

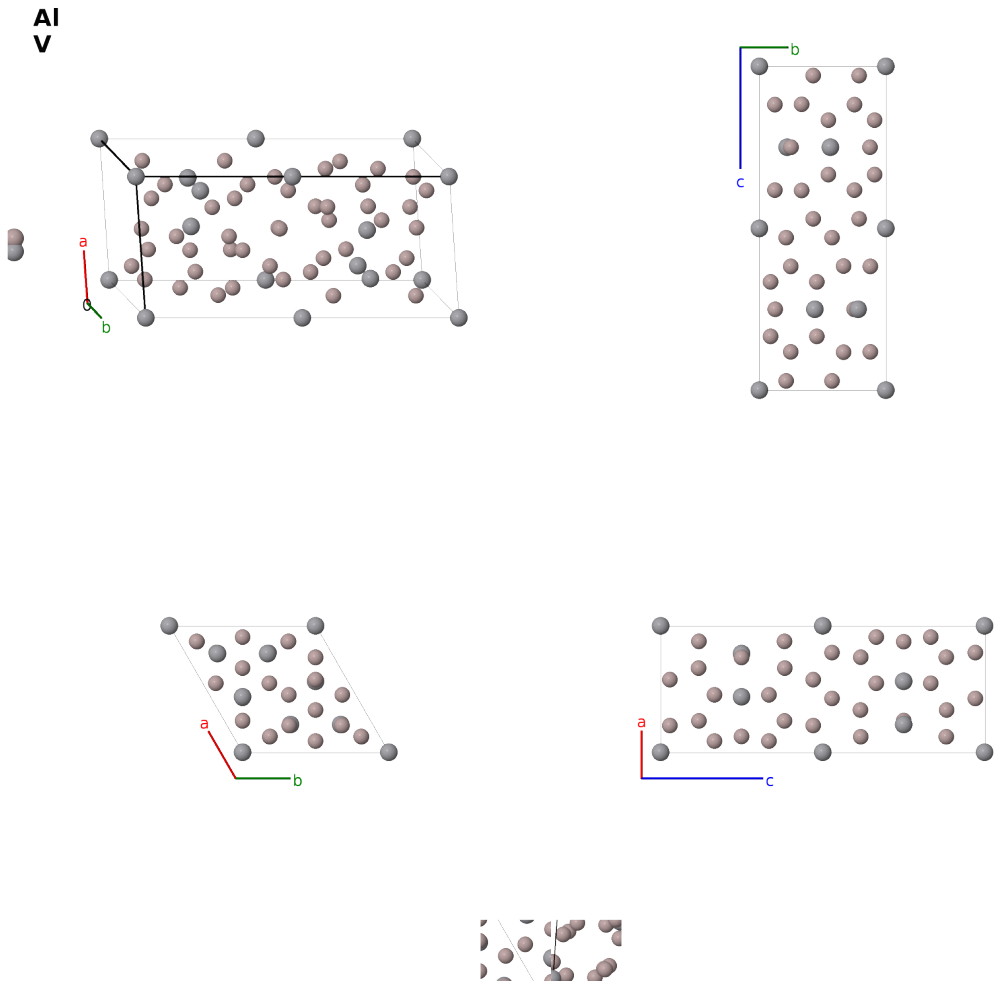
Al₂₃V₄ Structure: A23B4_hP54_194_fh3k_ah-001

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/W4P8>

https://aflow.org/prototype-encyclopedia/A23B4_hP54_194_fh3k_ah-001



Prototype	Al ₂₃ V ₄
AFLOW prototype label	A23B4_hP54_194_fh3k_ah-001
ICSD	174002
CCDC	1688895
Pearson symbol	hP54
Space group number	194
Space group symbol	$P6_3/mmc$

AFLOW prototype command `aflow --proto=A23B4_hP54_194_fh3k_ah-001`
 `--params=a, c/a, z2, x3, x4, x5, z5, x6, z6, x7, z7`

- (Smith, 1957) gives $z_2 = 0.167$ for their Al_5 (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



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

$\mathbf{B}_{24} =$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\sqrt{3}ax_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{28} =$	$-2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{29} =$	$x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Al III
$\mathbf{B}_{30} =$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{32} =$	$-2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(12k)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	Al V

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.

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.