$Al_{10}V$ Structure: A10B_cF176_227_cfg_d-001

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- 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.

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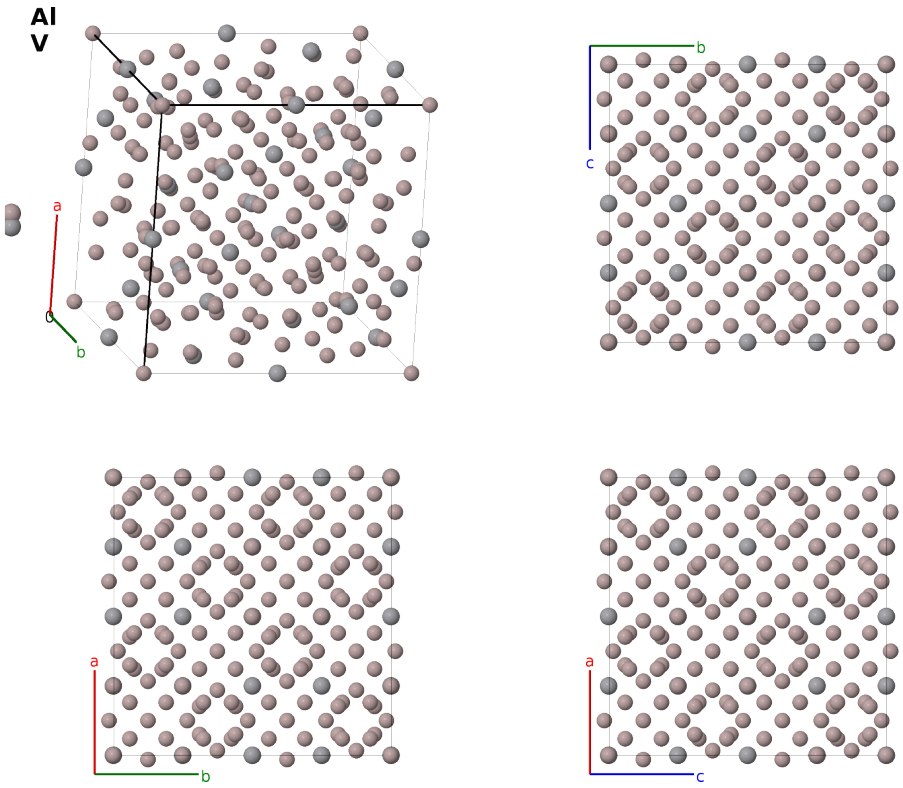
https://aflow.org/prototype-encyclopedia/WWX6

https://aflow.org/prototype-encyclopedia/A10B_cF176_227_cfg_d-001

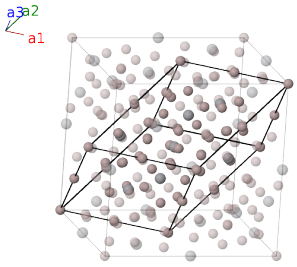


Prototype	$Al_{10}V$
AFLOW prototype label	A10B_cF176_227_cfg_d-001
ICSD	58202
CCDC	1622230
Pearson symbol	cF176
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A10B_cF176_227_cfg_d-001 --params=`a, x_3, x_4, z_4

- (Brown, 1957) gives the structural information in setting 1 of space group $Fd\bar{3}m$ #227. We shifted the origin by ($a/8$ $a/8$ $a/8$) to change this to the standard setting 2.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}\\ \mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(16c)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Al I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	V I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	V I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	V I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	V I
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{12}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{14}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{15}}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_3 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{17}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{18}}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{19}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{20}}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + a\left(x_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Al II
$\mathbf{B_{21}}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + (2x_4 - z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{22}}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{23}}$	=	$(2x_4 - z_4)\,\mathbf{a}_1 - \left(2x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al III

$\mathbf{B_{24}}$	$= -\left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_1 + (2x_4 - z_4)\mathbf{a}_2 + z_4\mathbf{a}_3$	$= ax_4\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{25}}$	$= (2x_4 - z_4)\mathbf{a}_1 + z_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$= az_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{26}}$	$= -\left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_1 + z_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$= az_4\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{27}}$	$= z_4\mathbf{a}_1 + (2x_4 - z_4)\mathbf{a}_2 - \left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$= -a\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{28}}$	$= z_4\mathbf{a}_1 - \left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_2 + (2x_4 - z_4)\mathbf{a}_3$	$= -a\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{29}}$	$= z_4\mathbf{a}_1 + (2x_4 - z_4)\mathbf{a}_2 + z_4\mathbf{a}_3$	$= ax_4\hat{\mathbf{x}} + az_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{30}}$	$= z_4\mathbf{a}_1 - \left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_2 + z_4\mathbf{a}_3$	$= -a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{x}} + az_4\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{31}}$	$= -\left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_1 + z_4\mathbf{a}_2 + (2x_4 - z_4)\mathbf{a}_3$	$= ax_4\hat{\mathbf{x}} - a\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{32}}$	$= (2x_4 - z_4)\mathbf{a}_1 + z_4\mathbf{a}_2 - \left(2x_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$= -a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{x}} - a\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{33}}$	$= -z_4\mathbf{a}_1 - z_4\mathbf{a}_2 + \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$= a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{y}} - az_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{34}}$	$= -z_4\mathbf{a}_1 - z_4\mathbf{a}_2 - (2x_4 - z_4)\mathbf{a}_3$	$= -ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - az_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{35}}$	$= -(2x_4 - z_4)\mathbf{a}_1 + \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_2 - z_4\mathbf{a}_3$	$= a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + a\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{36}}$	$= \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_1 - (2x_4 - z_4)\mathbf{a}_2 - z_4\mathbf{a}_3$	$= -ax_4\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{y}} + a\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{37}}$	$= -(2x_4 - z_4)\mathbf{a}_1 - z_4\mathbf{a}_2 + \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$= a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{x}} + a\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{38}}$	$= \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_1 - z_4\mathbf{a}_2 - (2x_4 - z_4)\mathbf{a}_3$	$= -ax_4\hat{\mathbf{x}} + a\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{39}}$	$= -z_4\mathbf{a}_1 - (2x_4 - z_4)\mathbf{a}_2 - z_4\mathbf{a}_3$	$= -ax_4\hat{\mathbf{x}} - az_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{40}}$	$= -z_4\mathbf{a}_1 + \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_2 - z_4\mathbf{a}_3$	$= a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{x}} - az_4\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{41}}$	$= -z_4\mathbf{a}_1 - (2x_4 - z_4)\mathbf{a}_2 + \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$= a\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{42}}$	$= -z_4\mathbf{a}_1 + \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_2 - (2x_4 - z_4)\mathbf{a}_3$	$= a\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{43}}$	$= \left(2x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_1 - z_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$= -az_4\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(96g)	Al III
$\mathbf{B_{44}}$	$= -(2x_4 - z_4)\mathbf{a}_1 - z_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$= -az_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(96g)	Al III

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