

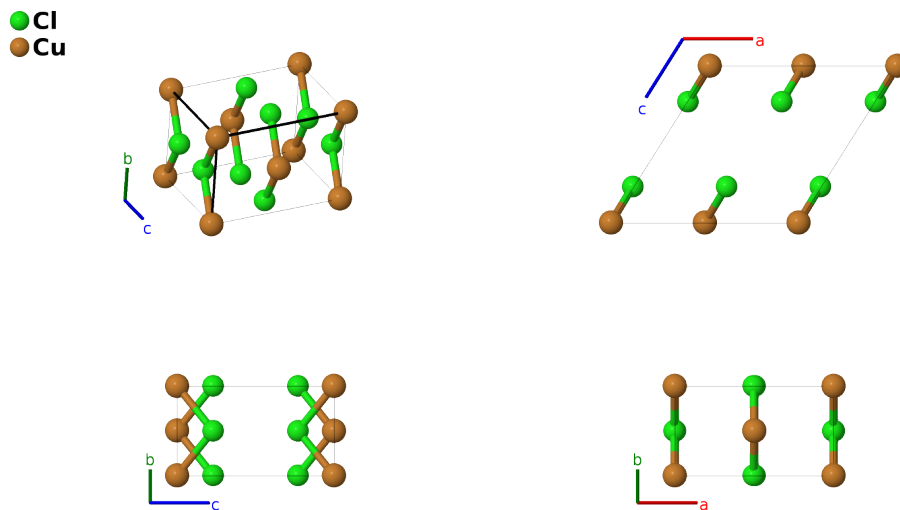
# Tolbachite (CuCl<sub>2</sub>) Structure: A2B\_mC6\_12\_i\_a-001

This structure originally had the label **A2B\_mC6\_12\_i\_a**. Calls to that address will be redirected here.

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

[https://aflow.org/p/A2B\\_mC6\\_12\\_i\\_a-001](https://aflow.org/p/A2B_mC6_12_i_a-001)



<b>Prototype</b>	Cl <sub>2</sub> Cu
<b>AFLOW prototype label</b>	A2B_mC6_12_i_a-001
<b>Mineral name</b>	tolbachite
<b>ICSD</b>	66645
<b>Pearson symbol</b>	mC6
<b>Space group number</b>	12
<b>Space group symbol</b>	<i>C</i> 2/ <i>m</i>
<b>AFLOW prototype command</b>	<code>aflow --proto=A2B_mC6_12_i_a-001 --params=a, b/a, c/a, β, x<sub>2</sub>, z<sub>2</sub></code>

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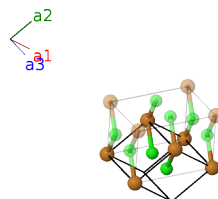
## Other compounds with this structure

CuBr<sub>2</sub>

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## Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$




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### Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	= 0	=	0	(2a)	Cu I
$\mathbf{B}_2$	= $x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B}_3$	= $-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Cl I

### References

- [1] P. C. Burns and F. C. Hawthorne, *Tolbachite,  $\text{CuCl}^{2+}$ , the first example of  $\text{Cu}_2$  octahedrally coordinated by  $\text{Cl}^-$* , American Mineralogist **78**, 187–189 (1993).