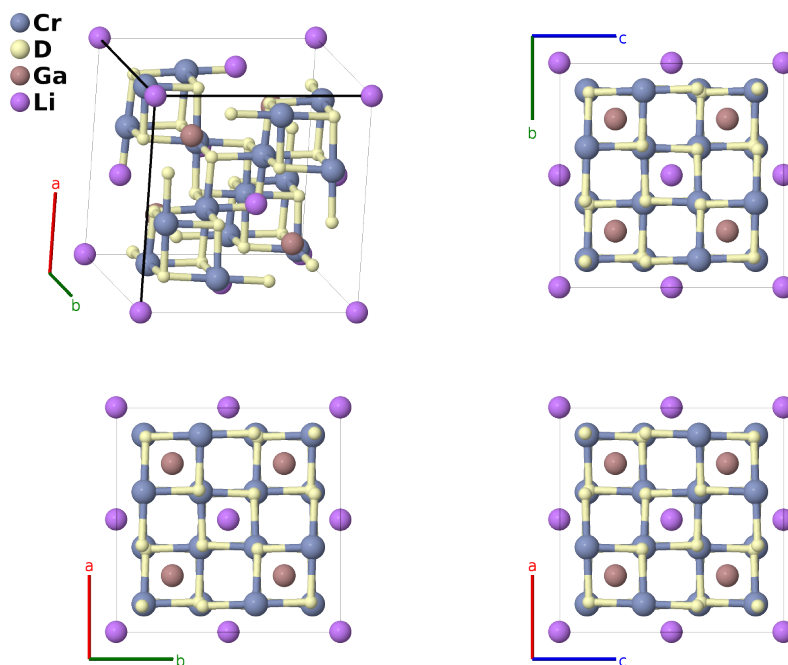


LiGaCr₄O₈ Structure: A4BCD8_cF56_216_e_a_c_2e-001

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<https://aflow.org/p/1XJV>

https://aflow.org/p/A4BCD8_cF56_216_e_a_c_2e-001



Prototype	Cr ₄ GaLiO ₈
AFLOW prototype label	A4BCD8_cF56_216_e_a_c_2e-001
ICSD	259392
Pearson symbol	cF56
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A4BCD8_cF56_216_e_a_c_2e-001 --params=a, x₃, x₄, x₅</code>

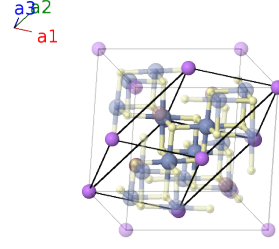
Other compounds with this structure

CuFeCr₄S₈, CuInCr₄S₈, FeInCr₄S₈, LiGaCr₄S₈

- This structure can be regarded as a distorted spinel structure, or a filled GaMo₄S₈ structure.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(4a) Ga I
\mathbf{B}_2	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(4c) Li I
\mathbf{B}_3	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x} + ax_3\hat{y} + ax_3\hat{z}$	(16e) Cr I
\mathbf{B}_4	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - 3x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} - ax_3\hat{y} + ax_3\hat{z}$	(16e) Cr I
\mathbf{B}_5	$=$	$x_3\mathbf{a}_1 - 3x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} + ax_3\hat{y} - ax_3\hat{z}$	(16e) Cr I
\mathbf{B}_6	$=$	$-3x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x} - ax_3\hat{y} - ax_3\hat{z}$	(16e) Cr I
\mathbf{B}_7	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} + ax_4\hat{y} + ax_4\hat{z}$	(16e) D I
\mathbf{B}_8	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - 3x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} - ax_4\hat{y} + ax_4\hat{z}$	(16e) D I
\mathbf{B}_9	$=$	$x_4\mathbf{a}_1 - 3x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} + ax_4\hat{y} - ax_4\hat{z}$	(16e) D I
\mathbf{B}_{10}	$=$	$-3x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} - ax_4\hat{y} - ax_4\hat{z}$	(16e) D I
\mathbf{B}_{11}	$=$	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} + ax_5\hat{y} + ax_5\hat{z}$	(16e) D II
\mathbf{B}_{12}	$=$	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 - 3x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} - ax_5\hat{y} + ax_5\hat{z}$	(16e) D II
\mathbf{B}_{13}	$=$	$x_5\mathbf{a}_1 - 3x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} + ax_5\hat{y} - ax_5\hat{z}$	(16e) D II
\mathbf{B}_{14}	$=$	$-3x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} - ax_5\hat{y} - ax_5\hat{z}$	(16e) D II

References

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- [1] G. Pokharel, A. F. May, D. S. Parker, S. Calder, G. Ehlers, A. Huq, S. A. J. Kimber, H. S. Arachchige, L. Poudel, M. A. McGuire, D. Mandrus, and A. D. Christianson, *Negative thermal expansion and magnetoelastic coupling in the breathing pyrochlore lattice material $\text{LiGaCr}_4\text{S}_8$* , Phys. Rev. B **97**, 134117 (2018), doi:10.1103/PhysRevB.97.134117.