Room Temperature $GaMo_4S_8$ Structure: AB4C8_cF52_216_a_e_2e-001

This structure originally had the label `AB4C8_cF52_216_a_e_2e`. Calls to that address will be redirected here.

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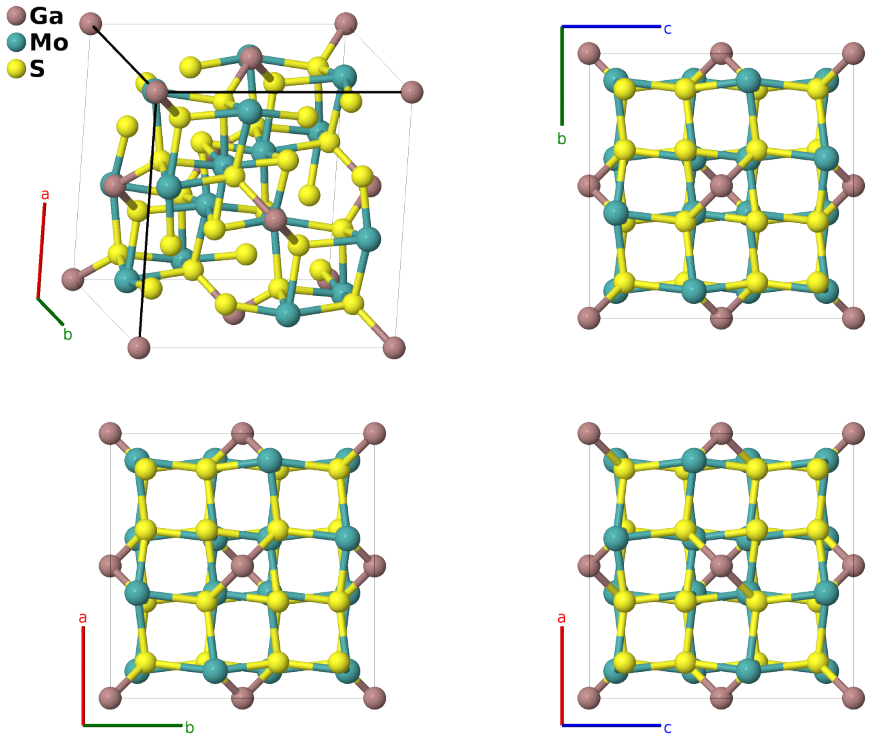
https://aflow.org/p/BEEG

https://aflow.org/p/AB4C8_cF52_216_a_e_2e-001



Prototype	$GaMo_4S_8$
AFLOW prototype label	AB4C8_cF52_216_a_e_2e-001
ICSD	49566
Pearson symbol	cF52
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB4C8_cF52_216_a_e_2e-001 --params=`a, x_2, x_3, x_4

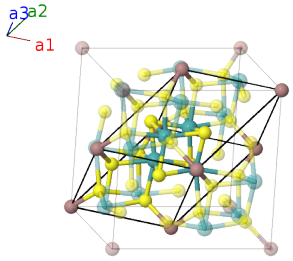
Other compounds with this structure

$AlMo_4S_8$, $Co(Mo_2Re_2)S_8$, $Fe(Mo_2Re_2)S_8$, $GaMo_4S_4Te_4$, $GaMo_4S_8$, $GaMo_4Se_4Te_4$, $GaMo_4Se_8$, $GaMo_4Te_8$, $GaNb_4S_8$, $GaNb_4Se_8$, $GaNb_4Te_8$, $GaRe_4S_8$, $GaRe_4Se_8$, $GaRe_4Te_8$, $GaTa_4S_8$, $GaTa_4Se_8$, $GaTa_4Te_8$, GaV_4S_8, GaV_4Se_8, GaV_4Te_8, $GeMo_4S_8$, $GeMo_4Se_8$, $GeMo_4Te_8$, $GeNb_4S_8$, $GeNb_4Se_8$, $GeNb_4Te_8$, $GeRe_4S_8$, $GeRe_4Se_8$, $GeRe_4Te_8$, $GeTa_4S_8$, $GeTa_4Se_8$, $GeTa_4Te_8$, GeV_4S_8, GeV_4Se_8, GeV_4Te_8, $LaMo_4S_8$, $Ni(Mo_2Re_2)S_8$, $Zn(Mo_2Re_2)S_8$

- This is the room temperature structure. Below 45K $GaMo_4S_8$ transforms into a rhombohedral structure.
- (Ben Yaich, 1984) do not give the lattice constant for $GaMo_4S_8$. We infer it from their interatomic distances and obtain a value of a = 9.7294Å. The ICSD entry uses a = 9.74Å.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Ga I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16e)	Mo I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - 3x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16e)	Mo I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - 3x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16e)	Mo I
$\mathbf{B_5}$	=	$-3x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16e)	Mo I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_9}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - 3x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - 3x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{13}}$	=	$-3x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(16e)	S II

References

[1] H. B. Yaich, J. C. Jegaden, M. P. R. Chevrel, M. Sergent, A. Berton, J. Chaussy, A. K. Rastogi, and R. Tournier, *Nouveaux chalcogenures mixtes $GaMo_4(XX)_8$ (X =S, Se, Te) à clusters tetraedriques Mo_4*, J. Solid State Chem. **51**, 212–217 (1984), doi:10.1016/0022-4596(84)90336-0.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).