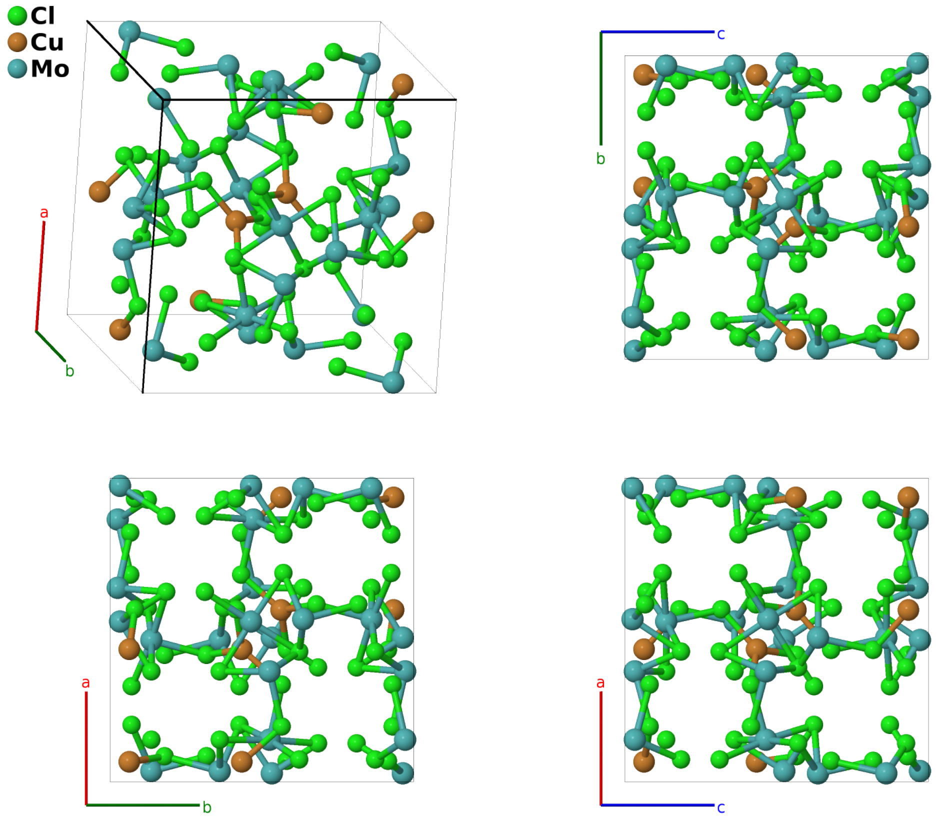
CuMo$_3$Cl$_7$ Structure: A7BC3_cP88_201_e2h_e_h-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/HF2G

https://aflow.org/p/A7BC3_cP88_201_e2h_e_h-001

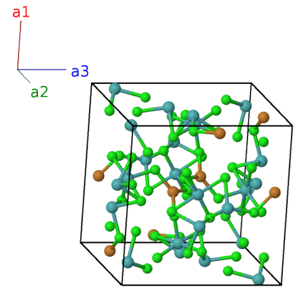


Prototype	Cl$_7$CuMo$_3$
AFLOW prototype label	A7BC3_cP88_201_e2h_e_h-001
ICSD	404375
Pearson symbol	cP88
Space group number	201
Space group symbol	$Pn\bar{3}$
AFLOW prototype command	`aflow --proto=A7BC3_cP88_201_e2h_e_h-001` `--params=`$a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Other compounds with this structure
CuMo$_3$Br$_7$, CuW$_3$Br$_7$

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_7}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_8}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cl I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{11}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{12}}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{15}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{16}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Cu I
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B_{18}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B_{19}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B_{20}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B_{21}}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B_{22}}$	=	$z_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B_{23}}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Cl II

$\mathbf{B}_{24}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a x_3\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{25}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$a y_3\,\hat{\mathbf{x}} + a z_3\,\hat{\mathbf{y}} + a x_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{26}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a z_3\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{27}$	=	$y_3\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a y_3\,\hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{28}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a x_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{29}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a x_3\,\hat{\mathbf{x}} - a y_3\,\hat{\mathbf{y}} - a z_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{30}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a z_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{31}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a y_3\,\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{32}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a x_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{33}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-a z_3\,\hat{\mathbf{x}} - a x_3\,\hat{\mathbf{y}} - a y_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{34}$	=	$-z_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a z_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{35}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a y_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{36}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a x_3\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{37}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-a y_3\,\hat{\mathbf{x}} - a z_3\,\hat{\mathbf{y}} - a x_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{38}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a z_3\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{39}$	=	$-y_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a y_3\,\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{40}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a x_3\,\hat{\mathbf{z}}$	(24h)	Cl II
$\mathbf{B}_{41}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a x_4\,\hat{\mathbf{x}} + a y_4\,\hat{\mathbf{y}} + a z_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{42}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a z_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{43}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a y_4\,\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{44}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a x_4\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{45}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$a z_4\,\hat{\mathbf{x}} + a x_4\,\hat{\mathbf{y}} + a y_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{46}$	=	$z_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a z_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{47}$	=	$-\left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$-a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a y_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{48}$	=	$-\left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a x_4\,\hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{49}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$a y_4\,\hat{\mathbf{x}} + a z_4\,\hat{\mathbf{y}} + a x_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{50}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a z_4\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{51}$	=	$y_4\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a y_4\,\hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{52}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a x_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{53}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-a x_4\,\hat{\mathbf{x}} - a y_4\,\hat{\mathbf{y}} - a z_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{54}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a z_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B}_{55}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a y_4\,\hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III

$\mathbf{B_{56}}$	=	$-x_4\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{57}}$	=	$-z_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-ay_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{58}}$	=	$-z_4\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{59}}$	=	$\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-ay_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{60}}$	=	$\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{61}}$	=	$-y_4\,\mathbf{a}_1-z_4\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{62}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{63}}$	=	$-y_4\,\mathbf{a}_1+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{64}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(24h)	Cl III
$\mathbf{B_{65}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{66}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{67}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+y_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{68}}$	=	$x_5\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{69}}$	=	$z_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{70}}$	=	$z_5\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{71}}$	=	$-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{72}}$	=	$-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1+x_5\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{73}}$	=	$y_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{74}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{75}}$	=	$y_5\,\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{76}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{77}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{78}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{79}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{80}}$	=	$-x_5\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{81}}$	=	$-z_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{82}}$	=	$-z_5\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{83}}$	=	$\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{84}}$	=	$\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{85}}$	=	$-y_5\,\mathbf{a}_1-z_5\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{86}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I
$\mathbf{B_{87}}$	=	$-y_5\,\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24h)	Mo I

$$\mathbf{B_{88}} = \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_2 - x_5 \, \mathbf{a}_3 = a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - a x_5 \, \hat{\mathbf{z}} \qquad (24h) \qquad \text{Mo I}$$

References

[1] A. Peppenhorst and H.-L. Keller, *Trigonal-planare CuX_3-Gruppen in $Cu_2Mo_6X_{14}$, X = Cl, Br, I*, Z. Anorganische und Allgemeine Chemie **622**, 663–669 (1996), doi:10.1524/ncrs.2006.0001.

Found in

[1] W. Xu, P. Wang, and Y.-Q. Zheng, *Crystal structure of dipotassium octakis(μ_3-bromo)hexabromo-octahedro-hexamolybdenate, $K_2[Mo_6Br_{14}]$*, Z. Kristallogr. NCS **221**, 107–108 (2006).