Trigonal (h') Al_5Mo Structure: A5B_hP60_143_7a7b6c10d_3a3b4c-001

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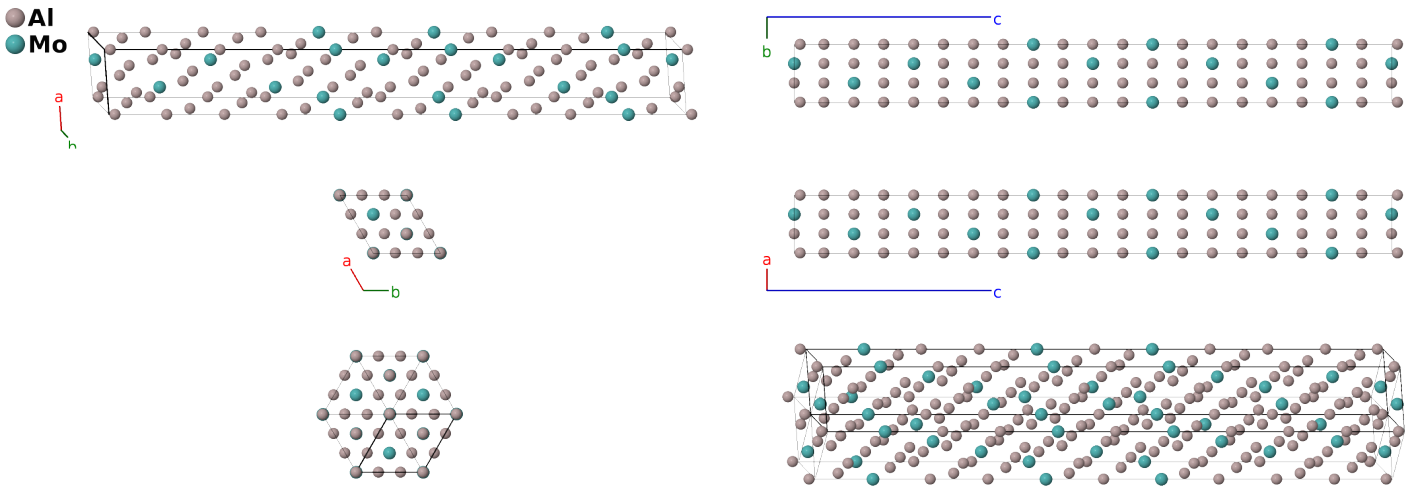
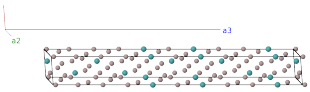


Prototype	Al_5Mo
AFLOW prototype label	A5B_hP60_143_7a7b6c10d_3a3b4c-001
ICSD	105519
Pearson symbol	hP60
Space group number	143
Space group symbol	$P3$
AFLOW prototype command	`aflow --proto=A5B_hP60_143_7a7b6c10d_3a3b4c-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}, z_{12}, z_{13}, z_{14}, z_{15}, z_{16}, z_{17}, z_{18}, z_{19}, z_{20}, z_{21}, z_{22}, z_{23}, z_{24}, z_{25}, z_{26}, z_{27}, z_{28}, z_{29}, z_{30}, x_{31}, y_{31}, z_{31}, x_{32}, y_{32}, z_{32}, x_{33}, y_{33}, z_{33}, x_{34}, y_{34}, z_{34}, x_{35}, y_{35}, z_{35}, x_{36}, y_{36}, z_{36}, x_{37}, y_{37}, z_{37}, x_{38}, y_{38}, z_{38}, x_{39}, y_{39}, z_{39}, x_{40}, y_{40}, z_{40}$

- Al_5Mo is known to have three phases (Schuster, 1991):
  - Below 650K it is in a rhombohedral structure, Al_5Mo (r).
  - Between 650K and 750-800K it is in a trigonal structure, Al_5Mo(h') (this structure).
  - Above 750-800K up to 846K it is in the Al_5W structure.
- The Al_5Mo(h') atomic positions in (Schuster, 1991) are highly symmetric and approximate, and put the system in space group $P321$ #150. To show the correct $P3$ 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_{32}}$	=	$-y_{31}\,\mathbf{a}_1 + (x_{31}-y_{31})\,\mathbf{a}_2 + z_{31}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{31}-2y_{31})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{31}\,\hat{\mathbf{y}} + cz_{31}\,\hat{\mathbf{z}}$	(3d)	Al XXI
$\mathbf{B_{33}}$	=	$-(x_{31}-y_{31})\,\mathbf{a}_1 - x_{31}\,\mathbf{a}_2 + z_{31}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_{31}-y_{31})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{31}\,\hat{\mathbf{y}} + cz_{31}\,\hat{\mathbf{z}}$	(3d)	Al XXI

$$\mathbf{B_{34}} = x_{32}\,\mathbf{a}_1 + y_{32}\,\mathbf{a}_2 + z_{32}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{32}+y_{32})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{32}-y_{32})\,\hat{\mathbf{y}} + cz_{32}\,\hat{\mathbf{z}}$$ (3d) Al XXII

$$\mathbf{B_{35}} = -y_{32}\,\mathbf{a}_1 + (x_{32}-y_{32})\,\mathbf{a}_2 + z_{32}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{32}-2y_{32})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{32}\,\hat{\mathbf{y}} + cz_{32}\,\hat{\mathbf{z}}$$ (3d) Al XXII

$$\mathbf{B_{36}} = -(x_{32}-y_{32})\,\mathbf{a}_1 - x_{32}\,\mathbf{a}_2 + z_{32}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{32}-y_{32})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{32}\,\hat{\mathbf{y}} + cz_{32}\,\hat{\mathbf{z}}$$ (3d) Al XXII

$$\mathbf{B_{37}} = x_{33}\,\mathbf{a}_1 + y_{33}\,\mathbf{a}_2 + z_{33}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{33}+y_{33})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{33}-y_{33})\,\hat{\mathbf{y}} + cz_{33}\,\hat{\mathbf{z}}$$ (3d) Al XXIII

$$\mathbf{B_{38}} = -y_{33}\,\mathbf{a}_1 + (x_{33}-y_{33})\,\mathbf{a}_2 + z_{33}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{33}-2y_{33})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{33}\,\hat{\mathbf{y}} + cz_{33}\,\hat{\mathbf{z}}$$ (3d) Al XXIII

$$\mathbf{B_{39}} = -(x_{33}-y_{33})\,\mathbf{a}_1 - x_{33}\,\mathbf{a}_2 + z_{33}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{33}-y_{33})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{33}\,\hat{\mathbf{y}} + cz_{33}\,\hat{\mathbf{z}}$$ (3d) Al XXIII

$$\mathbf{B_{40}} = x_{34}\,\mathbf{a}_1 + y_{34}\,\mathbf{a}_2 + z_{34}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{34}+y_{34})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{34}-y_{34})\,\hat{\mathbf{y}} + cz_{34}\,\hat{\mathbf{z}}$$ (3d) Al XXIV

$$\mathbf{B_{41}} = -y_{34}\,\mathbf{a}_1 + (x_{34}-y_{34})\,\mathbf{a}_2 + z_{34}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{34}-2y_{34})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{34}\,\hat{\mathbf{y}} + cz_{34}\,\hat{\mathbf{z}}$$ (3d) Al XXIV

$$\mathbf{B_{42}} = -(x_{34}-y_{34})\,\mathbf{a}_1 - x_{34}\,\mathbf{a}_2 + z_{34}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{34}-y_{34})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{34}\,\hat{\mathbf{y}} + cz_{34}\,\hat{\mathbf{z}}$$ (3d) Al XXIV

$$\mathbf{B_{43}} = x_{35}\,\mathbf{a}_1 + y_{35}\,\mathbf{a}_2 + z_{35}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{35}+y_{35})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{35}-y_{35})\,\hat{\mathbf{y}} + cz_{35}\,\hat{\mathbf{z}}$$ (3d) Al XXV

$$\mathbf{B_{44}} = -y_{35}\,\mathbf{a}_1 + (x_{35}-y_{35})\,\mathbf{a}_2 + z_{35}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{35}-2y_{35})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{35}\,\hat{\mathbf{y}} + cz_{35}\,\hat{\mathbf{z}}$$ (3d) Al XXV

$$\mathbf{B_{45}} = -(x_{35}-y_{35})\,\mathbf{a}_1 - x_{35}\,\mathbf{a}_2 + z_{35}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{35}-y_{35})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{35}\,\hat{\mathbf{y}} + cz_{35}\,\hat{\mathbf{z}}$$ (3d) Al XXV

$$\mathbf{B_{46}} = x_{36}\,\mathbf{a}_1 + y_{36}\,\mathbf{a}_2 + z_{36}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{36}+y_{36})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{36}-y_{36})\,\hat{\mathbf{y}} + cz_{36}\,\hat{\mathbf{z}}$$ (3d) Al XXVI

$$\mathbf{B_{47}} = -y_{36}\,\mathbf{a}_1 + (x_{36}-y_{36})\,\mathbf{a}_2 + z_{36}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{36}-2y_{36})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{36}\,\hat{\mathbf{y}} + cz_{36}\,\hat{\mathbf{z}}$$ (3d) Al XXVI

$$\mathbf{B_{48}} = -(x_{36}-y_{36})\,\mathbf{a}_1 - x_{36}\,\mathbf{a}_2 + z_{36}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{36}-y_{36})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{36}\,\hat{\mathbf{y}} + cz_{36}\,\hat{\mathbf{z}}$$ (3d) Al XXVI

$$\mathbf{B_{49}} = x_{37}\,\mathbf{a}_1 + y_{37}\,\mathbf{a}_2 + z_{37}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{37}+y_{37})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{37}-y_{37})\,\hat{\mathbf{y}} + cz_{37}\,\hat{\mathbf{z}}$$ (3d) Al XXVII

$$\mathbf{B_{50}} = -y_{37}\,\mathbf{a}_1 + (x_{37}-y_{37})\,\mathbf{a}_2 + z_{37}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{37}-2y_{37})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{37}\,\hat{\mathbf{y}} + cz_{37}\,\hat{\mathbf{z}}$$ (3d) Al XXVII

$$\mathbf{B_{51}} = -(x_{37}-y_{37})\,\mathbf{a}_1 - x_{37}\,\mathbf{a}_2 + z_{37}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{37}-y_{37})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{37}\,\hat{\mathbf{y}} + cz_{37}\,\hat{\mathbf{z}}$$ (3d) Al XXVII

$$\mathbf{B_{52}} = x_{38}\,\mathbf{a}_1 + y_{38}\,\mathbf{a}_2 + z_{38}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{38}+y_{38})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{38}-y_{38})\,\hat{\mathbf{y}} + cz_{38}\,\hat{\mathbf{z}}$$ (3d) Al XXVIII

$$\mathbf{B_{53}} = -y_{38}\,\mathbf{a}_1 + (x_{38}-y_{38})\,\mathbf{a}_2 + z_{38}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{38}-2y_{38})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{38}\,\hat{\mathbf{y}} + cz_{38}\,\hat{\mathbf{z}}$$ (3d) Al XXVIII

$$\mathbf{B_{54}} = -(x_{38}-y_{38})\,\mathbf{a}_1 - x_{38}\,\mathbf{a}_2 + z_{38}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{38}-y_{38})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{38}\,\hat{\mathbf{y}} + cz_{38}\,\hat{\mathbf{z}}$$ (3d) Al XXVIII

$$\mathbf{B_{55}} = x_{39}\,\mathbf{a}_1 + y_{39}\,\mathbf{a}_2 + z_{39}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{39}+y_{39})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{39}-y_{39})\,\hat{\mathbf{y}} + cz_{39}\,\hat{\mathbf{z}}$$ (3d) Al XXIX

$$\mathbf{B_{56}} = -y_{39}\,\mathbf{a}_1 + (x_{39}-y_{39})\,\mathbf{a}_2 + z_{39}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{39}-2y_{39})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{39}\,\hat{\mathbf{y}} + cz_{39}\,\hat{\mathbf{z}}$$ (3d) Al XXIX

$$\mathbf{B_{57}} = -(x_{39}-y_{39})\,\mathbf{a}_1 - x_{39}\,\mathbf{a}_2 + z_{39}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{39}-y_{39})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{39}\,\hat{\mathbf{y}} + cz_{39}\,\hat{\mathbf{z}}$$ (3d) Al XXIX

$$\mathbf{B_{58}} = x_{40}\,\mathbf{a}_1 + y_{40}\,\mathbf{a}_2 + z_{40}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{40}+y_{40})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{40}-y_{40})\,\hat{\mathbf{y}} + cz_{40}\,\hat{\mathbf{z}}$$ (3d) Al XXX

$$\mathbf{B_{59}} = -y_{40}\,\mathbf{a}_1 + (x_{40}-y_{40})\,\mathbf{a}_2 + z_{40}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{40}-2y_{40})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{40}\,\hat{\mathbf{y}} + cz_{40}\,\hat{\mathbf{z}}$$ (3d) Al XXX

$$\mathbf{B_{60}} = -(x_{40}-y_{40})\,\mathbf{a}_1 - x_{40}\,\mathbf{a}_2 + z_{40}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{40}-y_{40})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{40}\,\hat{\mathbf{y}} + cz_{40}\,\hat{\mathbf{z}}$$ (3d) Al XXX

References

[1] J. C. Schuster and H. Ipser, *The Al-Al_8Mo_3 section of the binary system aluminum-molybdenum*, Metall. Trans. A **22**, 1729–1736 (1991), doi:10.1007/BF02646496.