Blossite (α-$Cu_2V_2O_7$) Structure: A2B7C2_oF88_43_b_a3b_b-001

This structure originally had the label `A2B7C2_oF88_43_b_a3b_b`. Calls to that address will be redirected here.

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https://aflow.org/p/D9YZ

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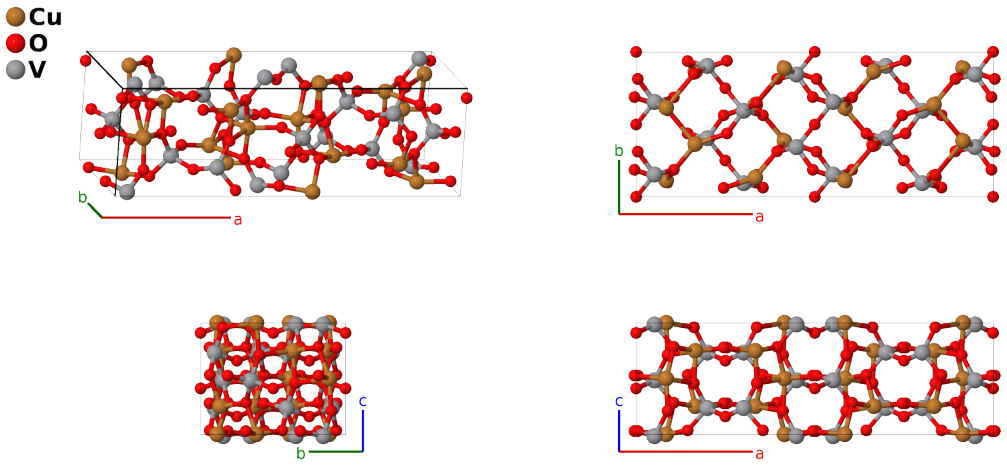
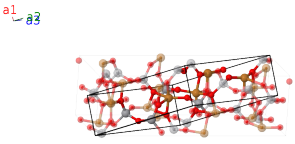


Prototype	$Cu_2O_7V_2$
AFLOW prototype label	A2B7C2_oF88_43_b_a3b_b-001
Mineral name	blossite
ICSD	1831
Pearson symbol	oF88
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=A2B7C2_oF88_43_b_a3b_b-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- 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 coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{4}\right)\,\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_3}$	=	$(-x_2+y_2+z_2)\,\mathbf{a}_1 + (x_2-y_2+z_2)\,\mathbf{a}_2 + (x_2+y_2-z_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Cu I
$\mathbf{B_4}$	=	$(x_2-y_2+z_2)\,\mathbf{a}_1 + (-x_2+y_2+z_2)\,\mathbf{a}_2 - (x_2+y_2+z_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Cu I
$\mathbf{B_5}$	=	$-\left(x_2+y_2-z_2-\frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_2+y_2+z_2+\frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_2-y_2-z_2+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Cu I
$\mathbf{B_6}$	=	$\left(x_2+y_2+z_2+\frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2+y_2-z_2-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2-y_2+z_2-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Cu I
$\mathbf{B_7}$	=	$(-x_3+y_3+z_3)\,\mathbf{a}_1 + (x_3-y_3+z_3)\,\mathbf{a}_2 + (x_3+y_3-z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_8}$	=	$(x_3-y_3+z_3)\,\mathbf{a}_1 + (-x_3+y_3+z_3)\,\mathbf{a}_2 - (x_3+y_3+z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_9}$	=	$-\left(x_3+y_3-z_3-\frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_3+y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_3-y_3-z_3+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_{10}}$	=	$\left(x_3+y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3+y_3-z_3-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3-y_3+z_3-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	O II
$\mathbf{B_{11}}$	=	$(-x_4+y_4+z_4)\,\mathbf{a}_1 + (x_4-y_4+z_4)\,\mathbf{a}_2 + (x_4+y_4-z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16b)	O III
$\mathbf{B_{12}}$	=	$(x_4-y_4+z_4)\,\mathbf{a}_1 + (-x_4+y_4+z_4)\,\mathbf{a}_2 - (x_4+y_4+z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16b)	O III
$\mathbf{B_{13}}$	=	$-\left(x_4+y_4-z_4-\frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_4+y_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_4-y_4-z_4+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	O III
$\mathbf{B_{14}}$	=	$\left(x_4+y_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_4+y_4-z_4-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_4-y_4+z_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	O III
$\mathbf{B_{15}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1 + (x_5-y_5+z_5)\,\mathbf{a}_2 + (x_5+y_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16b)	O IV
$\mathbf{B_{16}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1 + (-x_5+y_5+z_5)\,\mathbf{a}_2 - (x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16b)	O IV

$\mathbf{B_{17}}$	=	$-\left(x_5+y_5-z_5-\frac{1}{4}\right)\,\mathbf{a}_1+\left(x_5+y_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_5-y_5-z_5+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}-b\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	O IV
$\mathbf{B_{18}}$	=	$\left(x_5+y_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_1-\left(x_5+y_5-z_5-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_5-y_5+z_5-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+b\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	O IV
$\mathbf{B_{19}}$	=	$(-x_6+y_6+z_6)\,\mathbf{a}_1+(x_6-y_6+z_6)\,\mathbf{a}_2+(x_6+y_6-z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16b)	V I
$\mathbf{B_{20}}$	=	$(x_6-y_6+z_6)\,\mathbf{a}_1+(-x_6+y_6+z_6)\,\mathbf{a}_2-(x_6+y_6+z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16b)	V I
$\mathbf{B_{21}}$	=	$-\left(x_6+y_6-z_6-\frac{1}{4}\right)\,\mathbf{a}_1+\left(x_6+y_6+z_6+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_6-y_6-z_6+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{4}\right)\,\hat{\mathbf{x}}-b\left(y_6-\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	V I
$\mathbf{B_{22}}$	=	$\left(x_6+y_6+z_6+\frac{1}{4}\right)\,\mathbf{a}_1-\left(x_6+y_6-z_6-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_6-y_6+z_6-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{4}\right)\,\hat{\mathbf{x}}+b\left(y_6+\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	V I

References

[1] C. Calvo and R. Faggiani, *α Cupric Divanadate*, Acta Cryst. **31**, 603–605 (1975), doi:10.1107/S0567740875003354.

[2] P. D. Robinson, J. M. Hughs, and M. L. Malinconico, *Blossite, α-$Cu_2^{2+}V_2^{5+}O_7$, an new fumarlolic 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).