

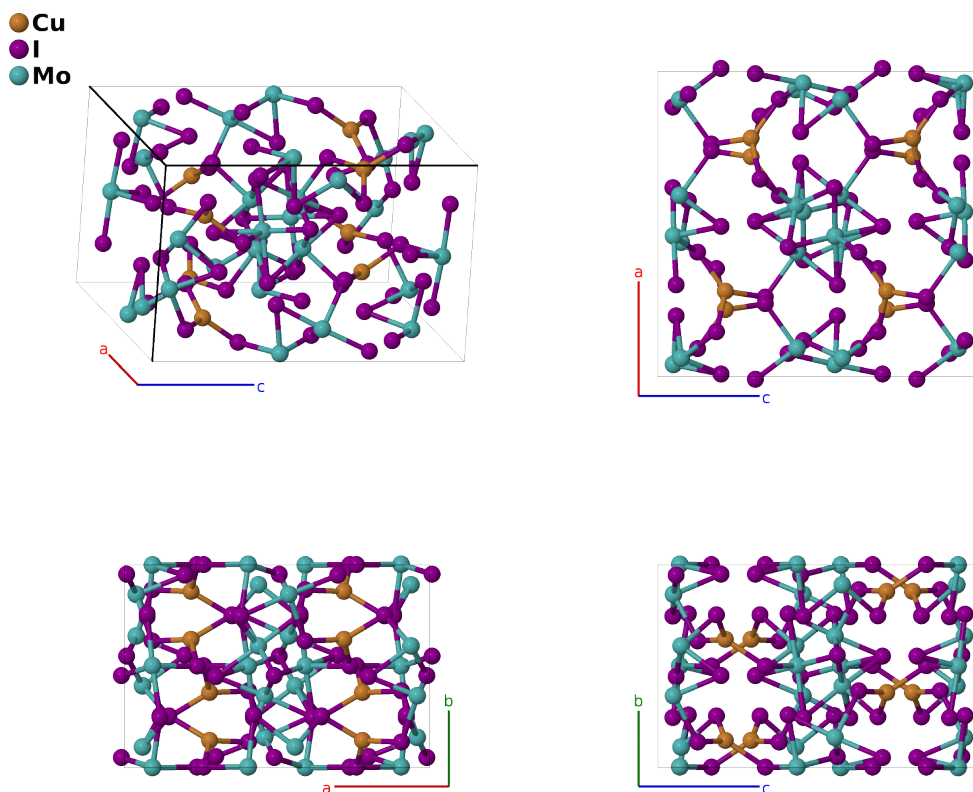
# CuMo<sub>3</sub>I<sub>7</sub> Structure:

## AB7C3\_oP88\_61\_c\_7c\_3c-001

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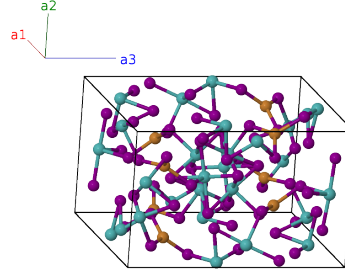
<https://aflow.org/p/WLBF>

[https://aflow.org/p/AB7C3\\_oP88\\_61\\_c\\_7c\\_3c-001](https://aflow.org/p/AB7C3_oP88_61_c_7c_3c-001)



Prototype	CuI <sub>7</sub> Mo <sub>3</sub>
AFLOW prototype label	AB7C3_oP88_61_c_7c_3c-001
ICSD	404377
Pearson symbol	oP88
Space group number	61
Space group symbol	<i>Pbca</i>
AFLOW prototype command	aflow --proto=AB7C3_oP88_61_c_7c_3c-001 --params=a, b/a, c/a, x <sub>1</sub> , y <sub>1</sub> , z <sub>1</sub> , x <sub>2</sub> , y <sub>2</sub> , z <sub>2</sub> , x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub> , x <sub>5</sub> , y <sub>5</sub> , z <sub>5</sub> , x <sub>6</sub> , y <sub>6</sub> , z <sub>6</sub> , x <sub>7</sub> , y <sub>7</sub> , z <sub>7</sub> , x <sub>8</sub> , y <sub>8</sub> , z <sub>8</sub> , x <sub>9</sub> , y <sub>9</sub> , z <sub>9</sub> , x <sub>10</sub> , y <sub>10</sub> , z <sub>10</sub> , x <sub>11</sub> , y <sub>11</sub> , z <sub>11</sub>

Simple Orthorhombic primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$

## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_8$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{12}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{16}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	I I
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8c)	I II
$\mathbf{B}_{18}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I II
$\mathbf{B}_{19}$	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I II
$\mathbf{B}_{20}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8c)	I II
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8c)	I II
$\mathbf{B}_{22}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I II
$\mathbf{B}_{23}$	$= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	I II





$$\mathbf{B}_{85} = -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} \quad (8c) \quad \text{Mo III}$$

$$\mathbf{B}_{86} = \begin{pmatrix} x_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{11} \mathbf{a}_2 - \mathbf{a}_3 = a \left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c \left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8c) \quad \text{Mo III}$$

$$\mathbf{B}_{87} = \begin{pmatrix} x_{11} \\ z_{11} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 + \mathbf{a}_3 = ax_{11} \hat{\mathbf{x}} - b \left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8c) \quad \text{Mo III}$$

$$\mathbf{B}_{88} = -\begin{pmatrix} x_{11} - \frac{1}{2} \\ z_{11} \end{pmatrix} \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \mathbf{a}_3 = -a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} \quad (8c) \quad \text{Mo III}$$

## References

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- [1] W. Xu, P. Wang, and Y.-Q. Zheng, *Crystal structure of dipotassium octakis( $\mu_3$ -bromo)hexabromo-octahedro-hexamolybdenate,  $K_2[\text{Mo}_6\text{Br}_{14}]$* , Z. Kristallogr. NCS **221**, 107–108 (2006).