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

This structure previously used the label(s) `A5B2_oP14_59_a2f_f`. Calls to these addresses will be redirected here.

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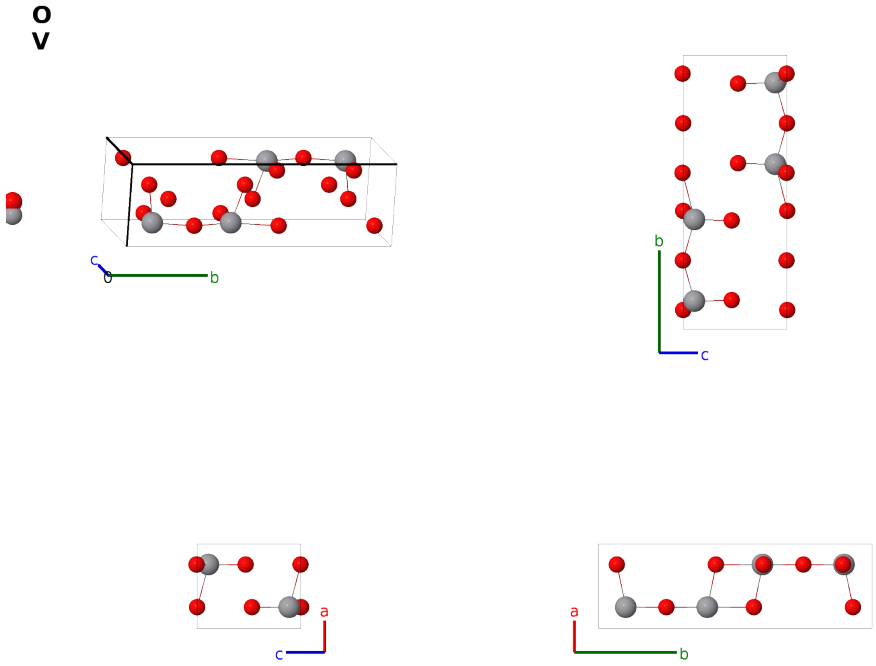
https://aflow.org/prototype-encyclopedia/KZMB

https://aflow.org/prototype-encyclopedia/A5B2_oP14_59_a2e_e-001

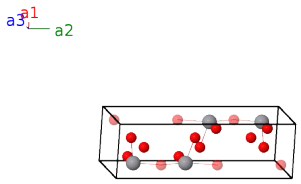



| | |
|---|---|
| **Prototype** | $O_5V_2$ |
| **AFLOW prototype label** | A5B2_oP14_59_a2e_e-001 |
| **Mineral name** | shcherbinaite |
| **ICSD** | 253957 |
| **CCDC** | 1553062 |
| **Pearson symbol** | oP14 |
| **Space group number** | 59 |
| **Space group symbol** | *Pmmn* |
| **AFLOW prototype command** | `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.
- The ICSD and CCDC entries are from (Lim, 2017). This ICSD is identical to the (Enjalbert, 1986) result, which has the ICSD number 60767 but is not recorded in the CCDC collection. If you have a subscription to the ICSD it can be found there.
- (Enjalbert, 1986) put the oxygen atoms on the (4f) (x,1/4,z) Wyckoff positions. The AFLOW prototype label protocol rotates the crystal by 90°, moving these atoms to the (4e) (1/4,y,z) sites.

**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] S.-C. Lim, J. Lee, H. H. Kwak, J. W. Heo, M. S. Chae, D. Ahn, Y. H. Jang, H. Lee, and S.-T. Hong, *Unraveling the Magnesium-Ion Intercalation Mechanism in Vanadium Pentoxide in a Wet Organic Electrolyte by Structural Determination*, Inorg. Chem. **56**, 7668–7678 (2017), doi:10.1021/acs.inorgchem.7b00204.

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

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