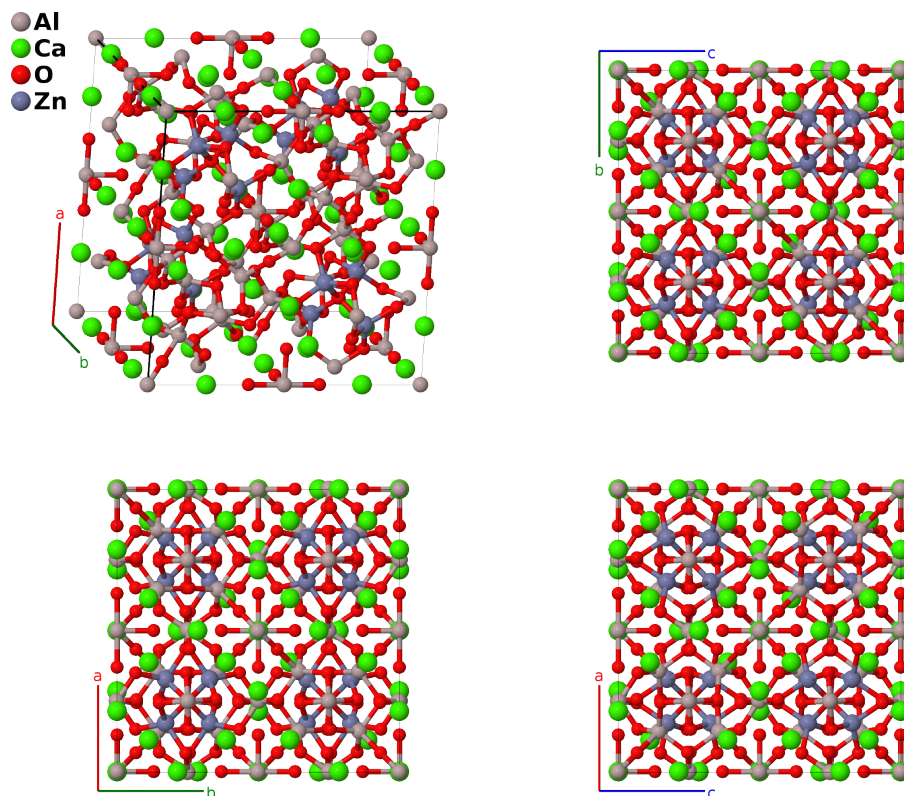


Ca₁₄Zn₆Al₁₀O₃₅ Structure: A12B14C35D4_cF260_196_abeg_2ef_cef2h_e-001

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<https://aflow.org/p/JELG>

https://aflow.org/p/A12B14C35D4_cF260_196_abeg_2ef_cef2h_e-001

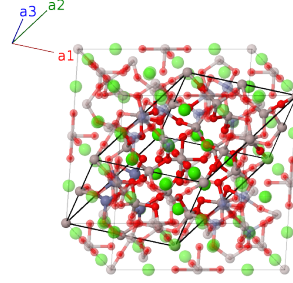


Prototype	Al ₁₀ Ca ₁₄ O ₃₅ Zn ₆
AFLOW prototype label	A12B14C35D4_cF260_196_abeg_2ef_cef2h_e-001
ICSD	50292
Pearson symbol	cF260
Space group number	196
Space group symbol	<i>F</i> 23
AFLOW prototype command	<code>aflow --proto=A12B14C35D4_cF260_196_abeg_2ef_cef2h_e-001 --params=a, x₄, x₅, x₆, x₇, x₈, x₉, x₁₀, x₁₁, x₁₂, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃</code>

- All of the sites labeled “aluminum” are actual 5 parts aluminum and 1 part zinc, giving the observed stoichiometry.

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) Al I
\mathbf{B}_2	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$	(4b) Al II
\mathbf{B}_3	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(4c) O I
\mathbf{B}_4	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} + ax_4\hat{y} + ax_4\hat{z}$	(16e) Al III
\mathbf{B}_5	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - 3x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} - ax_4\hat{y} + ax_4\hat{z}$	(16e) Al III
\mathbf{B}_6	$=$	$x_4\mathbf{a}_1 - 3x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} + ax_4\hat{y} - ax_4\hat{z}$	(16e) Al III
\mathbf{B}_7	$=$	$-3x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} - ax_4\hat{y} - ax_4\hat{z}$	(16e) Al III
\mathbf{B}_8	$=$	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} + ax_5\hat{y} + ax_5\hat{z}$	(16e) Ca I
\mathbf{B}_9	$=$	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 - 3x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} - ax_5\hat{y} + ax_5\hat{z}$	(16e) Ca I
\mathbf{B}_{10}	$=$	$x_5\mathbf{a}_1 - 3x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} + ax_5\hat{y} - ax_5\hat{z}$	(16e) Ca I
\mathbf{B}_{11}	$=$	$-3x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} - ax_5\hat{y} - ax_5\hat{z}$	(16e) Ca I
\mathbf{B}_{12}	$=$	$x_6\mathbf{a}_1 + x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$ax_6\hat{x} + ax_6\hat{y} + ax_6\hat{z}$	(16e) Ca II
\mathbf{B}_{13}	$=$	$x_6\mathbf{a}_1 + x_6\mathbf{a}_2 - 3x_6\mathbf{a}_3$	$=$	$-ax_6\hat{x} - ax_6\hat{y} + ax_6\hat{z}$	(16e) Ca II
\mathbf{B}_{14}	$=$	$x_6\mathbf{a}_1 - 3x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$-ax_6\hat{x} + ax_6\hat{y} - ax_6\hat{z}$	(16e) Ca II
\mathbf{B}_{15}	$=$	$-3x_6\mathbf{a}_1 + x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$ax_6\hat{x} - ax_6\hat{y} - ax_6\hat{z}$	(16e) Ca II
\mathbf{B}_{16}	$=$	$x_7\mathbf{a}_1 + x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$ax_7\hat{x} + ax_7\hat{y} + ax_7\hat{z}$	(16e) O II
\mathbf{B}_{17}	$=$	$x_7\mathbf{a}_1 + x_7\mathbf{a}_2 - 3x_7\mathbf{a}_3$	$=$	$-ax_7\hat{x} - ax_7\hat{y} + ax_7\hat{z}$	(16e) O II
\mathbf{B}_{18}	$=$	$x_7\mathbf{a}_1 - 3x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$-ax_7\hat{x} + ax_7\hat{y} - ax_7\hat{z}$	(16e) O II
\mathbf{B}_{19}	$=$	$-3x_7\mathbf{a}_1 + x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$ax_7\hat{x} - ax_7\hat{y} - ax_7\hat{z}$	(16e) O II
\mathbf{B}_{20}	$=$	$x_8\mathbf{a}_1 + x_8\mathbf{a}_2 + x_8\mathbf{a}_3$	$=$	$ax_8\hat{x} + ax_8\hat{y} + ax_8\hat{z}$	(16e) Zn I
\mathbf{B}_{21}	$=$	$x_8\mathbf{a}_1 + x_8\mathbf{a}_2 - 3x_8\mathbf{a}_3$	$=$	$-ax_8\hat{x} - ax_8\hat{y} + ax_8\hat{z}$	(16e) Zn I
\mathbf{B}_{22}	$=$	$x_8\mathbf{a}_1 - 3x_8\mathbf{a}_2 + x_8\mathbf{a}_3$	$=$	$-ax_8\hat{x} + ax_8\hat{y} - ax_8\hat{z}$	(16e) Zn I
\mathbf{B}_{23}	$=$	$-3x_8\mathbf{a}_1 + x_8\mathbf{a}_2 + x_8\mathbf{a}_3$	$=$	$ax_8\hat{x} - ax_8\hat{y} - ax_8\hat{z}$	(16e) Zn I
\mathbf{B}_{24}	$=$	$-x_9\mathbf{a}_1 + x_9\mathbf{a}_2 + x_9\mathbf{a}_3$	$=$	$ax_9\hat{x}$	(24f) Ca III
\mathbf{B}_{25}	$=$	$x_9\mathbf{a}_1 - x_9\mathbf{a}_2 - x_9\mathbf{a}_3$	$=$	$-ax_9\hat{x}$	(24f) Ca III
\mathbf{B}_{26}	$=$	$x_9\mathbf{a}_1 - x_9\mathbf{a}_2 + x_9\mathbf{a}_3$	$=$	$ax_9\hat{y}$	(24f) Ca III
\mathbf{B}_{27}	$=$	$-x_9\mathbf{a}_1 + x_9\mathbf{a}_2 - x_9\mathbf{a}_3$	$=$	$-ax_9\hat{y}$	(24f) Ca III
\mathbf{B}_{28}	$=$	$x_9\mathbf{a}_1 + x_9\mathbf{a}_2 - x_9\mathbf{a}_3$	$=$	$ax_9\hat{z}$	(24f) Ca III

$$\begin{aligned}
\mathbf{B}_{52} &= \begin{aligned} &-(x_{12} + y_{12} + z_{12}) \mathbf{a}_1 + \\ &(-x_{12} + y_{12} + z_{12}) \mathbf{a}_2 + \\ &(x_{12} + y_{12} - z_{12}) \mathbf{a}_3 \end{aligned} &= & ay_{12} \hat{\mathbf{x}} - az_{12} \hat{\mathbf{y}} - ax_{12} \hat{\mathbf{z}} & (48h) & \text{O IV} \\
\mathbf{B}_{53} &= \begin{aligned} &(x_{12} + y_{12} - z_{12}) \mathbf{a}_1 + \\ &(x_{12} - y_{12} + z_{12}) \mathbf{a}_2 - \\ &(x_{12} + y_{12} + z_{12}) \mathbf{a}_3 \end{aligned} &= & -ay_{12} \hat{\mathbf{x}} - az_{12} \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}} & (48h) & \text{O IV} \\
\mathbf{B}_{54} &= \begin{aligned} &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_1 + \\ &(x_{13} - y_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} + y_{13} - z_{13}) \mathbf{a}_3 \end{aligned} &= & ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} + az_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{55} &= \begin{aligned} &(x_{13} - y_{13} + z_{13}) \mathbf{a}_1 + \\ &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_2 - \\ &(x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & -ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} + az_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{56} &= \begin{aligned} &(x_{13} + y_{13} - z_{13}) \mathbf{a}_1 - \\ &(x_{13} + y_{13} + z_{13}) \mathbf{a}_2 + \\ &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & -ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} - az_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{57} &= \begin{aligned} &-(x_{13} + y_{13} + z_{13}) \mathbf{a}_1 + \\ &(x_{13} + y_{13} - z_{13}) \mathbf{a}_2 + \\ &(x_{13} - y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} - az_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{58} &= \begin{aligned} &(x_{13} + y_{13} - z_{13}) \mathbf{a}_1 + \\ &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} - y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & az_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + ay_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{59} &= \begin{aligned} &-(x_{13} + y_{13} + z_{13}) \mathbf{a}_1 + \\ &(x_{13} - y_{13} + z_{13}) \mathbf{a}_2 + \\ &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & az_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} - ay_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{60} &= \begin{aligned} &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_1 + \\ &(x_{13} + y_{13} - z_{13}) \mathbf{a}_2 - \\ &(x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & -az_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} + ay_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{61} &= \begin{aligned} &(x_{13} - y_{13} + z_{13}) \mathbf{a}_1 - \\ &(x_{13} + y_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} + y_{13} - z_{13}) \mathbf{a}_3 \end{aligned} &= & -az_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} - ay_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{62} &= \begin{aligned} &(x_{13} - y_{13} + z_{13}) \mathbf{a}_1 + \\ &(x_{13} + y_{13} - z_{13}) \mathbf{a}_2 + \\ &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & ay_{13} \hat{\mathbf{x}} + az_{13} \hat{\mathbf{y}} + ax_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{63} &= \begin{aligned} &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_1 - \\ &(x_{13} + y_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} - y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & -ay_{13} \hat{\mathbf{x}} + az_{13} \hat{\mathbf{y}} - ax_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{64} &= \begin{aligned} &-(x_{13} + y_{13} + z_{13}) \mathbf{a}_1 + \\ &(-x_{13} + y_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} + y_{13} - z_{13}) \mathbf{a}_3 \end{aligned} &= & ay_{13} \hat{\mathbf{x}} - az_{13} \hat{\mathbf{y}} - ax_{13} \hat{\mathbf{z}} & (48h) & \text{O V} \\
\mathbf{B}_{65} &= \begin{aligned} &(x_{13} + y_{13} - z_{13}) \mathbf{a}_1 + \\ &(x_{13} - y_{13} + z_{13}) \mathbf{a}_2 - \\ &(x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{aligned} &= & -ay_{13} \hat{\mathbf{x}} - az_{13} \hat{\mathbf{y}} + ax_{13} \hat{\mathbf{z}} & (48h) & \text{O V}
\end{aligned}$$

References

- [1] V. D. Barbanyagre, T. I. Timoshenko, A. M. Il'inets, and V. M. Shamshurov, *Calcium aluminozincates of $Ca_xAl_yZn_kO_n$ composition*, Powder Diff. **12**, 22–26 (1997), doi:10.1017/S0885715600009398.

Found in

- [1] ICSD, *Inorganic Crystal Structure Database. ID 50292.*