

Cu(PtS₂)₂ Structure:

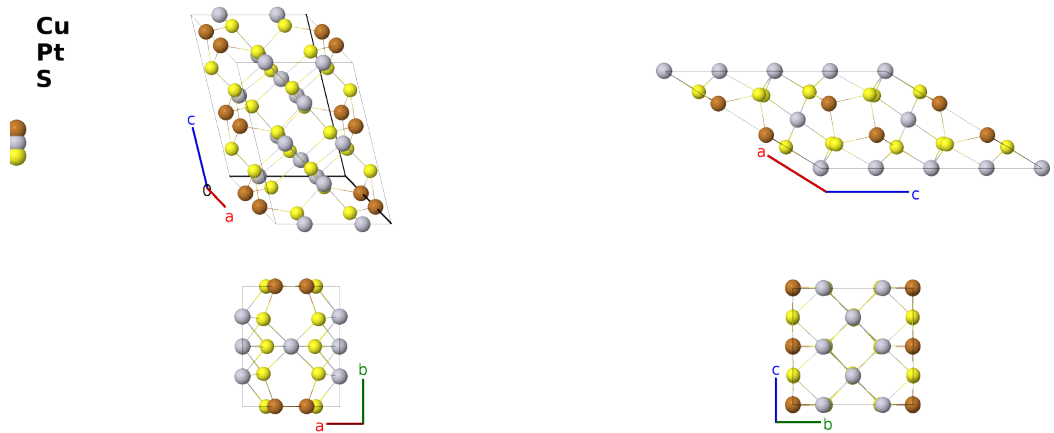
AB2C4_mP28_13_g_efg_4g-001

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<https://aflow.org/prototype-encyclopedia/HFY3>

https://aflow.org/prototype-encyclopedia/AB2C4_mP28_13_g_efg_4g-001

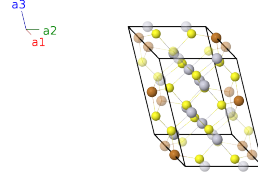


Prototype	CuPt ₂ S ₄
AFLOW prototype label	AB2C4_mP28_13_g_efg_4g-001
ICSD	74894
CCDC	1635564
Pearson symbol	mP28
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	<pre>aflow --proto=AB2C4_mP28_13_g_efg_4g-001 --params=a,b/a,c/a,β,y₁,y₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈, z₈</pre>

- (Gross, 1994) give the crystal structure in the $P2/n$ setting of space group #13. We use FINDSYM to change this to the standard $P2/c$ setting.
- With only a small uncertainty in the coordinates ($\approx 0.1\text{\AA}$) this could be placed in space group $P2/m$ #10 with the unit cell halved.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	Pt I
$\mathbf{B}_2$	$-y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	Pt I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{c \cos \beta}{4}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2f)	Pt II
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{3c \cos \beta}{4}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2f)	Pt II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B}_7$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B}_8$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B}_9$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	Pt III
$\mathbf{B}_{10}$	$-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Pt III
$\mathbf{B}_{11}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	Pt III
$\mathbf{B}_{12}$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Pt III
$\mathbf{B}_{13}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_{14}$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_{15}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_{16}$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S I
$\mathbf{B}_{17}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_{18}$	$-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_{19}$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_{20}$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S II
$\mathbf{B}_{21}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{22}$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{23}$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{24}$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{25}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4g)	S IV

$$\begin{aligned}
\mathbf{B}_{26} &= -x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_8 + c\left(z_8 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - &(4g) \quad \text{S IV} \\
&&& c\left(z_8 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{27} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} &(4g) \quad \text{S IV} \\
\mathbf{B}_{28} &= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_8 + c\left(z_8 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + &(4g) \quad \text{S IV} \\
&&& c\left(z_8 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] P. J. Gross and M. Jansen, *Synthese und Kristallstruktur von $\text{Cu}_2\text{Pt}^{II}\text{Pt}_3^V\text{S}_8$* , Z. Anorganische und Allgemeine Chemie **620**, 1909–1914 (1994), doi:10.1002/zaac.19946201112.

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