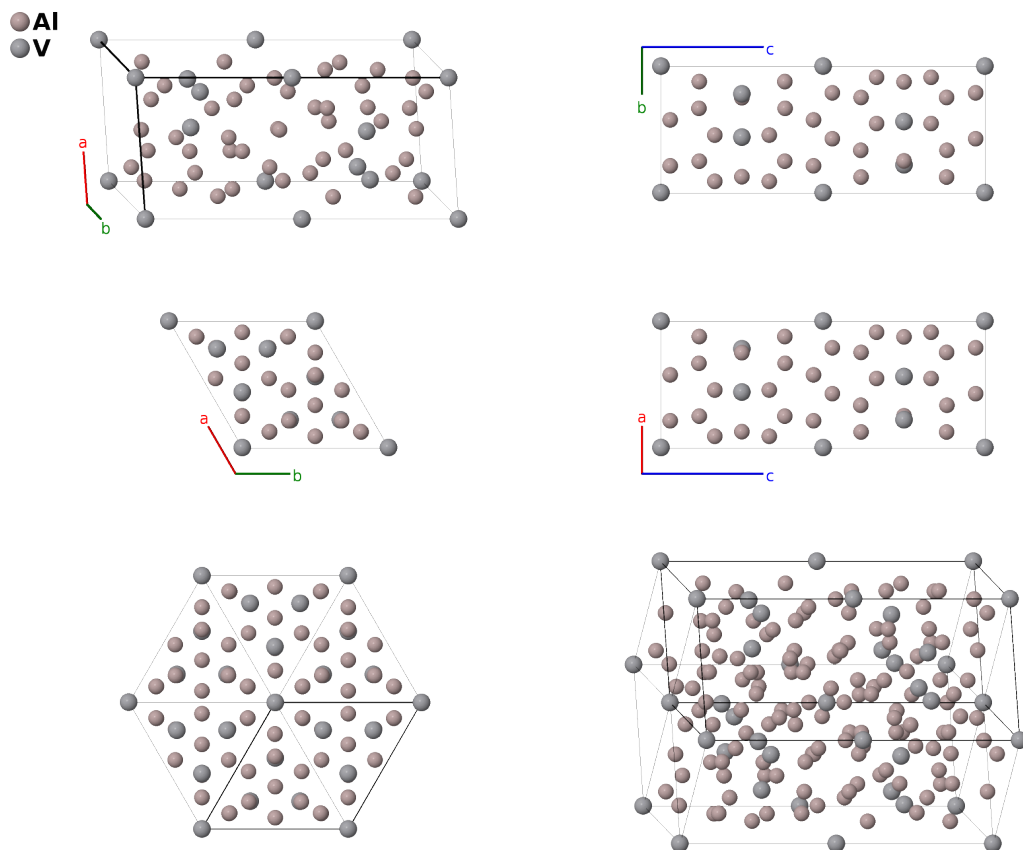


Al₂₃V₄ Structure: A23B4_hP54_194_fh3k_ah-001

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<https://aflow.org/p/W4P8>

https://aflow.org/p/A23B4_hP54_194_fh3k_ah-001

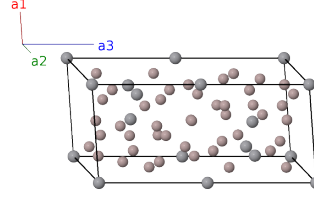


Prototype	Al ₂₃ V ₄
AFLOW prototype label	A23B4_hP54_194_fh3k_ah-001
ICSD	174002
Pearson symbol	hP54
Space group number	194
Space group symbol	<i>P</i> 6 ₃ / <i>mmc</i>
AFLOW prototype command	<code>aflow --proto=A23B4_hP54_194_fh3k_ah-001 --params=a, c/a, z₂, x₃, x₄, x₅, z₅, x₆, z₆, x₇, z₇</code>

- (Smith, 1957) gives $z_2 = 0.167$ for their Al₅ (our Al II) (4f) site, but the ICSD entry sets this to 0.617. The later value is consistent with the interatomic distances in the paper, so we use that value.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	V I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	V I
\mathbf{B}_3	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Al I
\mathbf{B}_4	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al I
\mathbf{B}_5	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Al I
\mathbf{B}_6	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Al I
\mathbf{B}_7	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Al II
\mathbf{B}_8	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Al II
\mathbf{B}_9	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Al II
\mathbf{B}_{10}	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Al II
\mathbf{B}_{11}	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Al II
\mathbf{B}_{12}	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Al II
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	V II
\mathbf{B}_{14}	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	V II
\mathbf{B}_{15}	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	V II
\mathbf{B}_{16}	$-x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	V II
\mathbf{B}_{17}	$2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	V II
\mathbf{B}_{18}	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	V II
\mathbf{B}_{19}	$x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{20}	$-2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{21}	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{22}	$-x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{23}	$2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{24}	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{25}	$2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{26}	$-x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{27}	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\sqrt{3}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{28}	$-2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{29}	$x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{30}	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Al III
\mathbf{B}_{31}	$x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(12k)	Al IV

$$\begin{aligned}
\mathbf{B}_{32} &= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= & -\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{33} &= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= & -\sqrt{3}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{34} &= -x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= & -\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{35} &= 2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{36} &= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= & \sqrt{3}ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{37} &= 2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & \frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{38} &= -x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & -\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{39} &= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & \sqrt{3}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{40} &= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= & -\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{41} &= x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{42} &= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= & -\sqrt{3}ax_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al IV} \\
\mathbf{B}_{43} &= x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & \frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{44} &= -2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -\frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{45} &= x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -\sqrt{3}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{46} &= -x_7 \mathbf{a}_1 - 2x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & -\frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{47} &= 2x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{48} &= -x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & \sqrt{3}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{49} &= 2x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & \frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{50} &= -x_7 \mathbf{a}_1 - 2x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & -\frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{51} &= -x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & \sqrt{3}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{52} &= -2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & -\frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{53} &= x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al V} \\
\mathbf{B}_{54} &= x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & -\sqrt{3}ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{Al V}
\end{aligned}$$

References

- [1] J. F. Smith and A. E. Ray, *The Structure of V_4Al_{23}* , Acta Cryst. **10**, 169–172 (1957), doi:10.1107/S0365110X57000559.