Approximate $Cu_3(TeO_4)(SO_4)\cdot H_2O$ Structure: A3B2C9DE_oP64_62_cd_2c_5c2d_c_c-001

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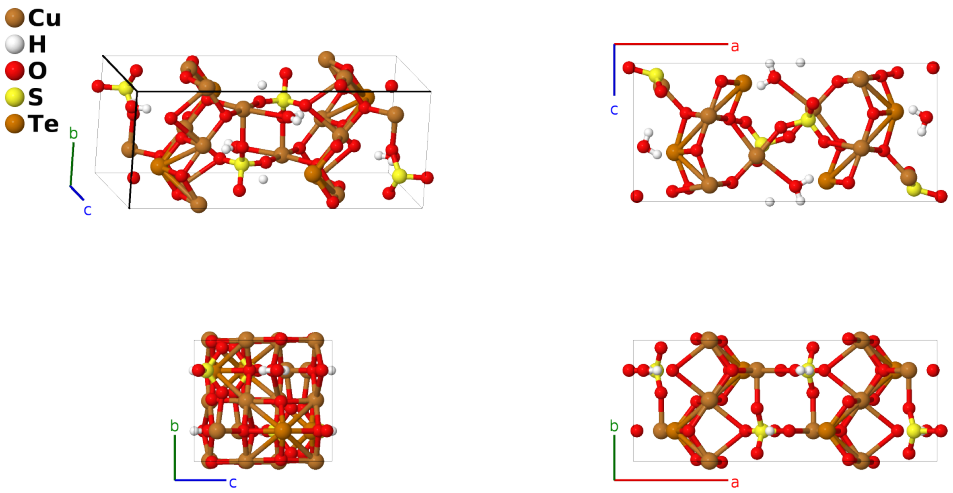
https://aflow.org/p/WLK8

https://aflow.org/p/A3B2C9DE_oP64_62_cd_2c_5c2d_c_c-001

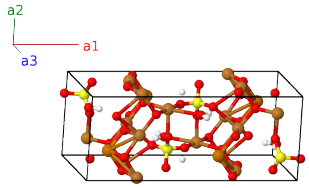


Prototype	$Cu_3H_4O_{10}STe$
AFLOW prototype label	A3B2C9DE_oP64_62_cd_2c_5c2d_c_c-001
ICSD	135754
Pearson symbol	oP64
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A3B2C9DE_oP64_62_cd_2c_5c2d_c_c-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

- This is an approximation of the structure proposed by (Wang, 2021). In their work, the water molecule formed by the H-I, H-II and O-V atoms can have two slightly different positions, with the two possible oxygen positions only 0.42Å apart, and two of the possible 4 hydrogen sites only 0.08Å apart. These short distances cannot be distinguished computationally, and AFLOW has difficulty determining the correct label. We address this problem by moving these atoms from (8d) Wyckoff positions to (4c) Wyckoff positions, changing the y coordinate of each from its given value to 1/4.
- The original structure can be found in the CIF provided by the ICSD.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{22}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{24}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B_{26}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B_{27}}$	=	$-x_7\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(4c)	O IV

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\begin{array}{lcccccc}
\mathbf{B_{28}} & = & \left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O IV}\\
\mathbf{B_{29}} & = & x_8\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & ax_8\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(4c)} & \text{O V}\\
\mathbf{B_{30}} & = & -\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O V}\\
\mathbf{B_{31}} & = & -x_8\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_8\,\mathbf{a}_3 & = & -ax_8\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}} & \text{(4c)} & \text{O V}\\
\mathbf{B_{32}} & = & \left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O V}\\
\mathbf{B_{33}} & = & x_9\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & ax_9\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(4c)} & \text{S I}\\
\mathbf{B_{34}} & = & -\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_9-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{S I}\\
\mathbf{B_{35}} & = & -x_9\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_9\,\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}} & \text{(4c)} & \text{S I}\\
\mathbf{B_{36}} & = & \left(x_9+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_9+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{S I}\\
\mathbf{B_{37}} & = & x_{10}\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(4c)} & \text{Te I}\\
\mathbf{B_{38}} & = & -\left(x_{10}-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{10}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{Te I}\\
\mathbf{B_{39}} & = & -x_{10}\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_{10}\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}} & \text{(4c)} & \text{Te I}\\
\mathbf{B_{40}} & = & \left(x_{10}+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_{10}+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{Te I}\\
\mathbf{B_{41}} & = & x_{11}\,\mathbf{a}_1+y_{11}\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{42}} & = & -\left(x_{11}-\frac{1}{2}\right)\,\mathbf{a}_1-y_{11}\,\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{11}-\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{43}} & = & -x_{11}\,\mathbf{a}_1+\left(y_{11}+\frac{1}{2}\right)\,\mathbf{a}_2-z_{11}\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}}+b\left(y_{11}+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{44}} & = & \left(x_{11}+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_{11}-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_{11}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_{11}-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{45}} & = & -x_{11}\,\mathbf{a}_1-y_{11}\,\mathbf{a}_2-z_{11}\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{46}} & = & \left(x_{11}+\frac{1}{2}\right)\,\mathbf{a}_1+y_{11}\,\mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_{11}+\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{47}} & = & x_{11}\,\mathbf{a}_1-\left(y_{11}-\frac{1}{2}\right)\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}}-b\left(y_{11}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{48}} & = & -\left(x_{11}-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_{11}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{11}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_{11}+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{Cu II}\\
\mathbf{B_{49}} & = & x_{12}\,\mathbf{a}_1+y_{12}\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3 & = & ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{50}} & = & -\left(x_{12}-\frac{1}{2}\right)\,\mathbf{a}_1-y_{12}\,\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{12}-\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{51}} & = & -x_{12}\,\mathbf{a}_1+\left(y_{12}+\frac{1}{2}\right)\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3 & = & -ax_{12}\,\hat{\mathbf{x}}+b\left(y_{12}+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{52}} & = & \left(x_{12}+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_{12}-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_{12}-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_{12}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_{12}-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_{12}-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{53}} & = & -x_{12}\,\mathbf{a}_1-y_{12}\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3 & = & -ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{54}} & = & \left(x_{12}+\frac{1}{2}\right)\,\mathbf{a}_1+y_{12}\,\mathbf{a}_2-\left(z_{12}-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_{12}+\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}-c\left(z_{12}-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{55}} & = & x_{12}\,\mathbf{a}_1-\left(y_{12}-\frac{1}{2}\right)\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3 & = & ax_{12}\,\hat{\mathbf{x}}-b\left(y_{12}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{56}} & = & -\left(x_{12}-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_{12}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{12}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_{12}+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VI}\\
\mathbf{B_{57}} & = & x_{13}\,\mathbf{a}_1+y_{13}\,\mathbf{a}_2+z_{13}\,\mathbf{a}_3 & = & ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VII}\\
\mathbf{B_{58}} & = & -\left(x_{13}-\frac{1}{2}\right)\,\mathbf{a}_1-y_{13}\,\mathbf{a}_2+\left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_{13}-\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+c\left(z_{13}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8d)} & \text{O VII}
\end{array}
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$\mathbf{B_{59}}$	=	$-x_{13}\,\mathbf{a}_1 + \left(y_{13}+\frac{1}{2}\right)\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} + b\left(y_{13}+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{13}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{60}}$	=	$\left(x_{13}+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{13}-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{13}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{13}+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{13}-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{13}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{61}}$	=	$-x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{62}}$	=	$\left(x_{13}+\frac{1}{2}\right)\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 - \left(z_{13}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{13}+\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - c\left(z_{13}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{63}}$	=	$x_{13}\,\mathbf{a}_1 - \left(y_{13}-\frac{1}{2}\right)\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} - b\left(y_{13}-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(8d)	O VII
$\mathbf{B_{64}}$	=	$-\left(x_{13}-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{13}+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{13}-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{13}+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O VII

References

[1] Z.-C. Wang, K. Thanabalasingam, J. P. Scheifers, A. Streeter, G. T. McCandless, J. Gaudet, C. M. Brown, C. U. Segre, J. Y. Chan, and F. Tafti, *Antiferromagnetic Order and Spin-Canting Transition in the Corrugated Square Net Compound $Cu_3(TeO_4)(SO_4)\cdot H_2O$* (2021), doi:10.1021/acs.inorgchem.1c01220.