$VPCl_9$ Structure: A9BC_oC44_39_3c3d_a_c-001

This structure originally had the label `A9BC_oC44_39_3c3d_a_c`. Calls to that address will be redirected here.

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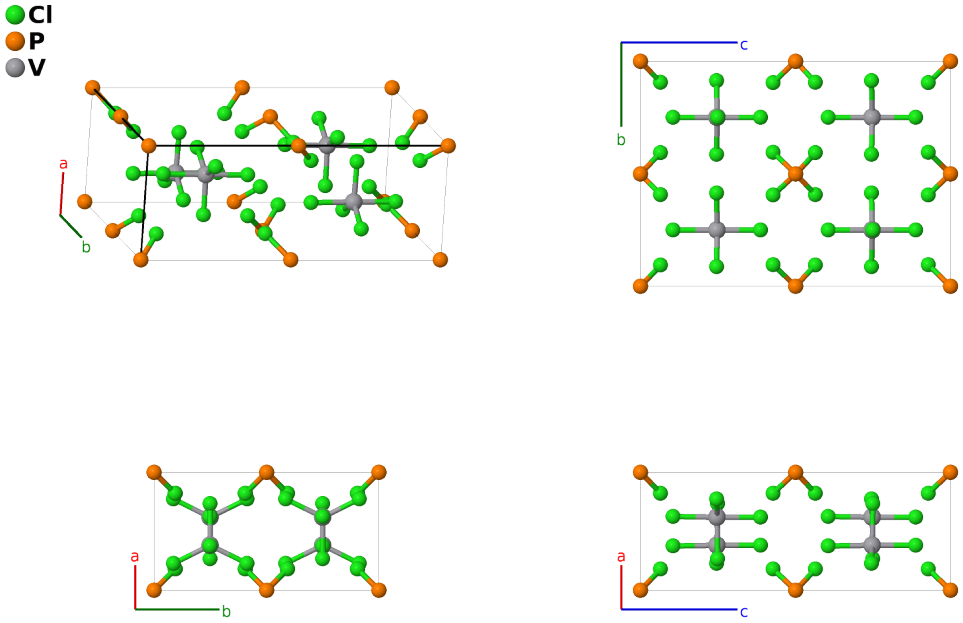
https://aflow.org/p/5ZH7

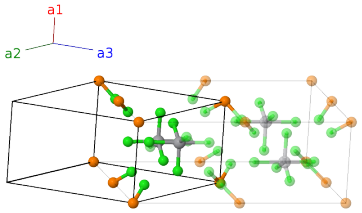
https://aflow.org/p/A9BC_oC44_39_3c3d_a_c-001



Prototype	Cl_9PV
AFLOW prototype label	A9BC_oC44_39_3c3d_a_c-001
ICSD	1047
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

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

References

[1] M. L. Ziegler, B. Nuber, K. Weidenhammer, and G. Hoch, *Die Molekül- und Kristallstruktur von Tetrachlorophosphoniumpentachlorovanadat(IV), [PCl_4] [VCl_5]*, Z. Naturforsch. B **32**, 18–21 (1977), doi:10.1515/znb-1977-0106.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.