Low Temperature $GaMo_4S_8$ Structure: AB4C8_hR13_160_a_ab_2a2b-001

This structure originally had the label `AB4C8_hR13_160_a_ab_2a2b`. Calls to that address will be redirected here.

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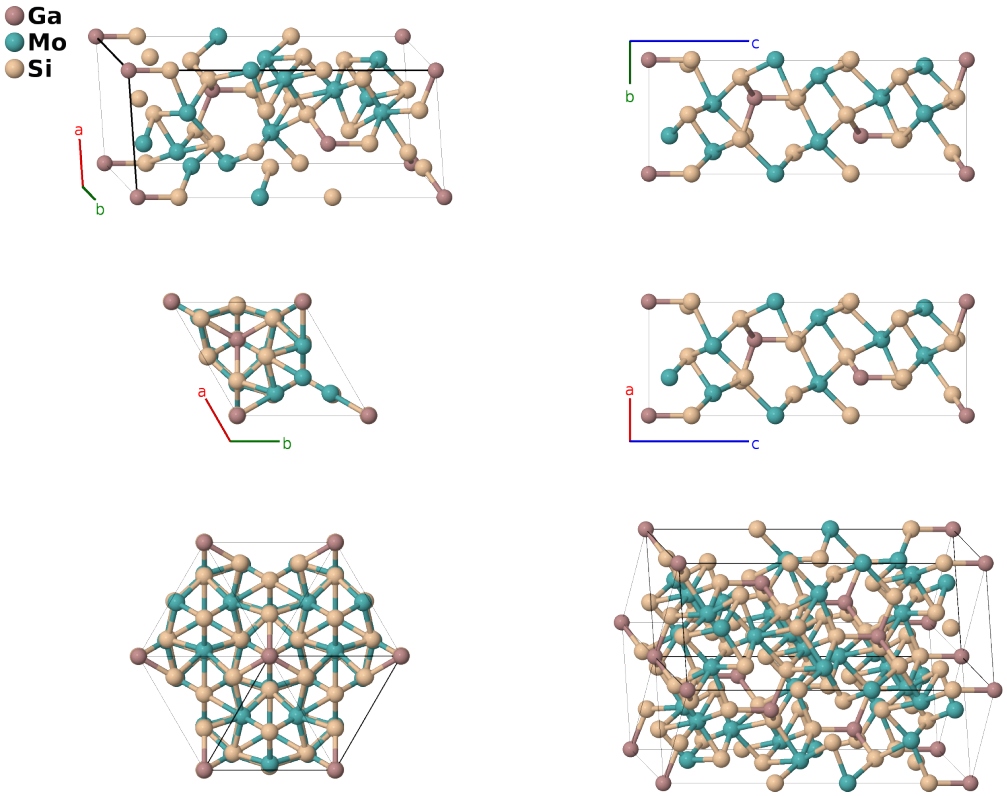
https://aflow.org/p/5V5H

https://aflow.org/p/AB4C8_hR13_160_a_ab_2a2b-001



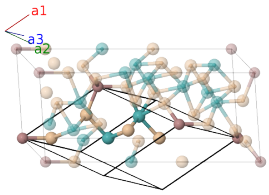
Prototype	$GaMo_4S_8$
AFLOW prototype label	AB4C8_hR13_160_a_ab_2a2b-001
ICSD	33995
Pearson symbol	hR13
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB4C8_hR13_160_a_ab_2a2b-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, z_5, x_6, z_6, x_7, z_7$

Other compounds with this structure
GaV_4S_8

- At temperatures below 45K $GaMo_4S_8$ 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



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
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(3b)	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.