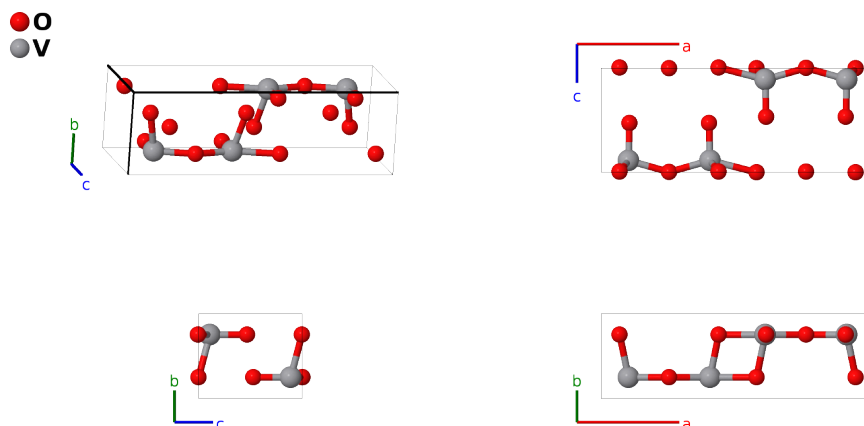# Shcherbinaite (V_2O_5) Structure (*Revised*): A5B2_oP14_59_a2e_e-001

This structure originally had the label `A5B2_oP14_59_a2f_f`. Calls to that address will be redirected here.

https://aflow.org/p/KZMB

https://aflow.org/p/A5B2_oP14_59_a2e_e-001

Prototype	O_5V_2
AFLOW prototype label	A5B2_oP14_59_a2e_e-001
Mineral name	shcherbinaite
ICSD	60767
Pearson symbol	oP14
Space group number	59
Space group symbol	$Pmmn$
AFLOW prototype command	`aflow --proto=A5B2_oP14_59_a2e_e-001` `--params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4$

- An earlier version of this structure found by (Ketelaar, 1936) was given the $D8_7$ *Strukturbericht* designation in (Gottfried, 1938). It was later realized that this structure had a rather unexpected arrangement of vanadium atoms, and the structure was revised by (Enjalbert, 1986) and others.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
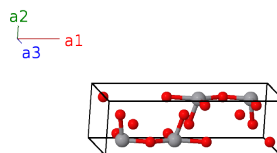
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + z_1\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - z_1\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$=$	$\frac{1}{4}\mathbf{a}_1 + y_2\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_4$	$=$	$\frac{1}{4}\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_5$	$=$	$\frac{3}{4}\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_6$	$=$	$\frac{3}{4}\mathbf{a}_1 - y_2\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_7$	$=$	$\frac{1}{4}\mathbf{a}_1 + y_3\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_8$	$=$	$\frac{1}{4}\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_9$	$=$	$\frac{3}{4}\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{10}$	$=$	$\frac{3}{4}\mathbf{a}_1 - y_3\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{11}$	$=$	$\frac{1}{4}\mathbf{a}_1 + y_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	V I
$\mathbf{B}_{12}$	$=$	$\frac{1}{4}\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	V I
$\mathbf{B}_{13}$	$=$	$\frac{3}{4}\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	V I
$\mathbf{B}_{14}$	$=$	$\frac{3}{4}\mathbf{a}_1 - y_4\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	V I

References

[1] R. Enjalbert and J. Galy, *A Refinement of the Structure of V_2O_5*, Acta Crystallogr. Sect. C **42**, 1467–1469 (1986), doi:10.1107/S0108270186091825.

[2] J. A. A. Ketelaar, *Crystal Structure and Shape of Colloidal Particles of Vanadium Pentoxide*, Nature **137**, 316 (1936), doi:10.1038/137316a0.

[3] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).