

# Cs<sub>2</sub>CuCl<sub>4</sub> Structure:

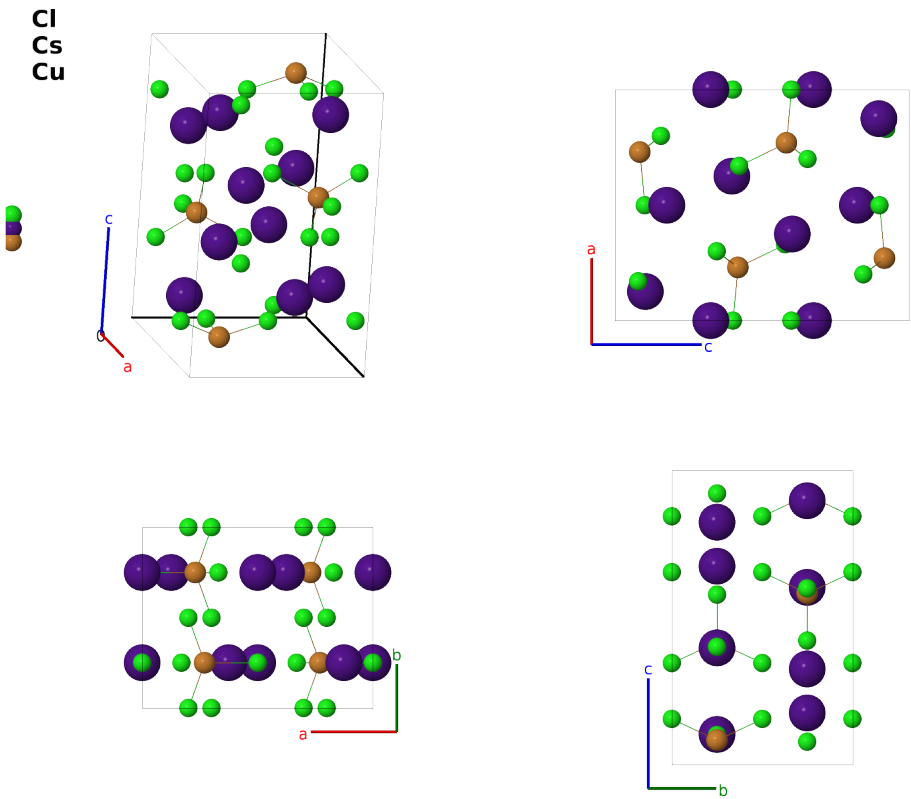
## A4B2C\_oP28\_62\_2cd\_2c\_c-001

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<https://aflow.org/prototype-encyclopedia/B1GA>

[https://aflow.org/prototype-encyclopedia/A4B2C\\_oP28\\_62\\_2cd\\_2c\\_c-001](https://aflow.org/prototype-encyclopedia/A4B2C_oP28_62_2cd_2c_c-001)



|                         |                                                                                                                                                                                                                                                              |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | Cl <sub>4</sub> Cs <sub>2</sub> Cu                                                                                                                                                                                                                           |
| AFLOW prototype label   | A4B2C_oP28_62_2cd_2c_c-001                                                                                                                                                                                                                                   |
| ICSD                    | 36175                                                                                                                                                                                                                                                        |
| CCDC                    | 1607951                                                                                                                                                                                                                                                      |
| Pearson symbol          | oP28                                                                                                                                                                                                                                                         |
| Space group number      | 62                                                                                                                                                                                                                                                           |
| Space group symbol      | <i>Pnma</i>                                                                                                                                                                                                                                                  |
| AFLOW prototype command | <pre>aflow --proto=A4B2C_oP28_62_2cd_2c_c-001 --params=a,b/a,c/a,x<sub>1</sub>,z<sub>1</sub>,x<sub>2</sub>,z<sub>2</sub>,x<sub>3</sub>,z<sub>3</sub>,x<sub>4</sub>,z<sub>4</sub>,x<sub>5</sub>,z<sub>5</sub>,x<sub>6</sub>,y<sub>6</sub>,z<sub>6</sub></pre> |

### Other compounds with this structure

Cs<sub>2</sub>BeCl<sub>4</sub>, Cs<sub>2</sub>CdBr<sub>4</sub>, Cs<sub>2</sub>CdI<sub>4</sub>, Cs<sub>2</sub>CoCl<sub>4</sub>, Cs<sub>2</sub>CoI<sub>4</sub>, Cs<sub>2</sub>CuBr<sub>4</sub>, Cs<sub>2</sub>FeCl<sub>4</sub>, Cs<sub>2</sub>HgBr<sub>4</sub>, Cs<sub>2</sub>HgCl<sub>4</sub>, Cs<sub>2</sub>MgCl<sub>4</sub>, Cs<sub>2</sub>MgH<sub>4</sub>, Cs<sub>2</sub>MnBr<sub>4</sub>, Cs<sub>2</sub>ZnBr<sub>4</sub>, Cs<sub>2</sub>ZnCl<sub>4</sub>, Cs<sub>2</sub>ZnI<sub>4</sub>, K<sub>2</sub>BeF<sub>4</sub>, K<sub>2</sub>ZnBr<sub>4</sub>, K<sub>2</sub>ZnCl<sub>4</sub>, Rb<sub>2</sub>CoBr<sub>4</sub>, Rb<sub>2</sub>CoCl<sub>4</sub>, Rb<sub>2</sub>MgH<sub>4</sub>, Rb<sub>2</sub>ZnBr<sub>4</sub>, Rb<sub>2</sub>ZnCl<sub>4</sub>, (NH<sub>4</sub>)<sub>2</sub>ZnBr<sub>4</sub>, (NH<sub>4</sub>)<sub>2</sub>ZnCl<sub>4</sub>

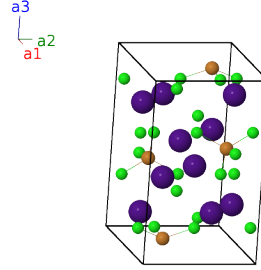
- This structure is somewhat similar to Arcanite (K<sub>2</sub>SO<sub>4</sub>, *H1*<sub>6</sub>), but the ICSD recognizes them as different structure types and AFLOW finds a misfit value of 0.2, sufficiently large to justify making this a new prototype.

### 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)             | Cl 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)             | Cl 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)             | Cl 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)             | Cl 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)             | Cl II     |
| $\mathbf{B}_6$    | $= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)             | Cl II     |
| $\mathbf{B}_7$    | $= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$                                                       | $=$ | $-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$                                                       | (4c)             | Cl II     |
| $\mathbf{B}_8$    | $= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)             | Cl II     |
| $\mathbf{B}_9$    | $= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$                                                        | $=$ | $ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                                        | (4c)             | Cs I      |
| $\mathbf{B}_{10}$ | $= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)             | Cs I      |
| $\mathbf{B}_{11}$ | $= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$                                                       | $=$ | $-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                                                       | (4c)             | Cs I      |
| $\mathbf{B}_{12}$ | $= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)             | Cs I      |
| $\mathbf{B}_{13}$ | $= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$                                                        | $=$ | $ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                                        | (4c)             | Cs II     |
| $\mathbf{B}_{14}$ | $= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4c)             | Cs II     |
| $\mathbf{B}_{15}$ | $= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$                                                       | $=$ | $-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$                                                       | (4c)             | Cs II     |
| $\mathbf{B}_{16}$ | $= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$  | $=$ | $a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$  | (4c)             | Cs II     |
| $\mathbf{B}_{17}$ | $= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$                                                        | $=$ | $ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$                                                        | (4c)             | Cu I      |

$$\begin{aligned}
\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) &\text{Cu I} \\
\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) &\text{Cu I} \\
\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) &\text{Cu I} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{22} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + b \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{25} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{26} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{27} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} - b \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8d) &\text{Cl III} \\
\mathbf{B}_{28} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\text{Cl III}
\end{aligned}$$

## References

- [1] L. Helmholz and R. F. Kruh, *The Crystal Structure of Cesium Chlorocuprate,  $\text{Cs}_2\text{CuCl}_4$ , and the Spectrum of the Chlorocuprate Ion*, J. Am. Chem. Soc. **74**, 1176–1181 (1952), doi:10.1021/ja01125a012.

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