

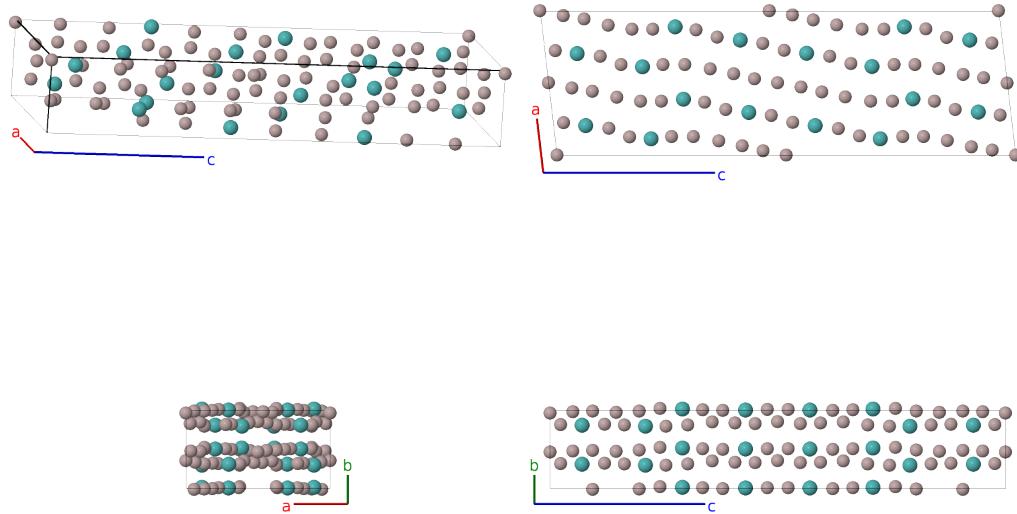
# Al<sub>17</sub>Mo<sub>4</sub> Structure: A17B4\_mC84\_5\_ab16c\_4c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/QL9A>

[https://aflow.org/p/A17B4\\_mC84\\_5\\_ab16c\\_4c-001](https://aflow.org/p/A17B4_mC84_5_ab16c_4c-001)

● Al  
● Mo

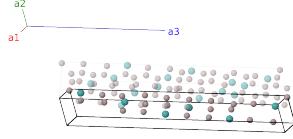


Prototype	Al <sub>17</sub> Mo <sub>4</sub>
AFLOW prototype label	A17B4_mC84_5_ab16c_4c-001
ICSD	400887
Pearson symbol	mC84
Space group number	5
Space group symbol	<i>C</i> 2
AFLOW prototype command	<pre>aflow --proto=A17B4_mC84_5_ab16c_4c-001 --params=a,b/a,c/a,\beta,y1,y2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8, z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16, y16,z16,x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22,z22</pre>

- Space group *C*2 #5 allows an arbitrary choice of the origin of the *y*-axis. Here we follow (Grin, 1995) and set  $y_{19} = 0$  for the Mo-I atom.

## 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
$\mathbf{B}_1$	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$b y_1 \hat{\mathbf{y}}$	(2a)	Al I
$\mathbf{B}_2$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B}_3$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Al III
$\mathbf{B}_4$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Al III
$\mathbf{B}_5$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	Al IV
$\mathbf{B}_6$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	Al IV
$\mathbf{B}_7$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	Al V
$\mathbf{B}_8$	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	Al V
$\mathbf{B}_9$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	Al VI
$\mathbf{B}_{10}$	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	Al VI
$\mathbf{B}_{11}$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	Al VII
$\mathbf{B}_{12}$	$-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	Al VII
$\mathbf{B}_{13}$	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	Al VIII
$\mathbf{B}_{14}$	$-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	Al VIII
$\mathbf{B}_{15}$	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	Al IX
$\mathbf{B}_{16}$	$-(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	Al IX
$\mathbf{B}_{17}$	$(x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	Al X
$\mathbf{B}_{18}$	$-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	Al X
$\mathbf{B}_{19}$	$(x_{11} - y_{11}) \mathbf{a}_1 + (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XI

$\mathbf{B}_{20}$	$=$	$-(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XI
$\mathbf{B}_{21}$	$=$	$(x_{12} - y_{12}) \mathbf{a}_1 + (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XII
$\mathbf{B}_{22}$	$=$	$-(x_{12} + y_{12}) \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XII
$\mathbf{B}_{23}$	$=$	$(x_{13} - y_{13}) \mathbf{a}_1 + (x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XIII
$\mathbf{B}_{24}$	$=$	$-(x_{13} + y_{13}) \mathbf{a}_1 - (x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XIII
$\mathbf{B}_{25}$	$=$	$(x_{14} - y_{14}) \mathbf{a}_1 + (x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XIV
$\mathbf{B}_{26}$	$=$	$-(x_{14} + y_{14}) \mathbf{a}_1 - (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - cz_{14} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XIV
$\mathbf{B}_{27}$	$=$	$(x_{15} - y_{15}) \mathbf{a}_1 + (x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XV
$\mathbf{B}_{28}$	$=$	$-(x_{15} + y_{15}) \mathbf{a}_1 - (x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - cz_{15} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XV
$\mathbf{B}_{29}$	$=$	$(x_{16} - y_{16}) \mathbf{a}_1 + (x_{16} + y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XVI
$\mathbf{B}_{30}$	$=$	$-(x_{16} + y_{16}) \mathbf{a}_1 - (x_{16} - y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - cz_{16} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XVI
$\mathbf{B}_{31}$	$=$	$(x_{17} - y_{17}) \mathbf{a}_1 + (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XVII
$\mathbf{B}_{32}$	$=$	$-(x_{17} + y_{17}) \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XVII
$\mathbf{B}_{33}$	$=$	$(x_{18} - y_{18}) \mathbf{a}_1 + (x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XVIII
$\mathbf{B}_{34}$	$=$	$-(x_{18} + y_{18}) \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}}$	(4c)	Al XVIII
$\mathbf{B}_{35}$	$=$	$(x_{19} - y_{19}) \mathbf{a}_1 + (x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_{36}$	$=$	$-(x_{19} + y_{19}) \mathbf{a}_1 - (x_{19} - y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - cz_{19} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_{37}$	$=$	$(x_{20} - y_{20}) \mathbf{a}_1 + (x_{20} + y_{20}) \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo II
$\mathbf{B}_{38}$	$=$	$-(x_{20} + y_{20}) \mathbf{a}_1 - (x_{20} - y_{20}) \mathbf{a}_2 - z_{20} \mathbf{a}_3$	$=$	$-(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - cz_{20} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo II
$\mathbf{B}_{39}$	$=$	$(x_{21} - y_{21}) \mathbf{a}_1 + (x_{21} + y_{21}) \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo III
$\mathbf{B}_{40}$	$=$	$-(x_{21} + y_{21}) \mathbf{a}_1 - (x_{21} - y_{21}) \mathbf{a}_2 - z_{21} \mathbf{a}_3$	$=$	$-(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} - cz_{21} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo III
$\mathbf{B}_{41}$	$=$	$(x_{22} - y_{22}) \mathbf{a}_1 + (x_{22} + y_{22}) \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo IV
$\mathbf{B}_{42}$	$=$	$-(x_{22} + y_{22}) \mathbf{a}_1 - (x_{22} - y_{22}) \mathbf{a}_2 - z_{22} \mathbf{a}_3$	$=$	$-(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} - cz_{22} \sin \beta \hat{\mathbf{z}}$	(4c)	Mo IV

## References

- [1] Y. N. Grin, M. Ellner, K. Peters, and J. C. Schuster, *The crystal structures of Mo<sub>4</sub>Al<sub>17</sub> and Mo<sub>5</sub>Al<sub>22</sub>*, Z. Kristallogr. **210**, 96–99 (1995), doi:10.1524/zkri.1995.210.2.96.