Petzite (Ag_3AuTe_2) Structure: A3BC2_cI48_214_f_a_e-001

This structure originally had the label `A3BC2_cI48_214_f_a_e`. Calls to that address will be redirected here.

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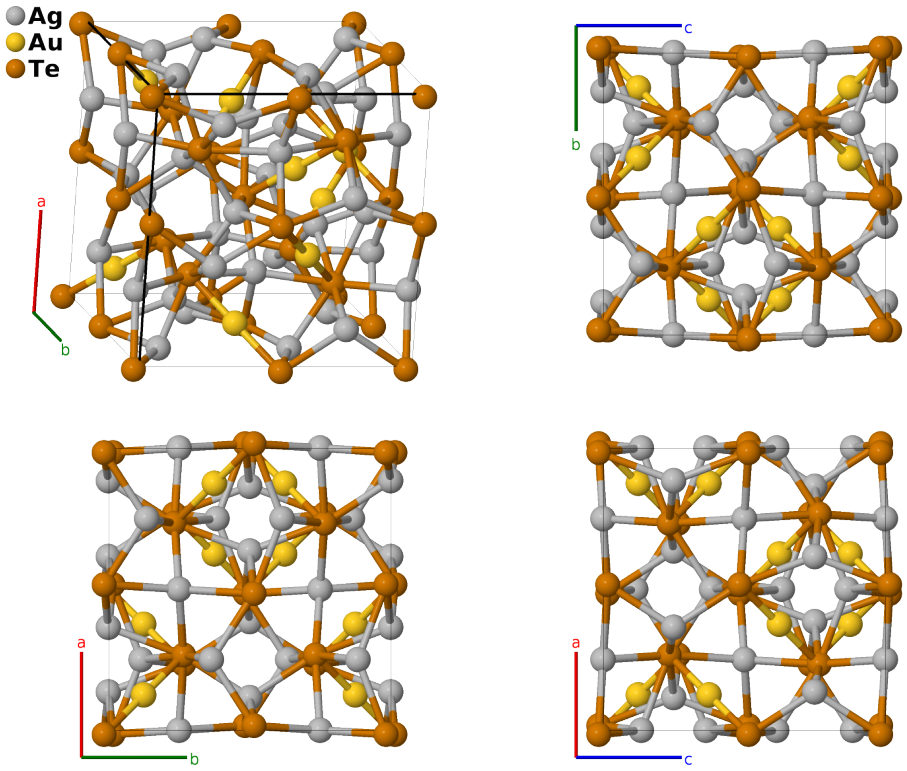
https://aflow.org/p/3JDV

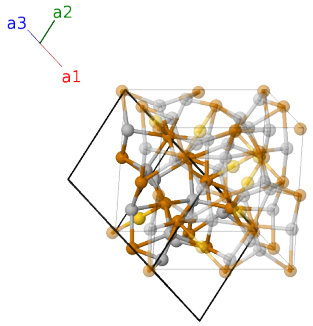
https://aflow.org/p/A3BC2_cI48_214_f_a_e-001



Prototype	Ag_3AuTe_2
AFLOW prototype label	A3BC2_cI48_214_f_a_e-001
Mineral name	petzite
ICSD	27539
Pearson symbol	cI48
Space group number	214
Space group symbol	$I4_132$
AFLOW prototype command	`aflow --proto=A3BC2_cI48_214_f_a_e-001 --params=`a, x_2, x_3

Body-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Au I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Au I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Au I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8a)	Au I
$\mathbf{B_5}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_7}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_8}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_3$	=	$a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_{10}}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_{11}}$	=	$2x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_{12}}$	=	$2x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B_{13}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{14}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{15}}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(24f)	Ag I
$\mathbf{B_{16}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{17}}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{18}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{19}}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{20}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}}$	(24f)	Ag I
$\mathbf{B_{21}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{22}}$	=	$\frac{1}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{23}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B_{24}}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24f)	Ag I

References

[1] J. A. J. Frueh, *Crystallography of petzite,* Ag_3AuTe_2, American Mineralogist **44**, 693–701 (1959).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).