

Petzite (Ag₃AuTe₂) Structure: A3BC2_cI48_214_f_a_e-001

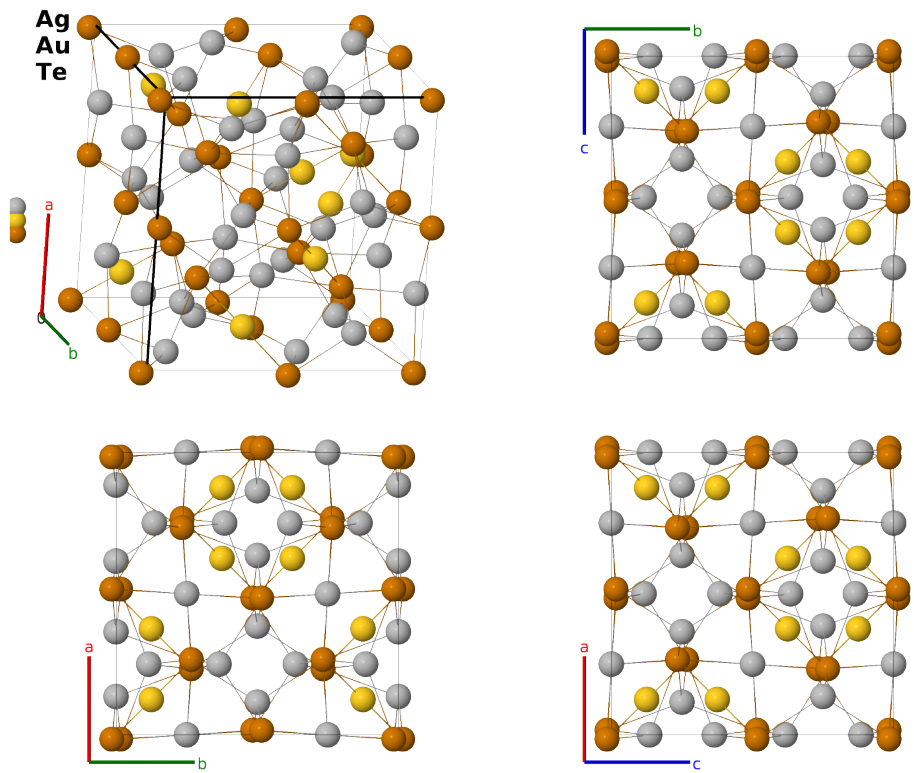
This structure previously used the label(s) **A3BC2.cI48.214.f.a.e.** Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/3JDV>

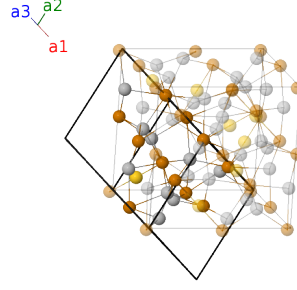
https://aflow.org/prototype-encyclopedia/A3BC2_cI48_214_f_a_e-001



Prototype	Ag ₃ AuTe ₂
AFLOW prototype label	A3BC2_cI48_214_f_a_e-001
Mineral name	petzite
ICSD	27539
CCDC	1602806
Pearson symbol	cI48
Space group number	214
Space group symbol	<i>I</i> 4 ₁ 32
AFLOW prototype command	<code>aflow --proto=A3BC2_cI48_214_f_a_e-001</code> <code>--params=<i>a</i>, <i>x</i>₂, <i>x</i>₃</code>

Body-centered Cubic primitive vectors

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



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
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_1 - (2x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - a(x_2 - \frac{1}{2})\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_7$	$= -(2x_2 - \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2})\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_8$	$= -(2x_2 - \frac{1}{2})\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$ax_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - a(x_2 - \frac{1}{2})\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_9$	$= \frac{1}{2}\mathbf{a}_1 + 2x_2\mathbf{a}_3$	$=$	$a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + a(x_2 + \frac{1}{4})\hat{\mathbf{y}} - a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_{10}$	$= -(2x_2 - \frac{1}{2})\mathbf{a}_1 - (2x_2 - \frac{1}{2})\mathbf{a}_2 - (2x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} - a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_{11}$	$= 2x_2\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4})\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_{12}$	$= 2x_2\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + a(x_2 + \frac{1}{4})\hat{\mathbf{z}}$	(16e)	Te I
$\mathbf{B}_{13}$	$= \frac{1}{4}\mathbf{a}_1 + (x_3 + \frac{1}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{14}$	$= \frac{3}{4}\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{15}$	$= x_3\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_3 + \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}}$	(24f)	Ag I
$\mathbf{B}_{16}$	$= -(x_3 - \frac{1}{2})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{17}$	$= (x_3 + \frac{1}{4})\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{18}$	$= -(x_3 - \frac{1}{4})\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{19}$	$= (x_3 + \frac{1}{4})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{20}$	$= -(x_3 - \frac{1}{4})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}}$	(24f)	Ag I
$\mathbf{B}_{21}$	$= \frac{3}{4}\mathbf{a}_1 + x_3\mathbf{a}_2 + (x_3 + \frac{1}{4})\mathbf{a}_3$	$=$	$a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{22}$	$= \frac{1}{4}\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{23}$	$= -(x_3 - \frac{1}{2})\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} - a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(24f)	Ag I
$\mathbf{B}_{24}$	$= x_3\mathbf{a}_1 + (x_3 + \frac{1}{4})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(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).

First cited in

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