

# Blossite ( $\alpha$ -Cu<sub>2</sub>V<sub>2</sub>O<sub>7</sub>) Structure: A2B7C2\_oF88\_43\_b\_a3b\_b-001

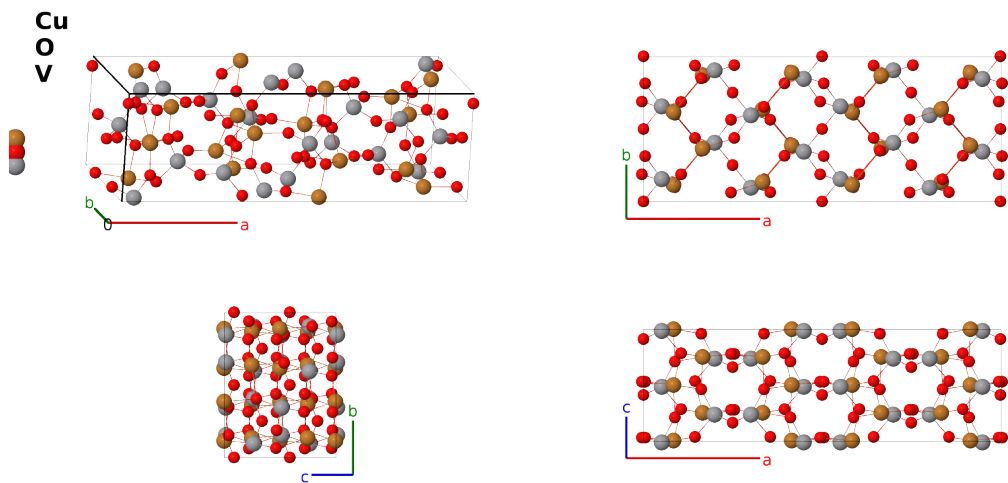
This structure previously used the label(s) **A2B7C2\_oF88\_43\_b\_a3b\_b**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/D9YZ>

[https://aflow.org/prototype-encyclopedia/A2B7C2\\_oF88\\_43\\_b\\_a3b\\_b-001](https://aflow.org/prototype-encyclopedia/A2B7C2_oF88_43_b_a3b_b-001)



|                         |                                                                                                                                                                                                                                                                                                              |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | Cu <sub>2</sub> O <sub>7</sub> V <sub>2</sub>                                                                                                                                                                                                                                                                |
| AFLOW prototype label   | A2B7C2_oF88_43_b_a3b_b-001                                                                                                                                                                                                                                                                                   |
| Mineral name            | blossite                                                                                                                                                                                                                                                                                                     |
| ICSD                    | 1831                                                                                                                                                                                                                                                                                                         |
| CCDC                    | 1591804                                                                                                                                                                                                                                                                                                      |
| Pearson symbol          | oF88                                                                                                                                                                                                                                                                                                         |
| Space group number      | 43                                                                                                                                                                                                                                                                                                           |
| Space group symbol      | <i>Fdd2</i>                                                                                                                                                                                                                                                                                                  |
| AFLOW prototype command | <pre>aflow --proto=A2B7C2_oF88_43_b_a3b_b-001       --params=a,b/a,c/a,z<sub>1</sub>,x<sub>2</sub>,y<sub>2</sub>,z<sub>2</sub>,x<sub>3</sub>,y<sub>3</sub>,z<sub>3</sub>,x<sub>4</sub>,y<sub>4</sub>,z<sub>4</sub>,x<sub>5</sub>,y<sub>5</sub>,z<sub>5</sub>,x<sub>6</sub>,y<sub>6</sub>,z<sub>6</sub></pre> |

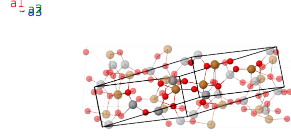
- This structure was given the name “blossite” by (Robinson, 1987).
- Space group *Fdd2* #43 does not fix the  $z = 0$  plane. We do this by setting  $z_2 = 3/4$  for the copper atom.

## Face-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$



## Basis vectors

|                   | Lattice<br>coordinates                                                                                                                          |     | Cartesian<br>coordinates                                                                                                 | Wyckoff<br>position | Atom<br>type |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|-----|--------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$                                                                                      | $=$ | $c z_1 \hat{\mathbf{z}}$                                                                                                 | (8a)                | O I          |
| $\mathbf{B}_2$    | $= (z_1 + \frac{1}{4}) \mathbf{a}_1 + (z_1 + \frac{1}{4}) \mathbf{a}_2 - (z_1 - \frac{1}{4}) \mathbf{a}_3$                                      | $=$ | $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$                  | (8a)                | O I          |
| $\mathbf{B}_3$    | $= (-x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3$                                           | $=$ | $a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$                                               | (16b)               | Cu I         |
| $\mathbf{B}_4$    | $= (x_2 - y_2 + z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3$                                           | $=$ | $-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$                                              | (16b)               | Cu I         |
| $\mathbf{B}_5$    | $= -(x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_1 + (x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_2 + (x_2 - y_2 - z_2 + \frac{1}{4}) \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$  | (16b)               | Cu I         |
| $\mathbf{B}_6$    | $= (x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_1 - (x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_2 - (x_2 - y_2 + z_2 - \frac{1}{4}) \mathbf{a}_3$  | $=$ | $-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$ | (16b)               | Cu I         |
| $\mathbf{B}_7$    | $= (-x_3 + y_3 + z_3) \mathbf{a}_1 + (x_3 - y_3 + z_3) \mathbf{a}_2 + (x_3 + y_3 - z_3) \mathbf{a}_3$                                           | $=$ | $a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$                                               | (16b)               | O II         |
| $\mathbf{B}_8$    | $= (x_3 - y_3 + z_3) \mathbf{a}_1 + (-x_3 + y_3 + z_3) \mathbf{a}_2 - (x_3 + y_3 + z_3) \mathbf{a}_3$                                           | $=$ | $-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$                                              | (16b)               | O II         |
| $\mathbf{B}_9$    | $= -(x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_1 + (x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 - y_3 - z_3 + \frac{1}{4}) \mathbf{a}_3$ | $=$ | $a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$  | (16b)               | O II         |
| $\mathbf{B}_{10}$ | $= (x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_1 - (x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_2 - (x_3 - y_3 + z_3 - \frac{1}{4}) \mathbf{a}_3$  | $=$ | $-a(x_3 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$ | (16b)               | O II         |
| $\mathbf{B}_{11}$ | $= (-x_4 + y_4 + z_4) \mathbf{a}_1 + (x_4 - y_4 + z_4) \mathbf{a}_2 + (x_4 + y_4 - z_4) \mathbf{a}_3$                                           | $=$ | $a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$                                               | (16b)               | O III        |
| $\mathbf{B}_{12}$ | $= (x_4 - y_4 + z_4) \mathbf{a}_1 + (-x_4 + y_4 + z_4) \mathbf{a}_2 - (x_4 + y_4 + z_4) \mathbf{a}_3$                                           | $=$ | $-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$                                              | (16b)               | O III        |
| $\mathbf{B}_{13}$ | $= -(x_4 + y_4 - z_4 - \frac{1}{4}) \mathbf{a}_1 + (x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + (x_4 - y_4 - z_4 + \frac{1}{4}) \mathbf{a}_3$ | $=$ | $a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$  | (16b)               | O III        |

$$\begin{aligned}
\mathbf{B}_{14} &= \begin{pmatrix} x_4 + y_4 + z_4 + \frac{1}{4} \\ x_4 + y_4 - z_4 - \frac{1}{4} \\ x_4 - y_4 + z_4 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - &= -a \left(x_4 - \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16b) & \text{O III} \\
\mathbf{B}_{15} &= \begin{pmatrix} -x_5 + y_5 + z_5 \\ x_5 - y_5 + z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{16} &= \begin{pmatrix} x_5 - y_5 + z_5 \\ -x_5 + y_5 + z_5 \\ x_5 + y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + &= -ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{17} &= \begin{pmatrix} -(x_5 + y_5 - z_5 - \frac{1}{4}) \\ x_5 + y_5 + z_5 + \frac{1}{4} \\ x_5 - y_5 - z_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + &= a \left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{18} &= \begin{pmatrix} x_5 + y_5 + z_5 + \frac{1}{4} \\ x_5 + y_5 - z_5 - \frac{1}{4} \\ x_5 - y_5 + z_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - &= -a \left(x_5 - \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{19} &= \begin{pmatrix} -x_6 + y_6 + z_6 \\ x_6 - y_6 + z_6 \\ x_6 + y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + &= ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16b) & \text{V I} \\
\mathbf{B}_{20} &= \begin{pmatrix} x_6 - y_6 + z_6 \\ -x_6 + y_6 + z_6 \\ x_6 + y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + &= -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16b) & \text{V I} \\
\mathbf{B}_{21} &= \begin{pmatrix} -(x_6 + y_6 - z_6 - \frac{1}{4}) \\ x_6 + y_6 + z_6 + \frac{1}{4} \\ x_6 - y_6 - z_6 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + &= a \left(x_6 + \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_6 - \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16b) & \text{V I} \\
\mathbf{B}_{22} &= \begin{pmatrix} x_6 + y_6 + z_6 + \frac{1}{4} \\ x_6 + y_6 - z_6 - \frac{1}{4} \\ x_6 - y_6 + z_6 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - &= -a \left(x_6 - \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_6 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16b) & \text{V I}
\end{aligned}$$

## References

- [1] C. Calvo and R. Faggiani,  *$\alpha$  Cupric Divanadate*, Acta Cryst. **31**, 603–605 (1975), doi:10.1107/S0567740875003354.
- [2] P. D. Robinson, J. M. Hughs, and M. L. Malinconico, *Blossite,  $\alpha$ -Cu<sub>2</sub><sup>2+</sup>V<sub>2</sub><sup>5+</sup>O<sub>7</sub>, an new fumarolic sublimate from Izalco volcano, El Salvador*, Am. Mineral. **72**, 397–400 (1987).

## Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

## First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.