Kapellasite ($Cu_3Zn(OH)_6Cl_2$) Structure: A2B3C6D_hP12_164_d_e_i_a-001

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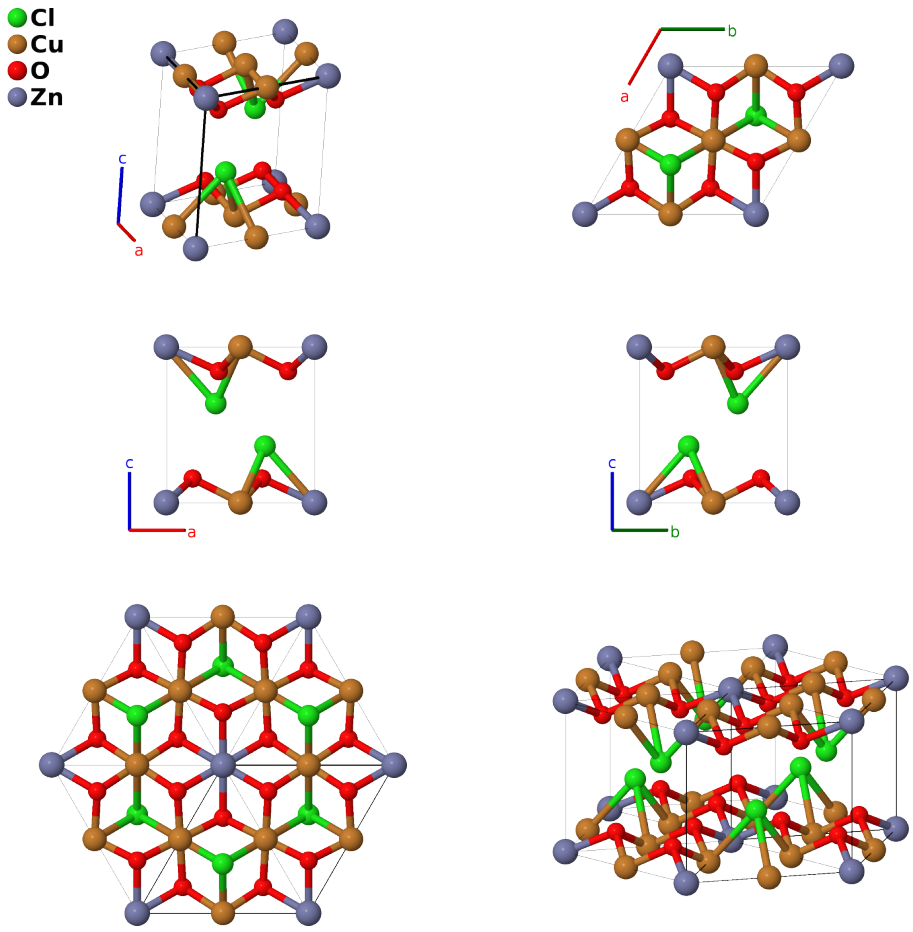
https://aflow.org/p/K216

https://aflow.org/p/A2B3C6D_hP12_164_d_e_i_a-001

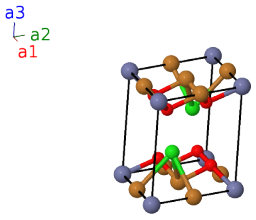


Prototype	$Cl_2Cu_3(OH)_6Zn$
AFLOW prototype label	A2B3C6D_hP12_164_d_e_i_a-001
Mineral name	kapellasite
ICSD	157870
Pearson symbol	hP12
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A2B3C6D_hP12_164_d_e_i_a-001 --params=`$a, c/a, z_2, x_4, z_4$

- Approximately 3% of the OH radicals are replace by chlorine atoms. We use "O" to represent all the OH/Cl sites.
- (Krause, 2006) placed the zinc atom at the (1b) Wyckoff position, (0 0 1/2). We shifted the origin of the structure so that the zinc atom is at the (1a) Wyckoff site.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Zn I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	Cl I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	Cl I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3e)	Cu I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3e)	Cu I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3e)	Cu I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_9}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{11}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6i)	O I

References

[1] W. Krause, H.-J. Bernhardt, R. S. W. Braithwaite, U. Kolitsch, and R. Pritchard, *Kapellasite, $Cu_3Zn(OH)_6Cl_2$, a new mineral from Lavrion, Greece, and its crystal structure*, Mineral. Mag. **70**, 329–340 (2006), doi:10.1180/0026461067030336.