

Monoclinic Co₄Al₁₃ Structure:

A13B4_mC102_8_17a11b_8a2b-001

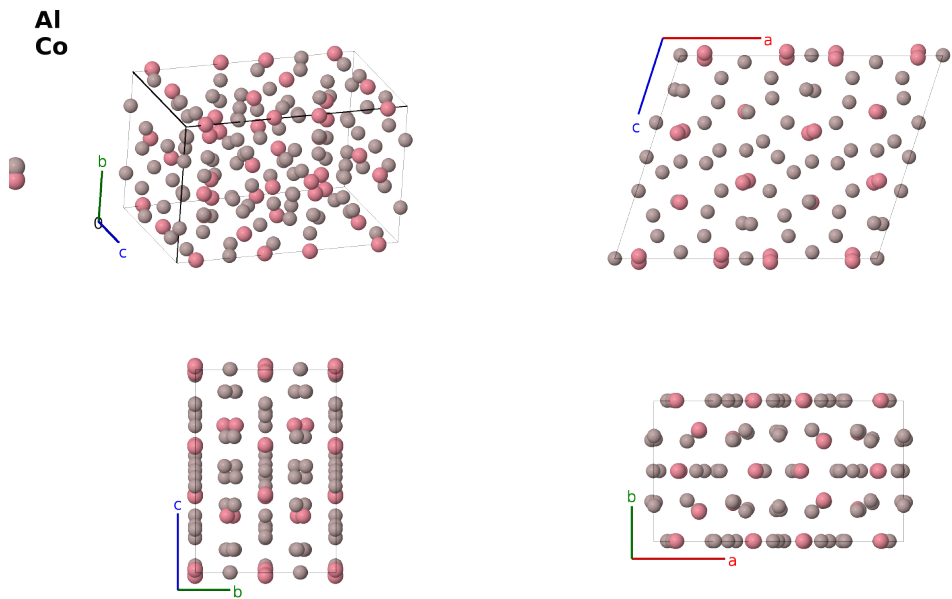
This structure previously used the label(s) **A13B4_mC102_8_17a11b_8a2b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/DU5A>

https://aflow.org/prototype-encyclopedia/A13B4_mC102_8_17a11b_8a2b-001

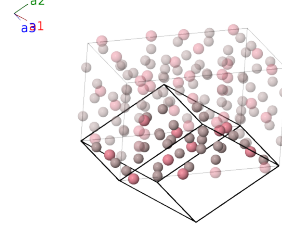


Prototype	Al ₁₃ Co ₄
AFLOW prototype label	A13B4_mC102_8_17a11b_8a2b-001
ICSD	57599
CCDC	1621648
Pearson symbol	mC102
Space group number	8
Space group symbol	<i>Cm</i>
AFLOW prototype command	<pre>aflow --proto=A13B4_mC102_8_17a11b_8a2b-001 --params=a,b/a,c/a,β,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀, z₁₀,x₁₁,z₁₁,x₁₂,z₁₂,x₁₃,z₁₃,x₁₄,z₁₄,x₁₅,z₁₅,x₁₆,z₁₆,x₁₇,z₁₇,x₁₈,z₁₈,x₁₉,z₁₉,x₂₀,z₂₀,x₂₁, z₂₁,x₂₂,z₂₂,x₂₃,z₂₃,x₂₄,z₂₄,x₂₅,z₂₅,x₂₆,z₂₆,x₂₇,z₂₇,x₂₈,z₂₈,x₂₉,z₂₉,x₃₀, y₃₀,z₃₀,x₃₁,y₃₁,z₃₁,x₃₂,y₃₂,z₃₂,x₃₃,y₃₃,z₃₃,x₃₄,y₃₄,z₃₄,x₃₅,y₃₅,z₃₅,x₃₆,y₃₆,z₃₆,x₃₇,y₃₇, z₃₇,x₃₈,y₃₈,z₃₈</pre>

- Following (Hudd, 1962), the Al-IV and Al-XIII sites are occupied 30% of the time, while the occupation of Al-VI, Al-IX, Al-XIV, and Al-XVII is 70%. This gives a nominal occupation of $\text{Al}_{91}\text{Co}_{30}$, though the authors state the actual composition is $\text{Al}_{68.3}\text{Co}_{24.4}$.
- Space group $Cm \#8$ allows an arbitrary choice for the origin of the z -axis. We follow (Hudd, 1962) and set $z_{26} = 0$.
- If we allow the rather large uncertainty of $0.3\text{\AA}$ in the atomic positions, FINDSYM sets the symmetry as $C2/m \#12$. That crystal has the $\text{Al}_{13}\text{Fe}_4$ prototype.
- Co_4 has also been observed in a orthorhombic structure.

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Al IV
$\mathbf{B}_5$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	Al V
$\mathbf{B}_6$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	Al VI
$\mathbf{B}_7$	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	Al VII
$\mathbf{B}_8$	$= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	Al VIII
$\mathbf{B}_9$	$= x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	Al IX
$\mathbf{B}_{10}$	$= x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	Al X
$\mathbf{B}_{11}$	$= x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XI
$\mathbf{B}_{12}$	$= x_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XII
$\mathbf{B}_{13}$	$= x_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XIII
$\mathbf{B}_{14}$	$= x_{14} \mathbf{a}_1 + x_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XIV
$\mathbf{B}_{15}$	$= x_{15} \mathbf{a}_1 + x_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XV
$\mathbf{B}_{16}$	$= x_{16} \mathbf{a}_1 + x_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XVI
$\mathbf{B}_{17}$	$= x_{17} \mathbf{a}_1 + x_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(2a)	Al XVII
$\mathbf{B}_{18}$	$= x_{18} \mathbf{a}_1 + x_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B}_{19}$	$= x_{19} \mathbf{a}_1 + x_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + cz_{19} \sin \beta \hat{\mathbf{z}}$	(2a)	Co II
$\mathbf{B}_{20}$	$= x_{20} \mathbf{a}_1 + x_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + cz_{20} \sin \beta \hat{\mathbf{z}}$	(2a)	Co III
$\mathbf{B}_{21}$	$= x_{21} \mathbf{a}_1 + x_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + cz_{21} \sin \beta \hat{\mathbf{z}}$	(2a)	Co IV
$\mathbf{B}_{22}$	$= x_{22} \mathbf{a}_1 + x_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + cz_{22} \sin \beta \hat{\mathbf{z}}$	(2a)	Co V
$\mathbf{B}_{23}$	$= x_{23} \mathbf{a}_1 + x_{23} \mathbf{a}_2 + z_{23} \mathbf{a}_3$	$=$	$(ax_{23} + cz_{23} \cos \beta) \hat{\mathbf{x}} + cz_{23} \sin \beta \hat{\mathbf{z}}$	(2a)	Co VI

$$\begin{aligned}
\mathbf{B}_{49} &= \begin{pmatrix} (x_{37} + y_{37}) \mathbf{a}_1 + \\ (x_{37} - y_{37}) \mathbf{a}_2 + z_{37} \mathbf{a}_3 \end{pmatrix} = (ax_{37} + cz_{37} \cos \beta) \hat{\mathbf{x}} - by_{37} \hat{\mathbf{y}} + cz_{37} \sin \beta \hat{\mathbf{z}} & (4b) & \text{Co IX} \\
\mathbf{B}_{50} &= \begin{pmatrix} (x_{38} - y_{38}) \mathbf{a}_1 + \\ (x_{38} + y_{38}) \mathbf{a}_2 + z_{38} \mathbf{a}_3 \end{pmatrix} = (ax_{38} + cz_{38} \cos \beta) \hat{\mathbf{x}} + by_{38} \hat{\mathbf{y}} + cz_{38} \sin \beta \hat{\mathbf{z}} & (4b) & \text{Co X} \\
\mathbf{B}_{51} &= \begin{pmatrix} (x_{38} + y_{38}) \mathbf{a}_1 + \\ (x_{38} - y_{38}) \mathbf{a}_2 + z_{38} \mathbf{a}_3 \end{pmatrix} = (ax_{38} + cz_{38} \cos \beta) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + cz_{38} \sin \beta \hat{\mathbf{z}} & (4b) & \text{Co X}
\end{aligned}$$

References

- [1] R. C. Hudd and W. H. Taylor, *The Structure of $\text{Co}_4\text{Al}_{13}$* , Acta Cryst. **15**, 441–442 (1962), doi:10.1107/S0365110X62001103.

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- [2] T. B. Massalski, H. Okamoto, P. R. Subramanian, and L. Kacprzak, eds., *Binary Alloy Phase Diagrams*, vol. 1 (ASM International, Materials Park, Ohio, USA, 1990), 2nd edn. Ac-Ag to Ca-Zn.

First cited in

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