

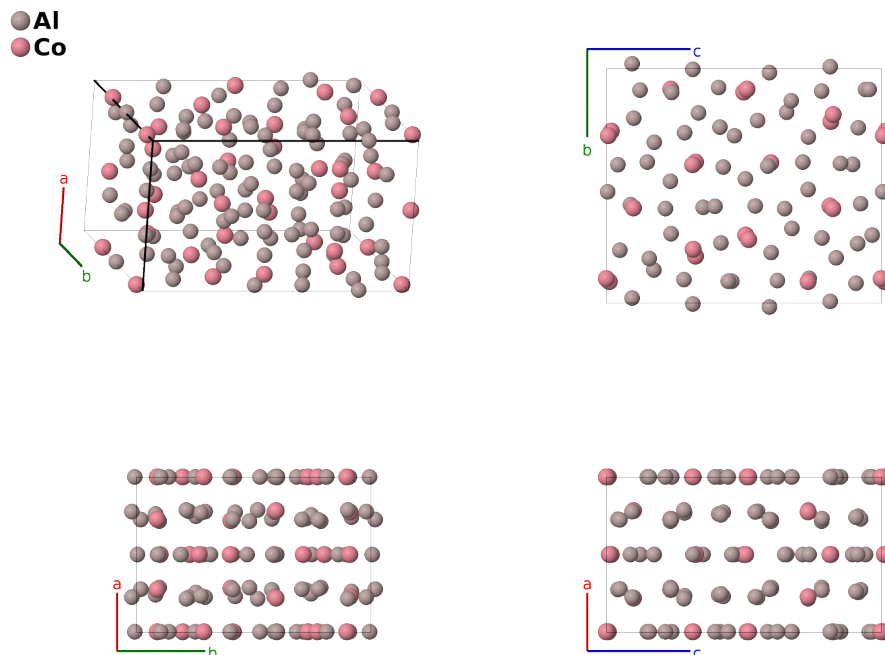
Orthorhombic $\text{Co}_4\text{Al}_{13}$ Structure (Approximate Quasicrystal): A13B4_oP102_31_17a11b_8a2b-001

This structure originally had the label A13B4_oP102_31_17a11b_8a2b. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://afLOW.org/p/DHFF>

https://afLOW.org/p/A13B4_oP102_31_17a11b_8a2b-001



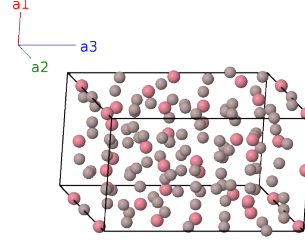
Prototype	$\text{Al}_{13}\text{Co}_4$
AFLOW prototype label	A13B4_oP102_31_17a11b_8a2b-001
ICSD	104638
Pearson symbol	oP102
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	<pre>afLOW --proto=A13B4_oP102_31_17a11b_8a2b-001 --params=a, b/a, c/a, y1, z1, y2, z2, y3, z3, y4, z4, y5, z5, y6, z6, y7, z7, y8, z8, y9, z9, y10, z10, y11, z11, y12, z12, y13, z13, y14, z14, y15, z15, y16, z16, y17, z17, y18, z18, y19, z19, y20, z20, y21, z21, y22, z22, y23, z23, y24, z24, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, 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>

- (Addou, 2009) consider this as an “approximate of the decagonal Al-Ni-Co quasicrystal.”

- Co_4 has also been observed in a monoclinic structure which has a large number of vacancies on the aluminum sites.
- Space group $Pmn2_1$ #31 allows an arbitrary choice for the origin of the z -axis. We follow (Grin, 1994) and set the $z_{25} = 0$.
- If we allow the rather large uncertainty of 0.6\AA in the atomic positions, FINDSYM sets the symmetry as $Pnmm$ #58.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	Al I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al I
\mathbf{B}_3	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	Al II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al II
\mathbf{B}_5	$= y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2a)	Al III
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al III
\mathbf{B}_7	$= y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2a)	Al IV
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al IV
\mathbf{B}_9	$= y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2a)	Al V
\mathbf{B}_{10}	$= \frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al V
\mathbf{B}_{11}	$= y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2a)	Al VI
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al VI
\mathbf{B}_{13}	$= y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(2a)	Al VII
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al VII
\mathbf{B}_{15}	$= y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(2a)	Al VIII
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al VIII
\mathbf{B}_{17}	$= y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(2a)	Al IX
\mathbf{B}_{18}	$= \frac{1}{2} \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al IX
\mathbf{B}_{19}	$= y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(2a)	Al X
\mathbf{B}_{20}	$= \frac{1}{2} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al X
\mathbf{B}_{21}	$= y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(2a)	Al XI
\mathbf{B}_{22}	$= \frac{1}{2} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al XI
\mathbf{B}_{23}	$= y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(2a)	Al XII
\mathbf{B}_{24}	$= \frac{1}{2} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al XII
\mathbf{B}_{25}	$= y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(2a)	Al XIII

$\mathbf{B}_{91} =$	$x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3$	$=$	$ax_{36} \hat{\mathbf{x}} + by_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}}$	(4b)	Al XXVIII
$\mathbf{B}_{92} =$	$-(x_{36} - \frac{1}{2}) \mathbf{a}_1 - y_{36} \mathbf{a}_2 +$ $(z_{36} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{36} - \frac{1}{2}) \hat{\mathbf{x}} - by_{36} \hat{\mathbf{y}} + c(z_{36} + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Al XXVIII
$\mathbf{B}_{93} =$	$(x_{36} + \frac{1}{2}) \mathbf{a}_1 - y_{36} \mathbf{a}_2 +$ $(z_{36} + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{36} + \frac{1}{2}) \hat{\mathbf{x}} - by_{36} \hat{\mathbf{y}} + c(z_{36} + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Al XXVIII
$\mathbf{B}_{94} =$	$-x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3$	$=$	$-ax_{36} \hat{\mathbf{x}} + by_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}}$	(4b)	Al XXVIII
$\mathbf{B}_{95} =$	$x_{37} \mathbf{a}_1 + y_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3$	$=$	$ax_{37} \hat{\mathbf{x}} + by_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}}$	(4b)	Co IX
$\mathbf{B}_{96} =$	$-(x_{37} - \frac{1}{2}) \mathbf{a}_1 - y_{37} \mathbf{a}_2 +$ $(z_{37} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{37} - \frac{1}{2}) \hat{\mathbf{x}} - by_{37} \hat{\mathbf{y}} + c(z_{37} + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Co IX
$\mathbf{B}_{97} =$	$(x_{37} + \frac{1}{2}) \mathbf{a}_1 - y_{37} \mathbf{a}_2 +$ $(z_{37} + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{37} + \frac{1}{2}) \hat{\mathbf{x}} - by_{37} \hat{\mathbf{y}} + c(z_{37} + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Co IX
$\mathbf{B}_{98} =$	$-x_{37} \mathbf{a}_1 + y_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3$	$=$	$-ax_{37} \hat{\mathbf{x}} + by_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}}$	(4b)	Co IX
$\mathbf{B}_{99} =$	$x_{38} \mathbf{a}_1 + y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3$	$=$	$ax_{38} \hat{\mathbf{x}} + by_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}}$	(4b)	Co X
$\mathbf{B}_{100} =$	$-(x_{38} - \frac{1}{2}) \mathbf{a}_1 - y_{38} \mathbf{a}_2 +$ $(z_{38} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{38} - \frac{1}{2}) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + c(z_{38} + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Co X
$\mathbf{B}_{101} =$	$(x_{38} + \frac{1}{2}) \mathbf{a}_1 - y_{38} \mathbf{a}_2 +$ $(z_{38} + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{38} + \frac{1}{2}) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + c(z_{38} + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Co X
$\mathbf{B}_{102} =$	$-x_{38} \mathbf{a}_1 + y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3$	$=$	$-ax_{38} \hat{\mathbf{x}} + by_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}}$	(4b)	Co X

References

- [1] J. Grin, U. Burkhard, M. Ellner, and K. Peters, *Crystal structure of orthorhombic Co_4Al_{13}* , J. Alloys Compd. **206**, 243–247 (1994), doi:10.1016/0925-8388(94)90043-4.

Found in

- [1] R. Addou, E. Gaudry, T. Deniozou, M. Heggen, M. Feuerbacher, P. Gille, Y. Grin, R. Widmer, O. Gröning, V. Fournée, J.-M. Dubois, , and J. Ledieu, *Structure investigation of the (100) surface of the orthorhombic $Al_{13}Co_4$ crystal*, Phys. Rev. B **80**, 014203 (2009), doi:10.1103/PhysRevB.80.014203.