

Shcherbinaite ($D8_7$, V_2O_5) Structure (*Obsolete*): A5B2_oP14_31_a2b_b-001

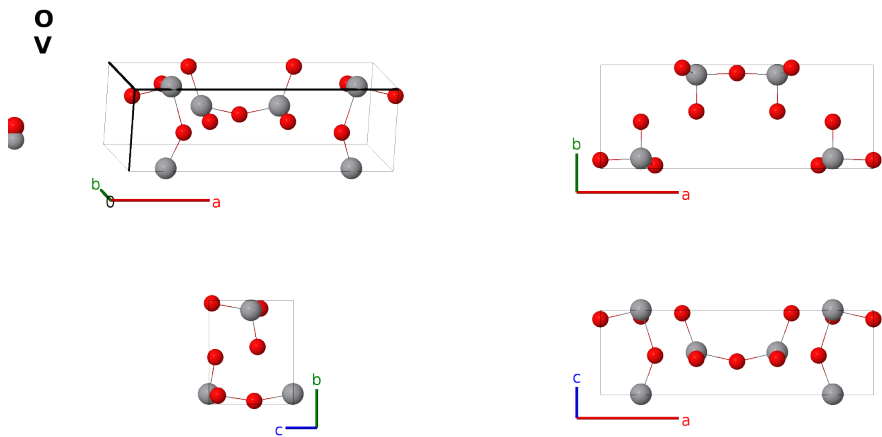
This structure previously used the label(s) **A5B2_oP14_31_a2b_b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/T4NG>

https://aflow.org/prototype-encyclopedia/A5B2_oP14_31_a2b_b-001



Prototype	O_5V_2
AFLOW prototype label	A5B2_oP14_31_a2b_b-001
<i>Strukturbericht</i> designation	$D8_7$
Mineral name	shcherbinaite
ICSD	15904
CCDC	1596576
Pearson symbol	oP14
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	<pre>aflow --proto=A5B2_oP14_31_a2b_b-001 --params=a, b/a, c/a, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4</pre>

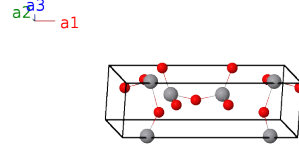
- This structure was reinvestigated by (Enjalbert, 1986) and others because of “[dissatisfaction with] some aspects of the crystal structure.” They proposed a revised structure in space group $Pmmn$ #59. We list this structure here for the historical record.

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
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_4$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_5$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_8$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_9$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	V I
$\mathbf{B}_{12}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	V I
$\mathbf{B}_{13}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	V I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	V I

References

- [1] J. A. A. Ketelaar, *Die Kristallstruktur des Vanadinpentoxyds*, Z. Kristallogr. **95**, 9–27 (1936), doi:10.1524/zkri.1936.95.1.9.
- [2] J. A. A. Ketelaar, *Crystal Structure and Shape of Colloidal Particles of Vanadium Pentoxide*, Nature **137**, 316 (1936), doi:10.1038/137316a0.

Found in

- [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.

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