$VPCl_9$ Structure: A9BC_oC44_39_3c3d_a_c-001

This structure previously used the label(s) `A9BC_oC44_39_3c3d_a_c`. Calls to these addresses will be redirected here.

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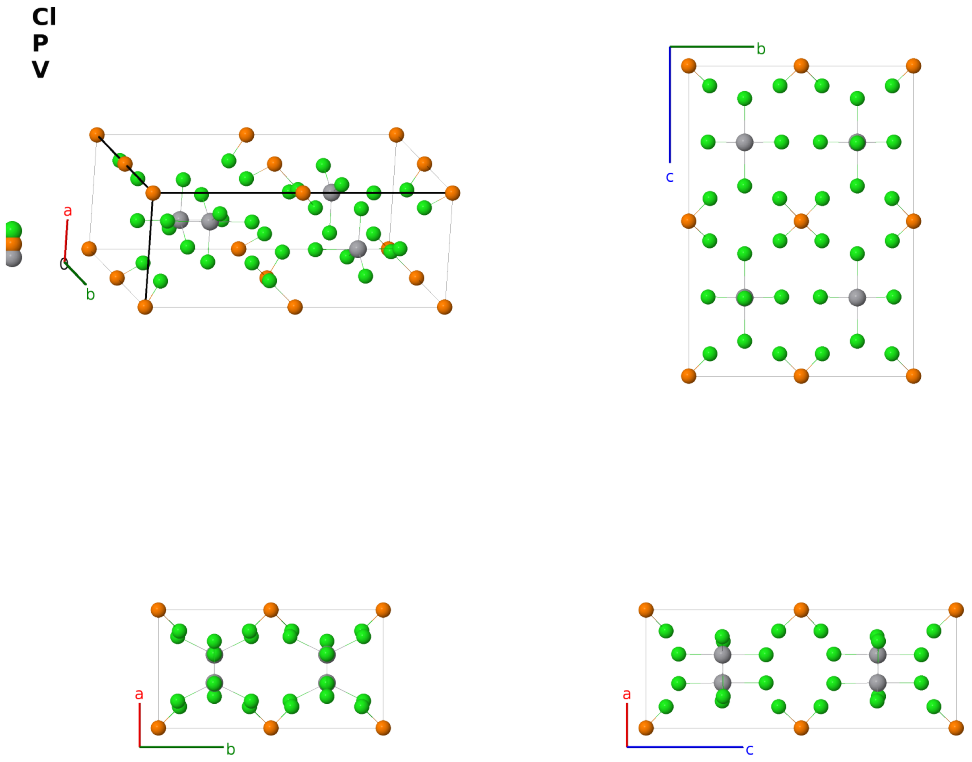
https://aflow.org/prototype-encyclopedia/5ZH7

https://aflow.org/prototype-encyclopedia/A9BC_oC44_39_3c3d_a_c-001

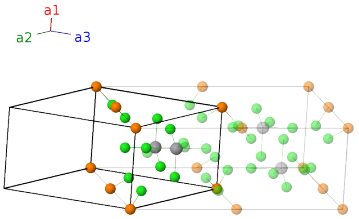


Prototype	Cl_9PV
AFLOW prototype label	A9BC_oC44_39_3c3d_a_c-001
ICSD	1047
CCDC	1591256
Pearson symbol	oC44
Space group number	39
Space group symbol	$Aem2$

AFLOW prototype command `aflow --proto=A9BC_oC44_39_3c3d_a_c-001 --params=`$a, b/a, c/a, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_2}$	=	$-\left(z_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - \left(z_2-\frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - \left(z_2-\frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_2+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - \left(z_3-\frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(z_3-\frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_3+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - \left(z_4-\frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Cl III
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - \left(z_4-\frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Cl III
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 - \left(z_5-\frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	V I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - \left(z_5-\frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_5+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	V I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + (y_6-z_6)\,\mathbf{a}_2 + (y_6+z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Cl IV
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - (y_6+z_6)\,\mathbf{a}_2 - (y_6-z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Cl IV
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6+z_6-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Cl IV
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6-z_6+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Cl IV
$\mathbf{B_{15}}$	=	$x_7\,\mathbf{a}_1 + (y_7-z_7)\,\mathbf{a}_2 + (y_7+z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	Cl V
$\mathbf{B_{16}}$	=	$-x_7\,\mathbf{a}_1 - (y_7+z_7)\,\mathbf{a}_2 - (y_7-z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	Cl V
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - b\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	Cl V
$\mathbf{B_{18}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + b\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	Cl V

$\mathbf{B_{19}}$	=	$x_8\,\mathbf{a}_1+(y_8-z_8)\,\mathbf{a}_2+(y_8+z_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	Cl VI
$\mathbf{B_{20}}$	=	$-x_8\,\mathbf{a}_1-(y_8+z_8)\,\mathbf{a}_2-(y_8-z_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	Cl VI
$\mathbf{B_{21}}$	=	$x_8\,\mathbf{a}_1-\left(y_8+z_8-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	Cl VI
$\mathbf{B_{22}}$	=	$-x_8\,\mathbf{a}_1+\left(y_8-z_8+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8d)	Cl VI

References

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First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043