$Al_{45}V_7$ Structure: A45B7_mC104_12_a8i7j_cij-001

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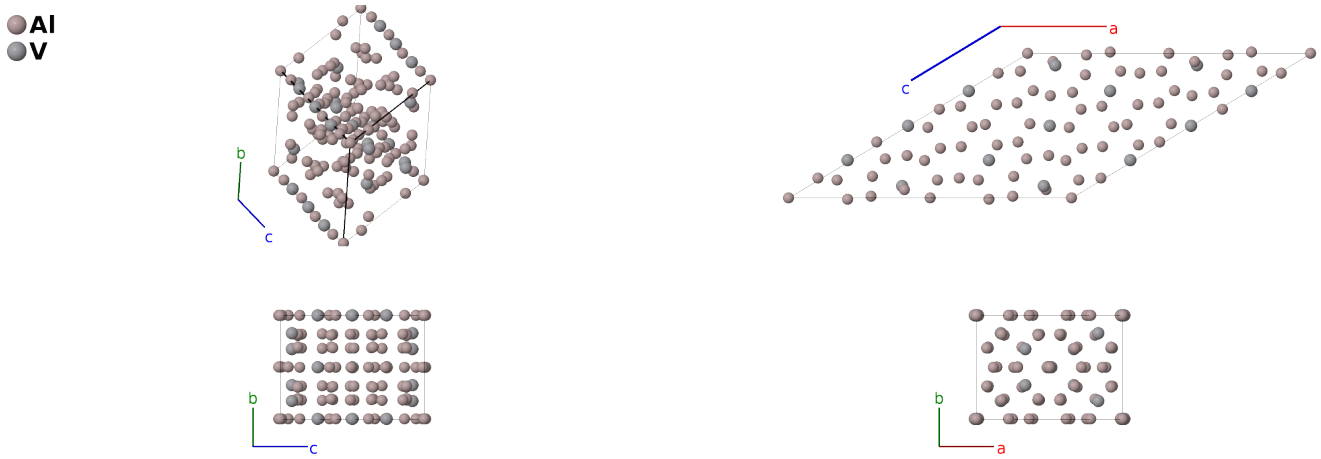
https://aflow.org/p/4Z2U

https://aflow.org/p/A45B7_mC104_12_a8i7j_cij-001



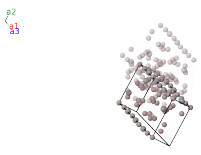
Prototype	$Al_{45}V_7$
AFLOW prototype label	A45B7_mC104_12_a8i7j_cij-001
ICSD	58204
Pearson symbol	mC104
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A45B7_mC104_12_a8i7j_cij-001 --params=`$a, b/a, c/a, \beta, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}$

Other compounds with this structure

$Al_{45}Cr_7$

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	V I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al II
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al II
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al III
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al III
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al IV
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al IV
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al V
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al V
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al VI
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al VI
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al VII
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al VII
$\mathbf{B_{15}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al VIII
$\mathbf{B_{16}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al VIII
$\mathbf{B_{17}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al IX
$\mathbf{B_{18}}$	=	$-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	Al IX
$\mathbf{B_{19}}$	=	$x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4i)	V II
$\mathbf{B_{20}}$	=	$-x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4i)	V II
$\mathbf{B_{21}}$	=	$(x_{12} - y_{12})\,\mathbf{a}_1 + (x_{12} + y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al X
$\mathbf{B_{22}}$	=	$-(x_{12} + y_{12})\,\mathbf{a}_1 - (x_{12} - y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al X
$\mathbf{B_{23}}$	=	$-(x_{12} - y_{12})\,\mathbf{a}_1 - (x_{12} + y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al X
$\mathbf{B_{24}}$	=	$(x_{12} + y_{12})\,\mathbf{a}_1 + (x_{12} - y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al X
$\mathbf{B_{25}}$	=	$(x_{13} - y_{13})\,\mathbf{a}_1 + (x_{13} + y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XI
$\mathbf{B_{26}}$	=	$-(x_{13} + y_{13})\,\mathbf{a}_1 - (x_{13} - y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XI
$\mathbf{B_{27}}$	=	$-(x_{13} - y_{13})\,\mathbf{a}_1 - (x_{13} + y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XI
$\mathbf{B_{28}}$	=	$(x_{13} + y_{13})\,\mathbf{a}_1 + (x_{13} - y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XI
$\mathbf{B_{29}}$	=	$(x_{14} - y_{14})\,\mathbf{a}_1 + (x_{14} + y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XII
$\mathbf{B_{30}}$	=	$-(x_{14} + y_{14})\,\mathbf{a}_1 - (x_{14} - y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	=	$-(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XII
$\mathbf{B_{31}}$	=	$-(x_{14} - y_{14})\,\mathbf{a}_1 - (x_{14} + y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	=	$-(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XII

$\mathbf{B_{32}}$	=	$(x_{14}+y_{14})\,\mathbf{a}_1+(x_{14}-y_{14})\,\mathbf{a}_2+z_{14}\,\mathbf{a}_3$	=	$(ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}+cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XII
$\mathbf{B_{33}}$	=	$(x_{15}-y_{15})\,\mathbf{a}_1+(x_{15}+y_{15})\,\mathbf{a}_2+z_{15}\,\mathbf{a}_3$	=	$(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}}+by_{15}\,\hat{\mathbf{y}}+cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B_{34}}$	=	$-(x_{15}+y_{15})\,\mathbf{a}_1-(x_{15}-y_{15})\,\mathbf{a}_2-z_{15}\,\mathbf{a}_3$	=	$-(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}}+by_{15}\,\hat{\mathbf{y}}-cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B_{35}}$	=	$-(x_{15}-y_{15})\,\mathbf{a}_1-(x_{15}+y_{15})\,\mathbf{a}_2-z_{15}\,\mathbf{a}_3$	=	$-(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}}-by_{15}\,\hat{\mathbf{y}}-cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B_{36}}$	=	$(x_{15}+y_{15})\,\mathbf{a}_1+(x_{15}-y_{15})\,\mathbf{a}_2+z_{15}\,\mathbf{a}_3$	=	$(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}}-by_{15}\,\hat{\mathbf{y}}+cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B_{37}}$	=	$(x_{16}-y_{16})\,\mathbf{a}_1+(x_{16}+y_{16})\,\mathbf{a}_2+z_{16}\,\mathbf{a}_3$	=	$(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}}+by_{16}\,\hat{\mathbf{y}}+cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B_{38}}$	=	$-(x_{16}+y_{16})\,\mathbf{a}_1-(x_{16}-y_{16})\,\mathbf{a}_2-z_{16}\,\mathbf{a}_3$	=	$-(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}}+by_{16}\,\hat{\mathbf{y}}-cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B_{39}}$	=	$-(x_{16}-y_{16})\,\mathbf{a}_1-(x_{16}+y_{16})\,\mathbf{a}_2-z_{16}\,\mathbf{a}_3$	=	$-(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}}-by_{16}\,\hat{\mathbf{y}}-cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B_{40}}$	=	$(x_{16}+y_{16})\,\mathbf{a}_1+(x_{16}-y_{16})\,\mathbf{a}_2+z_{16}\,\mathbf{a}_3$	=	$(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}}-by_{16}\,\hat{\mathbf{y}}+cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B_{41}}$	=	$(x_{17}-y_{17})\,\mathbf{a}_1+(x_{17}+y_{17})\,\mathbf{a}_2+z_{17}\,\mathbf{a}_3$	=	$(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}}+by_{17}\,\hat{\mathbf{y}}+cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B_{42}}$	=	$-(x_{17}+y_{17})\,\mathbf{a}_1-(x_{17}-y_{17})\,\mathbf{a}_2-z_{17}\,\mathbf{a}_3$	=	$-(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}}+by_{17}\,\hat{\mathbf{y}}-cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B_{43}}$	=	$-(x_{17}-y_{17})\,\mathbf{a}_1-(x_{17}+y_{17})\,\mathbf{a}_2-z_{17}\,\mathbf{a}_3$	=	$-(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}}-by_{17}\,\hat{\mathbf{y}}-cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B_{44}}$	=	$(x_{17}+y_{17})\,\mathbf{a}_1+(x_{17}-y_{17})\,\mathbf{a}_2+z_{17}\,\mathbf{a}_3$	=	$(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}}-by_{17}\,\hat{\mathbf{y}}+cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B_{45}}$	=	$(x_{18}-y_{18})\,\mathbf{a}_1+(x_{18}+y_{18})\,\mathbf{a}_2+z_{18}\,\mathbf{a}_3$	=	$(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}}+by_{18}\,\hat{\mathbf{y}}+cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B_{46}}$	=	$-(x_{18}+y_{18})\,\mathbf{a}_1-(x_{18}-y_{18})\,\mathbf{a}_2-z_{18}\,\mathbf{a}_3$	=	$-(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}}+by_{18}\,\hat{\mathbf{y}}-cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B_{47}}$	=	$-(x_{18}-y_{18})\,\mathbf{a}_1-(x_{18}+y_{18})\,\mathbf{a}_2-z_{18}\,\mathbf{a}_3$	=	$-(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}}-by_{18}\,\hat{\mathbf{y}}-cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B_{48}}$	=	$(x_{18}+y_{18})\,\mathbf{a}_1+(x_{18}-y_{18})\,\mathbf{a}_2+z_{18}\,\mathbf{a}_3$	=	$(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}}-by_{18}\,\hat{\mathbf{y}}+cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B_{49}}$	=	$(x_{19}-y_{19})\,\mathbf{a}_1+(x_{19}+y_{19})\,\mathbf{a}_2+z_{19}\,\mathbf{a}_3$	=	$(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}}+by_{19}\,\hat{\mathbf{y}}+cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B_{50}}$	=	$-(x_{19}+y_{19})\,\mathbf{a}_1-(x_{19}-y_{19})\,\mathbf{a}_2-z_{19}\,\mathbf{a}_3$	=	$-(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}}+by_{19}\,\hat{\mathbf{y}}-cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B_{51}}$	=	$-(x_{19}-y_{19})\,\mathbf{a}_1-(x_{19}+y_{19})\,\mathbf{a}_2-z_{19}\,\mathbf{a}_3$	=	$-(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}}-by_{19}\,\hat{\mathbf{y}}-cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B_{52}}$	=	$(x_{19}+y_{19})\,\mathbf{a}_1+(x_{19}-y_{19})\,\mathbf{a}_2+z_{19}\,\mathbf{a}_3$	=	$(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}}-by_{19}\,\hat{\mathbf{y}}+cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(8j)	V III

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