

# Orthorhombic Co<sub>4</sub>Al<sub>13</sub> Structure (Approximate Quasicrystal): A13B4\_oP102\_31\_17a11b\_8a2b-001

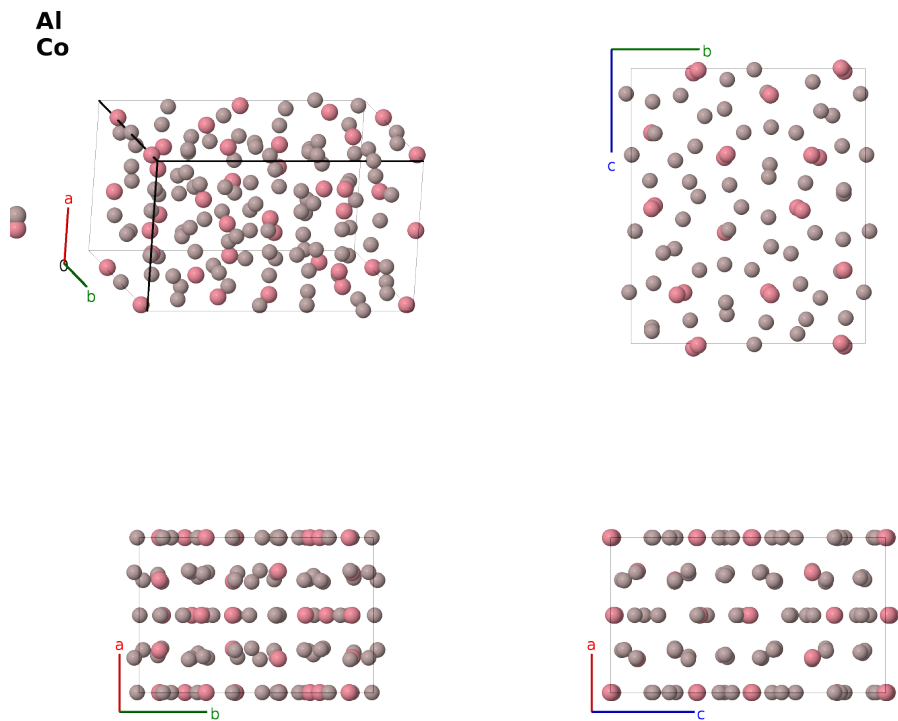
This structure previously used the label(s) **A13B4\_oP102\_31\_17a11b\_8a2b**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/DHFF>

[https://aflow.org/prototype-encyclopedia/A13B4\\_oP102\\_31\\_17a11b\\_8a2b-001](https://aflow.org/prototype-encyclopedia/A13B4_oP102_31_17a11b_8a2b-001)



|                       |                                  |
|-----------------------|----------------------------------|
| Prototype             | Al <sub>13</sub> Co <sub>4</sub> |
| AFLOW prototype label | A13B4_oP102_31_17a11b_8a2b-001   |
| ICSD                  | 104638                           |
| CCDC                  | 1662548                          |
| Pearson symbol        | oP102                            |
| Space group number    | 31                               |
| Space group symbol    | <i>Pmn</i> 2 <sub>1</sub>        |

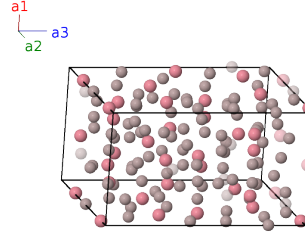
**AFLOW prototype command**      `aflow --proto=A13B4_oP102_31_17a11b_8a2b-001`  
                                          `--params=a, b/a, c/a, y1, z1, y2, z2, y3, z3, y4, z4, y5, z5, y6, z6, y7, z7, y8, z8, y9, z9, y10, z10,`  
                                          `y11, z11, y12, z12, y13, z13, 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`

---

- (Addou, 2009) consider this as an “approximate of the decagonal Al-Ni-Co quasicrystal.”
  - Co<sub>4</sub> 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 0.6Å in the atomic positions, FINDSYM sets the symmetry as  $Pnnm$  #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<br>coordinates                                                             |     | Cartesian<br>coordinates                                                                         | Wyckoff<br>position | Atom<br>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  |
| $\mathbf{B}_{26} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Al XIII  |
| $\mathbf{B}_{27} =$ | $y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$                                                        | $=$ | $by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$                                                             | (2a) | Al XIV   |
| $\mathbf{B}_{28} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Al XIV   |
| $\mathbf{B}_{29} =$ | $y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$                                                        | $=$ | $by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}}$                                                             | (2a) | Al XV    |
| $\mathbf{B}_{30} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{15} \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Al XV    |
| $\mathbf{B}_{31} =$ | $y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$                                                        | $=$ | $by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$                                                             | (2a) | Al XVI   |
| $\mathbf{B}_{32} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{16} \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Al XVI   |
| $\mathbf{B}_{33} =$ | $y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$                                                        | $=$ | $by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$                                                             | (2a) | Al XVII  |
| $\mathbf{B}_{34} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Al XVII  |
| $\mathbf{B}_{35} =$ | $y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$                                                        | $=$ | $by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$                                                             | (2a) | Co I     |
| $\mathbf{B}_{36} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co I     |
| $\mathbf{B}_{37} =$ | $y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$                                                        | $=$ | $by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}}$                                                             | (2a) | Co II    |
| $\mathbf{B}_{38} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + (z_{19} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co II    |
| $\mathbf{B}_{39} =$ | $y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$                                                        | $=$ | $by_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}}$                                                             | (2a) | Co III   |
| $\mathbf{B}_{40} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + (z_{20} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c(z_{20} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co III   |
| $\mathbf{B}_{41} =$ | $y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3$                                                        | $=$ | $by_{21} \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}}$                                                             | (2a) | Co IV    |
| $\mathbf{B}_{42} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{21} \mathbf{a}_2 + (z_{21} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} + c(z_{21} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co IV    |
| $\mathbf{B}_{43} =$ | $y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3$                                                        | $=$ | $by_{22} \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}}$                                                             | (2a) | Co V     |
| $\mathbf{B}_{44} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + (z_{22} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{22} \hat{\mathbf{y}} + c(z_{22} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co V     |
| $\mathbf{B}_{45} =$ | $y_{23} \mathbf{a}_2 + z_{23} \mathbf{a}_3$                                                        | $=$ | $by_{23} \hat{\mathbf{y}} + cz_{23} \hat{\mathbf{z}}$                                                             | (2a) | Co VI    |
| $\mathbf{B}_{46} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{23} \mathbf{a}_2 + (z_{23} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{23} \hat{\mathbf{y}} + c(z_{23} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co VI    |
| $\mathbf{B}_{47} =$ | $y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3$                                                        | $=$ | $by_{24} \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}}$                                                             | (2a) | Co VII   |
| $\mathbf{B}_{48} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{24} \mathbf{a}_2 + (z_{24} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} + c(z_{24} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co VII   |
| $\mathbf{B}_{49} =$ | $y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3$                                                        | $=$ | $by_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}}$                                                             | (2a) | Co VIII  |
| $\mathbf{B}_{50} =$ | $\frac{1}{2} \mathbf{a}_1 - y_{25} \mathbf{a}_2 + (z_{25} + \frac{1}{2}) \mathbf{a}_3$             | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} + c(z_{25} + \frac{1}{2}) \hat{\mathbf{z}}$            | (2a) | Co VIII  |
| $\mathbf{B}_{51} =$ | $x_{26} \mathbf{a}_1 + y_{26} \mathbf{a}_2 + z_{26} \mathbf{a}_3$                                  | $=$ | $ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \hat{\mathbf{z}}$                                  | (4b) | Al XVIII |
| $\mathbf{B}_{52} =$ | $-(x_{26} - \frac{1}{2}) \mathbf{a}_1 - y_{26} \mathbf{a}_2 + (z_{26} + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_{26} - \frac{1}{2}) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + c(z_{26} + \frac{1}{2}) \hat{\mathbf{z}}$ | (4b) | Al XVIII |
| $\mathbf{B}_{53} =$ | $(x_{26} + \frac{1}{2}) \mathbf{a}_1 - y_{26} \mathbf{a}_2 + (z_{26} + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_{26} + \frac{1}{2}) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + c(z_{26} + \frac{1}{2}) \hat{\mathbf{z}}$  | (4b) | Al XVIII |
| $\mathbf{B}_{54} =$ | $-x_{26} \mathbf{a}_1 + y_{26} \mathbf{a}_2 + z_{26} \mathbf{a}_3$                                 | $=$ | $-ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \hat{\mathbf{z}}$                                 | (4b) | Al XVIII |
| $\mathbf{B}_{55} =$ | $x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3$                                  | $=$ | $ax_{27} \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \hat{\mathbf{z}}$                                  | (4b) | Al XIX   |



|                    |     |                                                                                                                                              |     |                                                                                                                                               |      |           |
|--------------------|-----|----------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| $\mathbf{B}_{85}$  | $=$ | $\begin{pmatrix} x_{34} + \frac{1}{2} \\ z_{34} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{34} \mathbf{a}_2 + \mathbf{a}_3$               | $=$ | $a \left( x_{34} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{34} \hat{\mathbf{y}} + c \left( z_{34} + \frac{1}{2} \right) \hat{\mathbf{z}}$  | (4b) | Al XXVI   |
| $\mathbf{B}_{86}$  | $=$ | $-x_{34} \mathbf{a}_1 + y_{34} \mathbf{a}_2 + z_{34} \mathbf{a}_3$                                                                           | $=$ | $-ax_{34} \hat{\mathbf{x}} + by_{34} \hat{\mathbf{y}} + cz_{34} \hat{\mathbf{z}}$                                                             | (4b) | Al XXVI   |
| $\mathbf{B}_{87}$  | $=$ | $x_{35} \mathbf{a}_1 + y_{35} \mathbf{a}_2 + z_{35} \mathbf{a}_3$                                                                            | $=$ | $ax_{35} \hat{\mathbf{x}} + by_{35} \hat{\mathbf{y}} + cz_{35} \hat{\mathbf{z}}$                                                              | (4b) | Al XXVII  |
| $\mathbf{B}_{88}$  | $=$ | $-\left(x_{35} - \frac{1}{2}\right) \mathbf{a}_1 - y_{35} \mathbf{a}_2 + \begin{pmatrix} z_{35} + \frac{1}{2} \\ \end{pmatrix} \mathbf{a}_3$ | $=$ | $-a \left( x_{35} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{35} \hat{\mathbf{y}} + c \left( z_{35} + \frac{1}{2} \right) \hat{\mathbf{z}}$ | (4b) | Al XXVII  |
| $\mathbf{B}_{89}$  | $=$ | $\begin{pmatrix} x_{35} + \frac{1}{2} \\ z_{35} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{35} \mathbf{a}_2 + \mathbf{a}_3$               | $=$ | $a \left( x_{35} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{35} \hat{\mathbf{y}} + c \left( z_{35} + \frac{1}{2} \right) \hat{\mathbf{z}}$  | (4b) | Al XXVII  |
| $\mathbf{B}_{90}$  | $=$ | $-x_{35} \mathbf{a}_1 + y_{35} \mathbf{a}_2 + z_{35} \mathbf{a}_3$                                                                           | $=$ | $-ax_{35} \hat{\mathbf{x}} + by_{35} \hat{\mathbf{y}} + cz_{35} \hat{\mathbf{z}}$                                                             | (4b) | Al XXVII  |
| $\mathbf{B}_{91}$  | $=$ | $x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3$                                                                            | $=$ | $ax_{36} \hat{\mathbf{x}} + by_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}}$                                                              | (4b) | Al XXVIII |
| $\mathbf{B}_{92}$  | $=$ | $-\left(x_{36} - \frac{1}{2}\right) \mathbf{a}_1 - y_{36} \mathbf{a}_2 + \begin{pmatrix} z_{36} + \frac{1}{2} \\ \end{pmatrix} \mathbf{a}_3$ | $=$ | $-a \left( x_{36} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{36} \hat{\mathbf{y}} + c \left( z_{36} + \frac{1}{2} \right) \hat{\mathbf{z}}$ | (4b) | Al XXVIII |
| $\mathbf{B}_{93}$  | $=$ | $\begin{pmatrix} x_{36} + \frac{1}{2} \\ z_{36} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{36} \mathbf{a}_2 + \mathbf{a}_3$               | $=$ | $a \left( x_{36} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{36} \hat{\mathbf{y}} + c \left( z_{36} + \frac{1}{2} \right) \hat{\mathbf{z}}$  | (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     |
| $\mathbf{B}_{96}$  | $=$ | $-\left(x_{37} - \frac{1}{2}\right) \mathbf{a}_1 - y_{37} \mathbf{a}_2 + \begin{pmatrix} z_{37} + \frac{1}{2} \\ \end{pmatrix} \mathbf{a}_3$ | $=$ | $-a \left( x_{37} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{37} \hat{\mathbf{y}} + c \left( z_{37} + \frac{1}{2} \right) \hat{\mathbf{z}}$ | (4b) | Co IX     |
| $\mathbf{B}_{97}$  | $=$ | $\begin{pmatrix} x_{37} + \frac{1}{2} \\ z_{37} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{37} \mathbf{a}_2 + \mathbf{a}_3$               | $=$ | $a \left( x_{37} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{37} \hat{\mathbf{y}} + c \left( z_{37} + \frac{1}{2} \right) \hat{\mathbf{z}}$  | (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      |
| $\mathbf{B}_{100}$ | $=$ | $-\left(x_{38} - \frac{1}{2}\right) \mathbf{a}_1 - y_{38} \mathbf{a}_2 + \begin{pmatrix} z_{38} + \frac{1}{2} \\ \end{pmatrix} \mathbf{a}_3$ | $=$ | $-a \left( x_{38} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + c \left( z_{38} + \frac{1}{2} \right) \hat{\mathbf{z}}$ | (4b) | Co X      |
| $\mathbf{B}_{101}$ | $=$ | $\begin{pmatrix} x_{38} + \frac{1}{2} \\ z_{38} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{38} \mathbf{a}_2 + \mathbf{a}_3$               | $=$ | $a \left( x_{38} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + c \left( z_{38} + \frac{1}{2} \right) \hat{\mathbf{z}}$  | (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  $\text{Co}_4\text{Al}_{13}$* , 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  $\text{Al}_{13}\text{Co}_4$  crystal*, Phys. Rev. B **80**, 014203 (2009), doi:10.1103/PhysRevB.80.014203.

## First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.