

Krennerite (AuTe₂) Structure: AB2_oP24_28_acd_2c3d-001

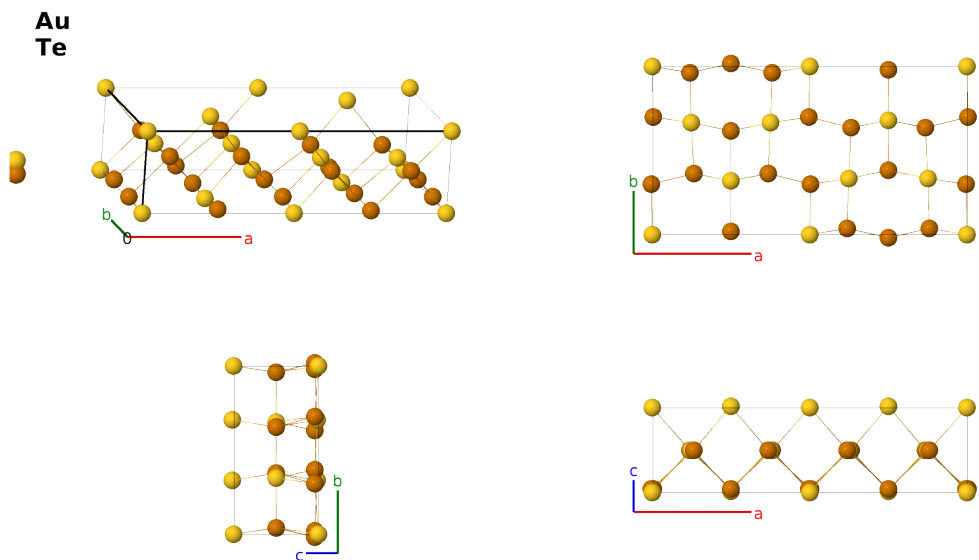
This structure previously used the label(s) AB2_oP24_28_acd_2c3d. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/A9SX>

https://aflow.org/prototype-encyclopedia/AB2_oP24_28_acd_2c3d-001



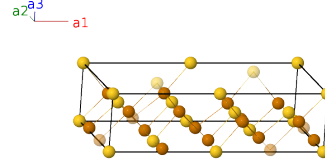
Prototype	AuTe ₂
AFLOW prototype label	AB2_oP24_28_acd_2c3d-001
Mineral name	krennerite
ICSD	612391
CCDC	1744822
Pearson symbol	oP24
Space group number	28
Space group symbol	<i>Pma</i> 2
AFLOW prototype command	<code>aflow --proto=AB2_oP24_28_acd_2c3d-001</code> <code>--params=a, b/a, c/a, z₁, y₂, z₂, y₃, z₃, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</code>

- The ICSD entry is from the much earlier work of (Tunnell, 1936).

- The current sample (Tunnell, 1950) has composition $(\text{Au}_{0.88}\text{Ag}_{0.12})\text{Te}_2$. For simplicity we label all of the Au/Ag sites as Au. (Pearson, 1972) states that this is a distortion of the trigonal ω phase, $C6$. Note that AuTe_2 also can be found as calaverite, $C34$.
- Space group $Pma2$ #28 allows an arbitrary placement of the origin of the z -axis. We follow (Tunell, 1950) and place the gold (2a) atom at the origin.
- We have corrected some numerical errors found in (Mehl, 2017).

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Au I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c z_1 \hat{\mathbf{z}}$	(2a)	Au I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2c)	Au II
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2c)	Au II
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B}_{11}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B}_{12}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B}_{14}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B}_{15}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B}_{16}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B}_{17}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B}_{18}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B}_{19}$	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a (x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B}_{20}$	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a (x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B}_{21}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$a x_8 \hat{\mathbf{x}} + b y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(4d)	Te V
$\mathbf{B}_{22}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a x_8 \hat{\mathbf{x}} - b y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(4d)	Te V
$\mathbf{B}_{23}$	$= (x_8 + \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$a (x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(4d)	Te V
$\mathbf{B}_{24}$	$= -(x_8 - \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a (x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(4d)	Te V

References

- [1] G. Tunell and K. J. Murata, *The atomic arrangement and chemical composition of krennerite*, Am. Mineral. **35**, 959–984 (1950).
- [2] G. Tunnell and C. J. Ksanda, *The crystal structure of krennerite*, J. Washington Academy Sci. **26**, 507–509 (1936).
- [3] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).
- [4] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1–828 (2017). doi: 10.1016/j.commatsci.2017.01.017