

CaV₄O₉ Structure:

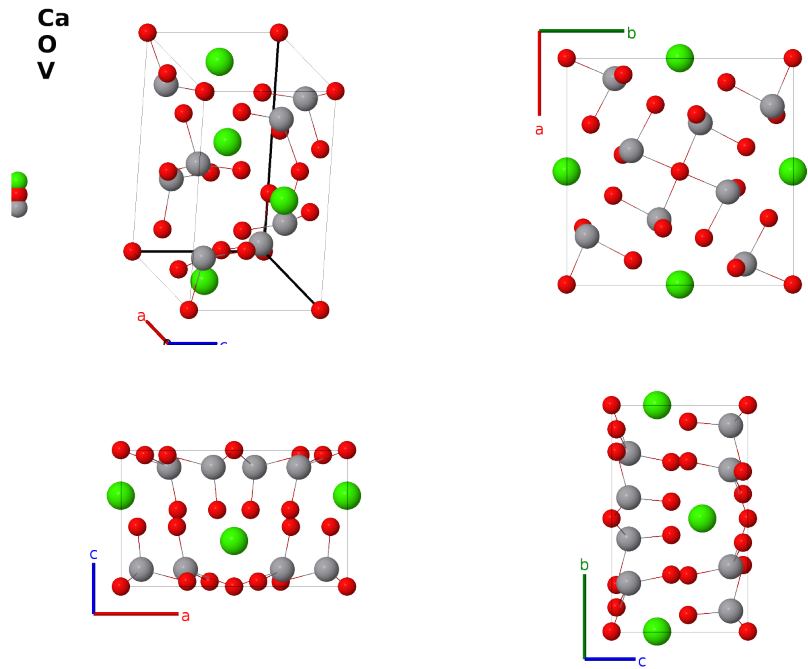
AB9C4_tP28_85_c_a2g_g-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osés, 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/HFAT>

https://aflow.org/prototype-encyclopedia/AB9C4_tP28_85_c_a2g_g-001



Prototype	CaO ₉ V ₄
AFLOW prototype label	AB9C4_tP28_85_c_a2g_g-001
ICSD	2556
CCDC	1592432
Pearson symbol	tP28
Space group number	85
Space group symbol	$P4/n$
AFLOW prototype command	<pre>aflow --proto=AB9C4_tP28_85_c_a2g_g-001 --params=a, c/a, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</pre>

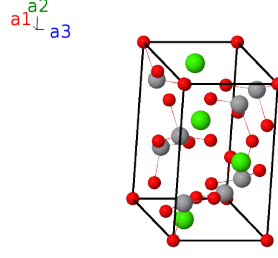
Other compounds with this structure

SrV₄O₉

- AFLOW moves the origin so that the published O I sited is moved from the (2b) Wyckoff position to the (2a) site.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_6$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_7$	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{10}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{11}$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{12}$	$= -y_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{15}$	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{18}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{19}$	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{20}$	$= -y_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{21}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_{22}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_{23}$	$= -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_{24}$	$= y_5 \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_{25}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_{26}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	V I

$$\mathbf{B}_{27} = \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (8g) \quad \text{V I}$$

$$\mathbf{B}_{28} = -y_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 = -ay_5 \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (8g) \quad \text{V I}$$

References

- [1] J.-C. Bouloux and J. Galy, *Structure cristalline de l'hypovanadate CaV_4O_9* , Acta Cryst. **29**, 1335–1338 (1973), doi:10.1107/S0567740873004462.

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