

- 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.