$YCu_3(OH)_6Cl_3$ Structure: ABC2D2E_hP21_164_bd_e_i_i_ac-001

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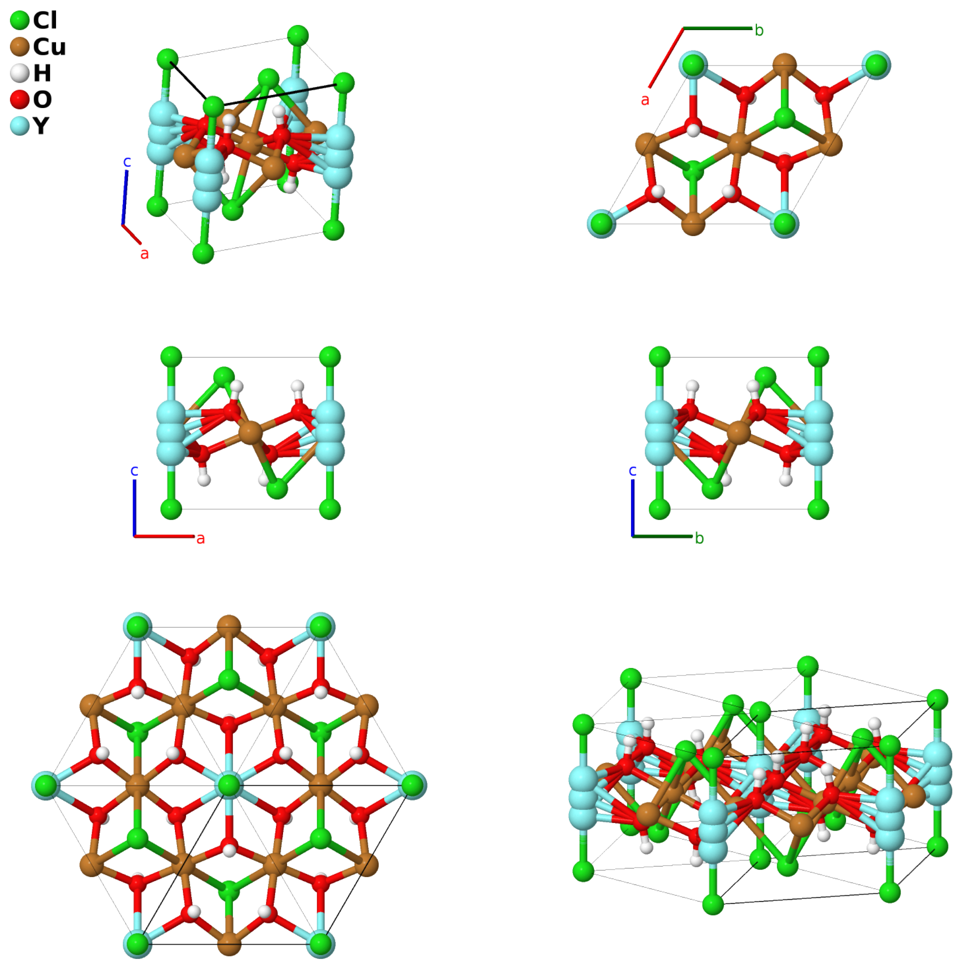
https://aflow.org/p/1PRT

https://aflow.org/p/ABC2D2E_hP21_164_bd_e_i_i_ac-001

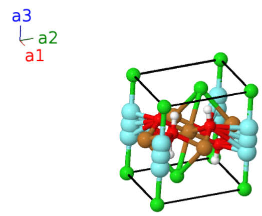


Prototype	$Cl_3Cu_3H_6O_6Y$
AFLOW prototype label	ABC2D2E_hP21_164_bd_e_i_i_ac-001
ICSD	32385
Pearson symbol	hP21
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=ABC2D2E_hP21_164_bd_e_i_i_ac-001` `--params=`$a, c/a, z_3, z_4, x_6, z_6, x_7, z_7$

- The Y-I (1b) site is occupied 95% of the time, with the other 5% of the yttrium atoms distributed on the Y-II (2c) sites. Thus only one of the triplet of yttrium atoms in the picture will be occupied at any one time, and most of the time it will be the central atom.
- (Zorko, 2019) give positions for the oxygen atoms which are not consistent with the (6i) Wyckoff positions. As the difference is slight, we assume that the x and z coordinates are correct and generate the y coordinate from the symmetry operations for the (6i) positions.
- The ICSD entry for this paper instead tries to solve the problem by placing the oxygen atoms on a half-filled (12j) site.

Trigonal (Hexagonal) primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Y I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Cl I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2c)	Y II
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2c)	Y II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	Cl II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	Cl II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3e)	Cu I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3e)	Cu I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3e)	Cu I
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	H I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	H I
$\mathbf{B_{12}}$	=	$-2x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	H I
$\mathbf{B_{13}}$	=	$-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\sqrt{3}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	H I
$\mathbf{B_{14}}$	=	$2x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	H I
$\mathbf{B_{15}}$	=	$-x_6\,\mathbf{a}_1 - 2x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	H I
$\mathbf{B_{16}}$	=	$x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\sqrt{3}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 + 2x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{18}}$	=	$-2x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{19}}$	=	$-x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\sqrt{3}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{20}}$	=	$2x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{21}}$	=	$-x_7\,\mathbf{a}_1 - 2x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6i)	O I

References

[1] A. Zorko, M. Pregelj, M. Gomilšek, M. Klanjšek, O. Zaharko, W. Sun, and J.-X. Mi, *Negative-vector-chirality 120° spin structure in the defect- and distortion-free quantum kagome antiferromagnet* $YCu_3(OH)_6Cl_3$, Phys. Rev. B **100**, 144420 (2019), doi:10.1103/PhysRevB.100.144420.