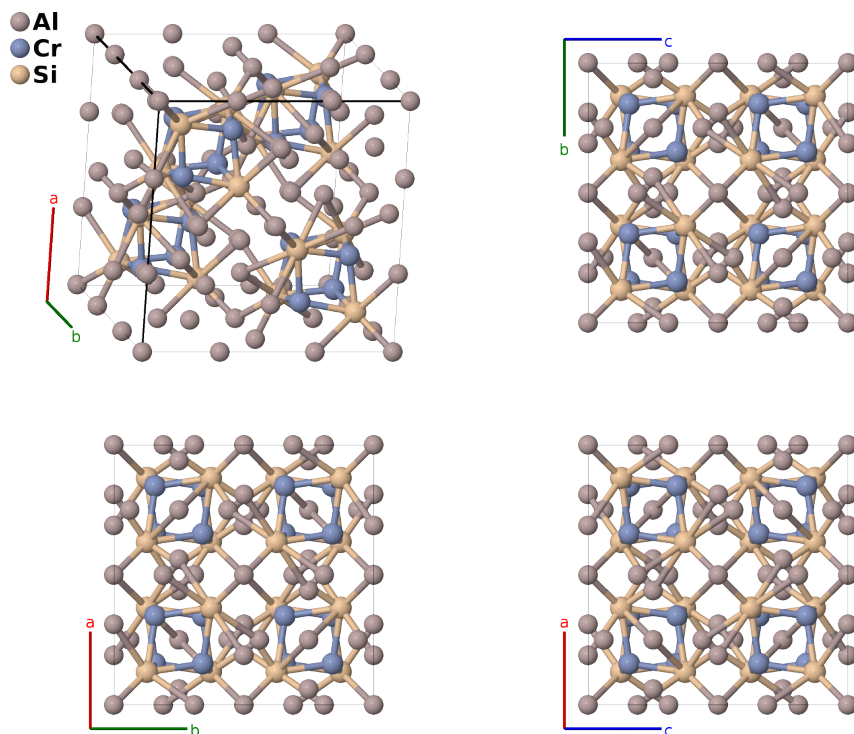


Al₁₃Cr₄Si₄ Structure: A13B4C4_cF84_216_afg_e_e-001

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<https://aflow.org/p/5ADG>

https://aflow.org/p/A13B4C4_cF84_216_afg_e_e-001



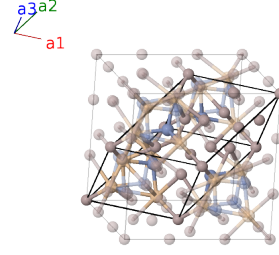
Prototype	Al ₁₃ Cr ₄ Si ₄
AFLOW prototype label	A13B4C4_cF84_216_afg_e_e-001
ICSD	76116
Pearson symbol	cF84
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A13B4C4_cF84_216_afg_e_e-001 --params=a, x2, x3, x4, x5</code>

Other compounds with this structure

Al₁₇Mn₄

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(4a) Al 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) Cr 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) Cr 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) Cr 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) Cr 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) Si 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) Si 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) Si 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) Si I
\mathbf{B}_{10}	$=$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}}$	(24f) Al II
\mathbf{B}_{11}	$=$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}}$	(24f) Al II
\mathbf{B}_{12}	$=$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{y}}$	(24f) Al II
\mathbf{B}_{13}	$=$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{y}}$	(24f) Al II
\mathbf{B}_{14}	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{z}}$	(24f) Al II
\mathbf{B}_{15}	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{z}}$	(24f) Al II
\mathbf{B}_{16}	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Al III
\mathbf{B}_{17}	$=$	$x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Al III
\mathbf{B}_{18}	$=$	$x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Al III
\mathbf{B}_{19}	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Al III
\mathbf{B}_{20}	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(24g) Al III
\mathbf{B}_{21}	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(24g) Al III

References

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