

Trigonal (h') Al₅Mo Structure: A5B_hP60_143_7a7b6c10d_3a3b4c-001

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/TWK7>

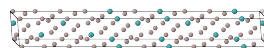
https://afLOW.org/prototype-encyclopedia/A5B_hP60_143_7a7b6c10d_3a3b4c-001

Prototype	Al ₅ Mo
AFLOW prototype label	A5B_hP60_143_7a7b6c10d_3a3b4c-001
ICSD	105519
CCDC	1663403
Pearson symbol	hP60
Space group number	143
Space group symbol	<i>P</i> 3
AFLOW prototype command	<code>afLOW --proto=A5B_hP60_143_7a7b6c10d_3a3b4c-001</code> <code>--params=a, c/a, z₁, z₂, z₃, z₄, z₅, z₆, z₇, z₈, z₉, z₁₀, z₁₁, z₁₂, z₁₃, z₁₄, z₁₅, z₁₆, z₁₇, z₁₈, z₁₉, z₂₀, z₂₁, z₂₂, z₂₃, z₂₄, z₂₅, z₂₆, z₂₇, z₂₈, z₂₉, 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, x₃₉, y₃₉, z₃₉, x₄₀, y₄₀, z₄₀</code>

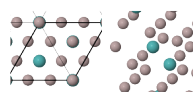
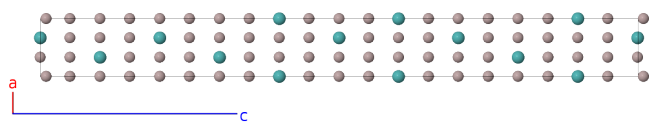
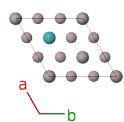
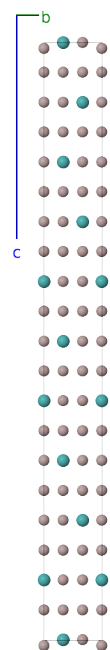
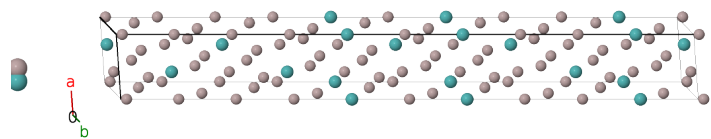
- Al₅Mo is known to have three phases (Schuster, 1991):
 - Below 650K it is in a rhombohedral structure, Al₅Mo (r).
 - Between 650K and 750-800K it is in a trigonal structure, Al₅Mo(h') (this structure).
 - Above 750-800K up to 846K it is in the Al₅W structure.
- The Al₅Mo(h') atomic positions in (Schuster, 1991) are highly symmetric and approximate, and put the system in space group *P*321 #150. To show the correct *P*3 space group we slightly shifted the Al-I atom's *z*-coordinate. Presumably further refinement of the coordinates would let us determine the correct space group.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Al
Mo



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(1a)	Al I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(1a)	Al II
$\mathbf{B}_3$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(1a)	Al III
$\mathbf{B}_4$	$= z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(1a)	Al IV
$\mathbf{B}_5$	$= z_5 \mathbf{a}_3$	$=$	$cz_5 \hat{\mathbf{z}}$	(1a)	Al V
$\mathbf{B}_6$	$= z_6 \mathbf{a}_3$	$=$	$cz_6 \hat{\mathbf{z}}$	(1a)	Al VI
$\mathbf{B}_7$	$= z_7 \mathbf{a}_3$	$=$	$cz_7 \hat{\mathbf{z}}$	(1a)	Al VII
$\mathbf{B}_8$	$= z_8 \mathbf{a}_3$	$=$	$cz_8 \hat{\mathbf{z}}$	(1a)	Mo I
$\mathbf{B}_9$	$= z_9 \mathbf{a}_3$	$=$	$cz_9 \hat{\mathbf{z}}$	(1a)	Mo II
$\mathbf{B}_{10}$	$= z_{10} \mathbf{a}_3$	$=$	$cz_{10} \hat{\mathbf{z}}$	(1a)	Mo III
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(1b)	Al VIII
$\mathbf{B}_{12}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(1b)	Al IX
$\mathbf{B}_{13}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(1b)	Al X
$\mathbf{B}_{14}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$	(1b)	Al XI
$\mathbf{B}_{15}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}}$	(1b)	Al XII
$\mathbf{B}_{16}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$	(1b)	Al XIII
$\mathbf{B}_{17}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	(1b)	Al XIV
$\mathbf{B}_{18}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	(1b)	Mo IV
$\mathbf{B}_{19}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}}$	(1b)	Mo V
$\mathbf{B}_{20}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}}$	(1b)	Mo VI
$\mathbf{B}_{21}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}}$	(1c)	Al XV
$\mathbf{B}_{22}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}}$	(1c)	Al XVI
$\mathbf{B}_{23}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{23} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{23} \hat{\mathbf{z}}$	(1c)	Al XVII
$\mathbf{B}_{24}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{24} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}}$	(1c)	Al XVIII
$\mathbf{B}_{25}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{25} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}}$	(1c)	Al XIX
$\mathbf{B}_{26}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{26} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{26} \hat{\mathbf{z}}$	(1c)	Al XX
$\mathbf{B}_{27}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{27} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{27} \hat{\mathbf{z}}$	(1c)	Mo VII
$\mathbf{B}_{28}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{28} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{28} \hat{\mathbf{z}}$	(1c)	Mo VIII
$\mathbf{B}_{29}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{29} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{29} \hat{\mathbf{z}}$	(1c)	Mo IX
$\mathbf{B}_{30}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_{30} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{30} \hat{\mathbf{z}}$	(1c)	Mo X
$\mathbf{B}_{31}$	$= x_{31} \mathbf{a}_1 + y_{31} \mathbf{a}_2 + z_{31} \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_{31} + y_{31}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a (x_{31} - y_{31}) \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}}$	(3d)	Al XXI
$\mathbf{B}_{32}$	$= -y_{31} \mathbf{a}_1 + (x_{31} - y_{31}) \mathbf{a}_2 + z_{31} \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_{31} - 2y_{31}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a x_{31} \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}}$	(3d)	Al XXI
$\mathbf{B}_{33}$	$= -(x_{31} - y_{31}) \mathbf{a}_1 - x_{31} \mathbf{a}_2 + z_{31} \mathbf{a}_3$	$=$	$-\frac{1}{2} a (2x_{31} - y_{31}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a y_{31} \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}}$	(3d)	Al XXI
$\mathbf{B}_{34}$	$= x_{32} \mathbf{a}_1 + y_{32} \mathbf{a}_2 + z_{32} \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_{32} + y_{32}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a (x_{32} - y_{32}) \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}}$	(3d)	Al XXII
$\mathbf{B}_{35}$	$= -y_{32} \mathbf{a}_1 + (x_{32} - y_{32}) \mathbf{a}_2 + z_{32} \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_{32} - 2y_{32}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} a x_{32} \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}}$	(3d)	Al XXII
$\mathbf{B}_{36}$	$= -(x_{32} - y_{32}) \mathbf{a}_1 - x_{32} \mathbf{a}_2 + z_{32} \mathbf{a}_3$	$=$	$-\frac{1}{2} a (2x_{32} - y_{32}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} a y_{32} \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}}$	(3d)	Al XXII

$\mathbf{B}_{37}$	$=$	$x_{33} \mathbf{a}_1 + y_{33} \mathbf{a}_2 + z_{33} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{33} + y_{33}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{33} - y_{33}) \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}}$	(3d)	Al XXIII
$\mathbf{B}_{38}$	$=$	$-y_{33} \mathbf{a}_1 + (x_{33} - y_{33}) \mathbf{a}_2 + z_{33} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{33} - 2y_{33}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{33} \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}}$	(3d)	Al XXIII
$\mathbf{B}_{39}$	$=$	$-(x_{33} - y_{33}) \mathbf{a}_1 - x_{33} \mathbf{a}_2 + z_{33} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{33} - y_{33}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{33} \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}}$	(3d)	Al XXIII
$\mathbf{B}_{40}$	$=$	$x_{34} \mathbf{a}_1 + y_{34} \mathbf{a}_2 + z_{34} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{34} + y_{34}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{34} - y_{34}) \hat{\mathbf{y}} + cz_{34} \hat{\mathbf{z}}$	(3d)	Al XXIV
$\mathbf{B}_{41}$	$=$	$-y_{34} \mathbf{a}_1 + (x_{34} - y_{34}) \mathbf{a}_2 + z_{34} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{34} - 2y_{34}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{34} \hat{\mathbf{y}} + cz_{34} \hat{\mathbf{z}}$	(3d)	Al XXIV
$\mathbf{B}_{42}$	$=$	$-(x_{34} - y_{34}) \mathbf{a}_1 - x_{34} \mathbf{a}_2 + z_{34} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{34} - y_{34}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{34} \hat{\mathbf{y}} + cz_{34} \hat{\mathbf{z}}$	(3d)	Al XXIV
$\mathbf{B}_{43}$	$=$	$x_{35} \mathbf{a}_1 + y_{35} \mathbf{a}_2 + z_{35} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{35} + y_{35}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{35} - y_{35}) \hat{\mathbf{y}} + cz_{35} \hat{\mathbf{z}}$	(3d)	Al XXV
$\mathbf{B}_{44}$	$=$	$-y_{35} \mathbf{a}_1 + (x_{35} - y_{35}) \mathbf{a}_2 + z_{35} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{35} - 2y_{35}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{35} \hat{\mathbf{y}} + cz_{35} \hat{\mathbf{z}}$	(3d)	Al XXV
$\mathbf{B}_{45}$	$=$	$-(x_{35} - y_{35}) \mathbf{a}_1 - x_{35} \mathbf{a}_2 + z_{35} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{35} - y_{35}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{35} \hat{\mathbf{y}} + cz_{35} \hat{\mathbf{z}}$	(3d)	Al XXV
$\mathbf{B}_{46}$	$=$	$x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{36} + y_{36}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{36} - y_{36}) \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}}$	(3d)	Al XXVI
$\mathbf{B}_{47}$	$=$	$-y_{36} \mathbf{a}_1 + (x_{36} - y_{36}) \mathbf{a}_2 + z_{36} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{36} - 2y_{36}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}}$	(3d)	Al XXVI
$\mathbf{B}_{48}$	$=$	$-(x_{36} - y_{36}) \mathbf{a}_1 - x_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{36} - y_{36}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}}$	(3d)	Al XXVI
$\mathbf{B}_{49}$	$=$	$x_{37} \mathbf{a}_1 + y_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{37} + y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{37} - y_{37}) \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}}$	(3d)	Al XXVII
$\mathbf{B}_{50}$	$=$	$-y_{37} \mathbf{a}_1 + (x_{37} - y_{37}) \mathbf{a}_2 + z_{37} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{37} - 2y_{37}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}}$	(3d)	Al XXVII
$\mathbf{B}_{51}$	$=$	$-(x_{37} - y_{37}) \mathbf{a}_1 - x_{37} \mathbf{a}_2 + z_{37} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{37} - y_{37}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{37} \hat{\mathbf{y}} + cz_{37} \hat{\mathbf{z}}$	(3d)	Al XXVII
$\mathbf{B}_{52}$	$=$	$x_{38} \mathbf{a}_1 + y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{38} + y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{38} - y_{38}) \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}}$	(3d)	Al XXVIII
$\mathbf{B}_{53}$	$=$	$-y_{38} \mathbf{a}_1 + (x_{38} - y_{38}) \mathbf{a}_2 + z_{38} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{38} - 2y_{38}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}}$	(3d)	Al XXVIII
$\mathbf{B}_{54}$	$=$	$-(x_{38} - y_{38}) \mathbf{a}_1 - x_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{38} - y_{38}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}}$	(3d)	Al XXVIII
$\mathbf{B}_{55}$	$=$	$x_{39} \mathbf{a}_1 + y_{39} \mathbf{a}_2 + z_{39} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{39} + y_{39}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{39} - y_{39}) \hat{\mathbf{y}} + cz_{39} \hat{\mathbf{z}}$	(3d)	Al XXIX
$\mathbf{B}_{56}$	$=$	$-y_{39} \mathbf{a}_1 + (x_{39} - y_{39}) \mathbf{a}_2 + z_{39} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{39} - 2y_{39}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{39} \hat{\mathbf{y}} + cz_{39} \hat{\mathbf{z}}$	(3d)	Al XXIX
$\mathbf{B}_{57}$	$=$	$-(x_{39} - y_{39}) \mathbf{a}_1 - x_{39} \mathbf{a}_2 + z_{39} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{39} - y_{39}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{39} \hat{\mathbf{y}} + cz_{39} \hat{\mathbf{z}}$	(3d)	Al XXIX
$\mathbf{B}_{58}$	$=$	$x_{40} \mathbf{a}_1 + y_{40} \mathbf{a}_2 + z_{40} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{40} + y_{40}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{40} - y_{40}) \hat{\mathbf{y}} + cz_{40} \hat{\mathbf{z}}$	(3d)	Al XXX
$\mathbf{B}_{59}$	$=$	$-y_{40} \mathbf{a}_1 + (x_{40} - y_{40}) \mathbf{a}_2 + z_{40} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{40} - 2y_{40}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{40} \hat{\mathbf{y}} + cz_{40} \hat{\mathbf{z}}$	(3d)	Al XXX
$\mathbf{B}_{60}$	$=$	$-(x_{40} - y_{40}) \mathbf{a}_1 - x_{40} \mathbf{a}_2 + z_{40} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{40} - y_{40}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{40} \hat{\mathbf{y}} + cz_{40} \hat{\mathbf{z}}$	(3d)	Al XXX

References

- [1] J. C. Schuster and H. Ipser, *The Al-Al₈Mo₃ section of the binary system aluminum-molybdenum*, Metall. Trans. A **22**, 1729–1736 (1991), doi:10.1007/BF02646496.

First cited in

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.