$Y_3Cu_9(OH)_{19}Cl_8$ Structure: A8B9C24D19E3_hR63_148_cf_df_4f_a3f_bc-001

https://aflow.org/p/GGPS

https://aflow.org/p/A8B9C24D19E3_hR63_148_cf_df_4f_a3f_bc-001
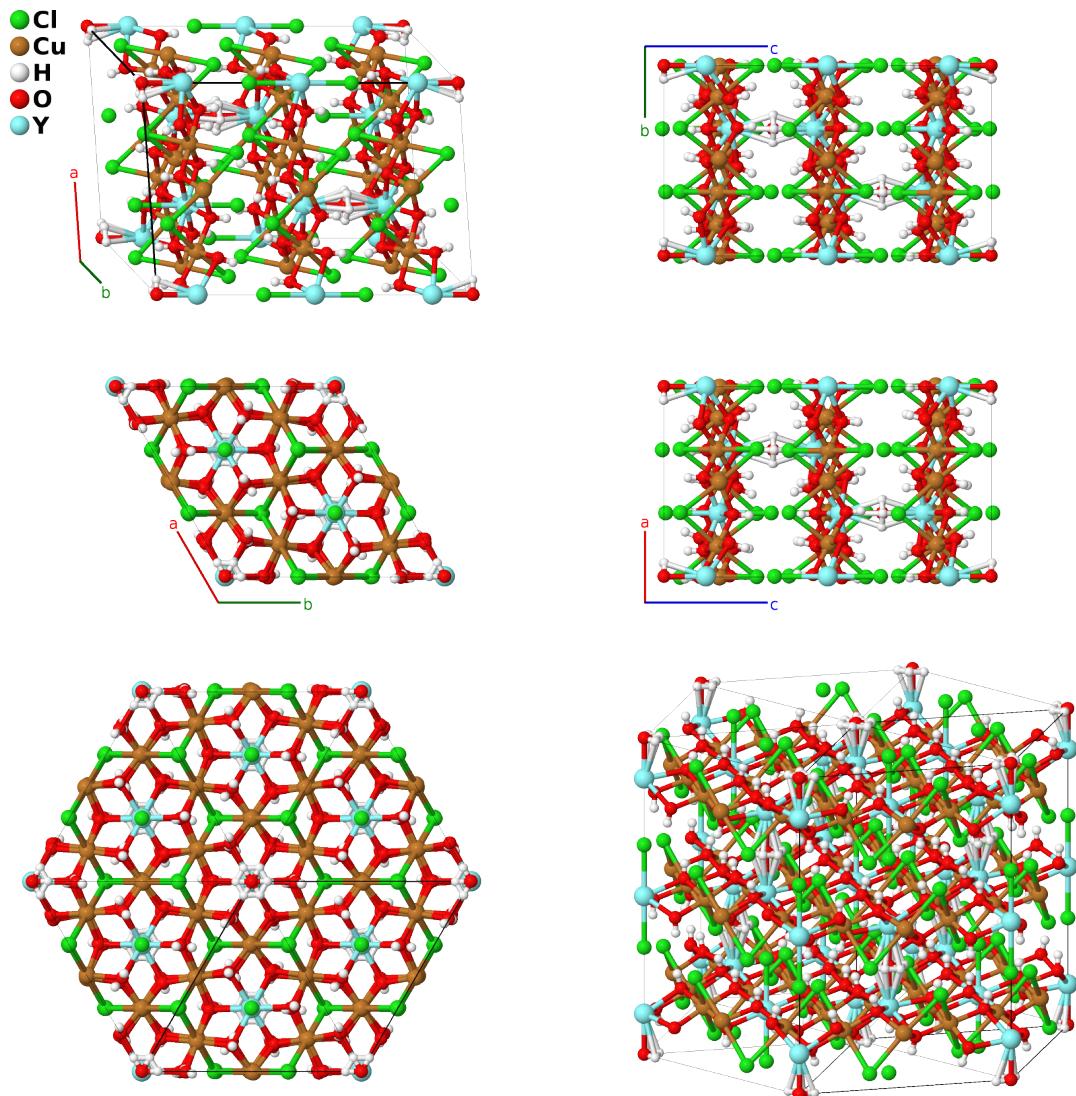
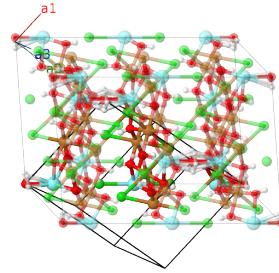|	
Prototype	$Cl_3Cu_9H_{19}O_{19}Y_3$
AFLOW prototype label	A8B9C24D19E3_hR63_148_cf_df_4f_a3f_bc-001
CCDC	1532410
Pearson symbol	hR63
Space group number	148
Space group symbol	$R\bar{3}$

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AFLOW prototype command   `aflow --proto=A8B9C24D19E3_hR63_148_cf_df_4f_a3f_bc-001`
                    `--params=`$a, c/a, x_3, x_4, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11},$
          $z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

- Only 1/6 of the sites allocated for H-I (18f) are occupied. These H-I hydrogen sites are arranged in hexagons around the oxygen O-I atoms. As the separation between them is only 0.82Å it is likely that the atoms are all in one of the two possible isosceles triangles surrounding each oxygen.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	O I
$\mathbf{B_2}$	=	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	=	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Y I
$\mathbf{B_3}$	=	$x_3\mathbf{a_1} + x_3\mathbf{a_2} + x_3\mathbf{a_3}$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Cl I
$\mathbf{B_4}$	=	$-x_3\mathbf{a_1} - x_3\mathbf{a_2} - x_3\mathbf{a_3}$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Cl I
$\mathbf{B_5}$	=	$x_4\mathbf{a_1} + x_4\mathbf{a_2} + x_4\mathbf{a_3}$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Y II
$\mathbf{B_6}$	=	$-x_4\mathbf{a_1} - x_4\mathbf{a_2} - x_4\mathbf{a_3}$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Y II
$\mathbf{B_7}$	=	$\tfrac{1}{2}\mathbf{a_1}$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Cu I
$\mathbf{B_8}$	=	$\tfrac{1}{2}\mathbf{a_2}$	=	$\tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Cu I
$\mathbf{B_9}$	=	$\tfrac{1}{2}\mathbf{a_3}$	=	$-\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Cu I
$\mathbf{B_{10}}$	=	$x_6\mathbf{a_1} + y_6\mathbf{a_2} + z_6\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{11}}$	=	$z_6\mathbf{a_1} + x_6\mathbf{a_2} + y_6\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{12}}$	=	$y_6\mathbf{a_1} + z_6\mathbf{a_2} + x_6\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{13}}$	=	$-x_6\mathbf{a_1} - y_6\mathbf{a_2} - z_6\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{14}}$	=	$-z_6\mathbf{a_1} - x_6\mathbf{a_2} - y_6\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{15}}$	=	$-y_6\mathbf{a_1} - z_6\mathbf{a_2} - x_6\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	Cl II
$\mathbf{B_{16}}$	=	$x_7\mathbf{a_1} + y_7\mathbf{a_2} + z_7\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	Cu II
$\mathbf{B_{17}}$	=	$z_7\mathbf{a_1} + x_7\mathbf{a_2} + y_7\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}}$	(6f)	Cu II

$$\mathbf{B_{18}} = y_7\,\mathbf{a_1} + z_7\,\mathbf{a_2} + x_7\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_7 - y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_7 + y_7 - 2z_7\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{Cu II}$$

$$\mathbf{B_{19}} = -x_7\,\mathbf{a_1} - y_7\,\mathbf{a_2} - z_7\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_7 - z_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_7 - 2y_7 + z_7\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{Cu II}$$

$$\mathbf{B_{20}} = -z_7\,\mathbf{a_1} - x_7\,\mathbf{a_2} - y_7\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_7 - z_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_7 - y_7 - z_7\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{Cu II}$$

$$\mathbf{B_{21}} = -y_7\,\mathbf{a_1} - z_7\,\mathbf{a_2} - x_7\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_7 - y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_7 + y_7 - 2z_7\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{Cu II}$$

$$\mathbf{B_{22}} = x_8\,\mathbf{a_1} + y_8\,\mathbf{a_2} + z_8\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_8 - z_8\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_8 - 2y_8 + z_8\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H I}$$

$$\mathbf{B_{23}} = z_8\,\mathbf{a_1} + x_8\,\mathbf{a_2} + y_8\,\mathbf{a_3} = -\tfrac{1}{2}a\left(y_8 - z_8\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_8 - y_8 - z_8\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H I}$$

$$\mathbf{B_{24}} = y_8\,\mathbf{a_1} + z_8\,\mathbf{a_2} + x_8\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_8 - y_8\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_8 + y_8 - 2z_8\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H I}$$

$$\mathbf{B_{25}} = -x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} - z_8\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_8 - z_8\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_8 - 2y_8 + z_8\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H I}$$

$$\mathbf{B_{26}} = -z_8\,\mathbf{a_1} - x_8\,\mathbf{a_2} - y_8\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_8 - z_8\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_8 - y_8 - z_8\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H I}$$

$$\mathbf{B_{27}} = -y_8\,\mathbf{a_1} - z_8\,\mathbf{a_2} - x_8\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_8 - y_8\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_8 + y_8 - 2z_8\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H I}$$

$$\mathbf{B_{28}} = x_9\,\mathbf{a_1} + y_9\,\mathbf{a_2} + z_9\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_9 - z_9\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_9 - 2y_9 + z_9\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H II}$$

$$\mathbf{B_{29}} = z_9\,\mathbf{a_1} + x_9\,\mathbf{a_2} + y_9\,\mathbf{a_3} = -\tfrac{1}{2}a\left(y_9 - z_9\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_9 - y_9 - z_9\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H II}$$

$$\mathbf{B_{30}} = y_9\,\mathbf{a_1} + z_9\,\mathbf{a_2} + x_9\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_9 - y_9\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_9 + y_9 - 2z_9\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H II}$$

$$\mathbf{B_{31}} = -x_9\,\mathbf{a_1} - y_9\,\mathbf{a_2} - z_9\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_9 - z_9\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_9 - 2y_9 + z_9\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H II}$$

$$\mathbf{B_{32}} = -z_9\,\mathbf{a_1} - x_9\,\mathbf{a_2} - y_9\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_9 - z_9\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_9 - y_9 - z_9\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H II}$$

$$\mathbf{B_{33}} = -y_9\,\mathbf{a_1} - z_9\,\mathbf{a_2} - x_9\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_9 - y_9\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_9 + y_9 - 2z_9\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H II}$$

$$\mathbf{B_{34}} = x_{10}\,\mathbf{a_1} + y_{10}\,\mathbf{a_2} + z_{10}\,\mathbf{a_3} = \tfrac{1}{2}a\left(x_{10} - z_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{10} - 2y_{10} + z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H III}$$

$$\mathbf{B_{35}} = z_{10}\,\mathbf{a_1} + x_{10}\,\mathbf{a_2} + y_{10}\,\mathbf{a_3} = -\tfrac{1}{2}a\left(y_{10} - z_{10}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{10} - y_{10} - z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H III}$$

$$\mathbf{B_{36}} = y_{10}\,\mathbf{a_1} + z_{10}\,\mathbf{a_2} + x_{10}\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_{10} - y_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{10} + y_{10} - 2z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H III}$$

$$\mathbf{B_{37}} = -x_{10}\,\mathbf{a_1} - y_{10}\,\mathbf{a_2} - z_{10}\,\mathbf{a_3} = -\tfrac{1}{2}a\left(x_{10} - z_{10}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_{10} - 2y_{10} + z_{10}\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H III}$$

$$\mathbf{B_{38}} = -z_{10}\,\mathbf{a_1} - x_{10}\,\mathbf{a_2} - y_{10}\,\mathbf{a_3} = \tfrac{1}{2}a\left(y_{10} - z_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_{10} - y_{10} - z_{10}\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad (6f) \qquad \text{H III}$$

$$\mathbf{B_{39}} = -y_{10}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_2 - x_{10}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(x_{10} + y_{10} - 2z_{10})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{10} + y_{10} + z_{10})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H III}$$

$$\mathbf{B_{40}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(x_{11} - z_{11})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(x_{11} - 2y_{11} + z_{11})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H IV}$$

$$\mathbf{B_{41}} = z_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + y_{11}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(y_{11} - z_{11})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(2x_{11} - y_{11} - z_{11})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H IV}$$

$$\mathbf{B_{42}} = y_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + x_{11}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(x_{11} - y_{11})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(x_{11} + y_{11} - 2z_{11})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H IV}$$

$$\mathbf{B_{43}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(x_{11} - z_{11})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(x_{11} - 2y_{11} + z_{11})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H IV}$$

$$\mathbf{B_{44}} = -z_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - y_{11}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(y_{11} - z_{11})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(2x_{11} - y_{11} - z_{11})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H IV}$$

$$\mathbf{B_{45}} = -y_{11}\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_2 - x_{11}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(x_{11} - y_{11})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(x_{11} + y_{11} - 2z_{11})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{H IV}$$

$$\mathbf{B_{46}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(x_{12} - 2y_{12} + z_{12})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O II}$$

$$\mathbf{B_{47}} = z_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + y_{12}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(y_{12} - z_{12})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(2x_{12} - y_{12} - z_{12})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O II}$$

$$\mathbf{B_{48}} = y_{12}\,\mathbf{a}_1 + z_{12}\,\mathbf{a}_2 + x_{12}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(x_{12} - y_{12})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(x_{12} + y_{12} - 2z_{12})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O II}$$

$$\mathbf{B_{49}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(x_{12} - 2y_{12} + z_{12})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O II}$$

$$\mathbf{B_{50}} = -z_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 - y_{12}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(y_{12} - z_{12})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(2x_{12} - y_{12} - z_{12})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O II}$$

$$\mathbf{B_{51}} = -y_{12}\,\mathbf{a}_1 - z_{12}\,\mathbf{a}_2 - x_{12}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(x_{12} - y_{12})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(x_{12} + y_{12} - 2z_{12})\,\hat{\mathbf{y}} -\\&\tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O II}$$

$$\mathbf{B_{52}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \begin{aligned}&\tfrac{1}{2}a\,(x_{13} - z_{13})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(x_{13} - 2y_{13} + z_{13})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{13} + y_{13} + z_{13})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O III}$$

$$\mathbf{B_{53}} = z_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + y_{13}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(y_{13} - z_{13})\,\hat{\mathbf{x}} +\\&\tfrac{\sqrt{3}}{6}a\,(2x_{13} - y_{13} - z_{13})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{13} + y_{13} + z_{13})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O III}$$

$$\mathbf{B_{54}} = y_{13}\,\mathbf{a}_1 + z_{13}\,\mathbf{a}_2 + x_{13}\,\mathbf{a}_3 = \begin{aligned}&-\tfrac{1}{2}a\,(x_{13} - y_{13})\,\hat{\mathbf{x}} -\\&\tfrac{\sqrt{3}}{6}a\,(x_{13} + y_{13} - 2z_{13})\,\hat{\mathbf{y}} +\\&\tfrac{1}{3}c\,(x_{13} + y_{13} + z_{13})\,\hat{\mathbf{z}}\end{aligned} \quad\text{(6f)}\qquad\text{O III}$$

$$\mathbf{B_{55}} = -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = \begin{aligned} &-\tfrac{1}{2}a\left(x_{13}-z_{13}\right)\hat{\mathbf{x}} + \\ &\tfrac{\sqrt{3}}{6}a\left(x_{13}-2y_{13}+z_{13}\right)\hat{\mathbf{y}} - \\ &\tfrac{1}{3}c\left(x_{13}+y_{13}+z_{13}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O III}$$

$$\mathbf{B_{56}} = -z_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 - y_{13}\,\mathbf{a}_3 = \begin{aligned} &\tfrac{1}{2}a\left(y_{13}-z_{13}\right)\hat{\mathbf{x}} - \\ &\tfrac{\sqrt{3}}{6}a\left(2x_{13}-y_{13}-z_{13}\right)\hat{\mathbf{y}} - \\ &\tfrac{1}{3}c\left(x_{13}+y_{13}+z_{13}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O III}$$

$$\mathbf{B_{57}} = -y_{13}\,\mathbf{a}_1 - z_{13}\,\mathbf{a}_2 - x_{13}\,\mathbf{a}_3 = \begin{aligned} &\tfrac{1}{2}a\left(x_{13}-y_{13}\right)\hat{\mathbf{x}} + \\ &\tfrac{\sqrt{3}}{6}a\left(x_{13}+y_{13}-2z_{13}\right)\hat{\mathbf{y}} - \\ &\tfrac{1}{3}c\left(x_{13}+y_{13}+z_{13}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O III}$$

$$\mathbf{B_{58}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \begin{aligned} &\tfrac{1}{2}a\left(x_{14}-z_{14}\right)\hat{\mathbf{x}} - \\ &\tfrac{\sqrt{3}}{6}a\left(x_{14}-2y_{14}+z_{14}\right)\hat{\mathbf{y}} + \\ &\tfrac{1}{3}c\left(x_{14}+y_{14}+z_{14}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O IV}$$

$$\mathbf{B_{59}} = z_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + y_{14}\,\mathbf{a}_3 = \begin{aligned} &-\tfrac{1}{2}a\left(y_{14}-z_{14}\right)\hat{\mathbf{x}} + \\ &\tfrac{\sqrt{3}}{6}a\left(2x_{14}-y_{14}-z_{14}\right)\hat{\mathbf{y}} + \\ &\tfrac{1}{3}c\left(x_{14}+y_{14}+z_{14}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O IV}$$

$$\mathbf{B_{60}} = y_{14}\,\mathbf{a}_1 + z_{14}\,\mathbf{a}_2 + x_{14}\,\mathbf{a}_3 = \begin{aligned} &-\tfrac{1}{2}a\left(x_{14}-y_{14}\right)\hat{\mathbf{x}} - \\ &\tfrac{\sqrt{3}}{6}a\left(x_{14}+y_{14}-2z_{14}\right)\hat{\mathbf{y}} + \\ &\tfrac{1}{3}c\left(x_{14}+y_{14}+z_{14}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O IV}$$

$$\mathbf{B_{61}} = -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = \begin{aligned} &-\tfrac{1}{2}a\left(x_{14}-z_{14}\right)\hat{\mathbf{x}} + \\ &\tfrac{\sqrt{3}}{6}a\left(x_{14}-2y_{14}+z_{14}\right)\hat{\mathbf{y}} - \\ &\tfrac{1}{3}c\left(x_{14}+y_{14}+z_{14}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O IV}$$

$$\mathbf{B_{62}} = -z_{14}\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 - y_{14}\,\mathbf{a}_3 = \begin{aligned} &\tfrac{1}{2}a\left(y_{14}-z_{14}\right)\hat{\mathbf{x}} - \\ &\tfrac{\sqrt{3}}{6}a\left(2x_{14}-y_{14}-z_{14}\right)\hat{\mathbf{y}} - \\ &\tfrac{1}{3}c\left(x_{14}+y_{14}+z_{14}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O IV}$$

$$\mathbf{B_{63}} = -y_{14}\,\mathbf{a}_1 - z_{14}\,\mathbf{a}_2 - x_{14}\,\mathbf{a}_3 = \begin{aligned} &\tfrac{1}{2}a\left(x_{14}-y_{14}\right)\hat{\mathbf{x}} + \\ &\tfrac{\sqrt{3}}{6}a\left(x_{14}+y_{14}-2z_{14}\right)\hat{\mathbf{y}} - \\ &\tfrac{1}{3}c\left(x_{14}+y_{14}+z_{14}\right)\hat{\mathbf{z}} \end{aligned} \qquad (6f) \qquad \text{O IV}$$

References

[1] P. Puphal, M. Bolte, D. Sheptyakov, A. Pustogow, K. Kliemt, M. Dressel, M. Baenitze, and C. Krellner, *Strong magnetic frustration in $Y_3Cu_9(OH)_{19}Cl_8$: a distorted kagome antiferromagnet*, J. Mater. Chem. C **5**, 2629–2635 (2017), doi:10.1039/C6TC05110C.