

# Valentinite ( $\text{Sb}_2\text{O}_3$ , $D5_{11}$ ) Structure: A3B2\_oP20\_56\_ce\_e-001

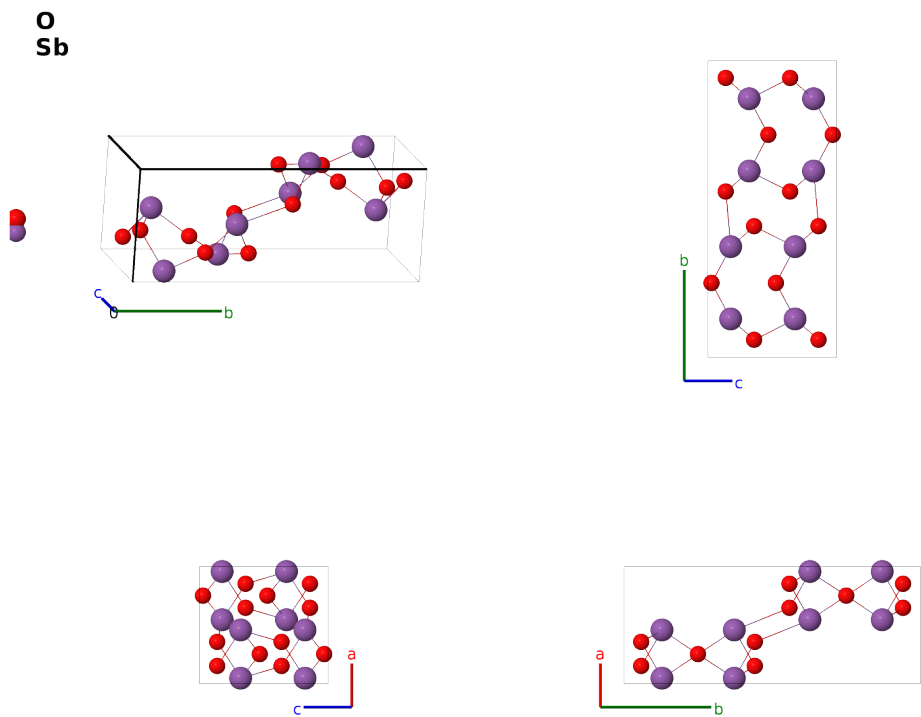
This structure previously used the label(s) **A3B2\_oP20\_56\_ce\_e**. Calls to these addresses will be redirected here.

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<https://afLOW.org/prototype-encyclopedia/HKUU>

[https://afLOW.org/prototype-encyclopedia/A3B2\\_oP20\\_56\\_ce\\_e-001](https://afLOW.org/prototype-encyclopedia/A3B2_oP20_56_ce_e-001)



|                                    |                         |
|------------------------------------|-------------------------|
| Prototype                          | $\text{O}_3\text{Sb}_2$ |
| AFLOW prototype label              | A3B2_oP20_56_ce_e-001   |
| <i>Strukturbericht</i> designation | $D5_{11}$               |
| Mineral name                       | valentinite             |
| ICSD                               | 2033                    |
| CCDC                               | 1591984                 |
| Pearson symbol                     | oP20                    |
| Space group number                 | 56                      |

|                         |                                                                                                   |
|-------------------------|---------------------------------------------------------------------------------------------------|
| Space group symbol      | $Pccn$                                                                                            |
| AFLOW prototype command | afLOW --proto=A3B2_oP20_56_ce_e-001<br>--params= $a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3$ |

- This is the orthorhombic form of  $\text{Sb}_2\text{O}_3$ . For the cubic form, see the senarmontite ( $D6_1$ ) page.

### Simple Orthorhombic primitive vectors



### Basis vectors

|                   | Lattice coordinates                                                                         |     | Cartesian coordinates                                                                                     | Wyckoff position | Atom type |
|-------------------|---------------------------------------------------------------------------------------------|-----|-----------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$                  | $=$ | $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$                 | (4c)             | O I       |
| $\mathbf{B}_2$    | $= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)             | O I       |
| $\mathbf{B}_3$    | $= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$                  | $=$ | $\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$                 | (4c)             | O I       |
| $\mathbf{B}_4$    | $= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)             | O I       |
| $\mathbf{B}_5$    | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$                                  | $=$ | $ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$                                   | (8e)             | O II      |
| $\mathbf{B}_6$    | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$  | (8e)             | O II      |
| $\mathbf{B}_7$    | $= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8e)             | O II      |
| $\mathbf{B}_8$    | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$   | (8e)             | O II      |
| $\mathbf{B}_9$    | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$                                 | $=$ | $-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$                                  | (8e)             | O II      |
| $\mathbf{B}_{10}$ | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$  | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$   | (8e)             | O II      |
| $\mathbf{B}_{11}$ | $= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$   | (8e)             | O II      |
| $\mathbf{B}_{12}$ | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8e)             | O II      |
| $\mathbf{B}_{13}$ | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                                  | $=$ | $ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                   | (8e)             | Sb I      |
| $\mathbf{B}_{14}$ | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$  | (8e)             | Sb I      |
| $\mathbf{B}_{15}$ | $= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8e)             | Sb I      |
| $\mathbf{B}_{16}$ | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$   | (8e)             | Sb I      |
| $\mathbf{B}_{17}$ | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$                                 | $=$ | $-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                                  | (8e)             | Sb I      |
| $\mathbf{B}_{18}$ | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$  | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$   | (8e)             | Sb I      |
| $\mathbf{B}_{19}$ | $= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$   | (8e)             | Sb I      |

$$\mathbf{B}_{20} = -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 = -a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8e) \quad \text{Sb I}$$

## References

- [1] C. Svensson, *The crystal structure of orthorhombic antimony trioxide,  $\text{Sb}_2\text{O}_3$* , Acta Crystallogr. Sect. B **30**, 458–461 (1974), doi:10.1107/S0567740874002986.

## First cited in

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