Krennerite ($AuTe_2$) Structure: AB2_oP24_28_acd_2c3d-001

This structure originally had the label `AB2_oP24_28_acd_2c3d`. Calls to that address will be redirected here.

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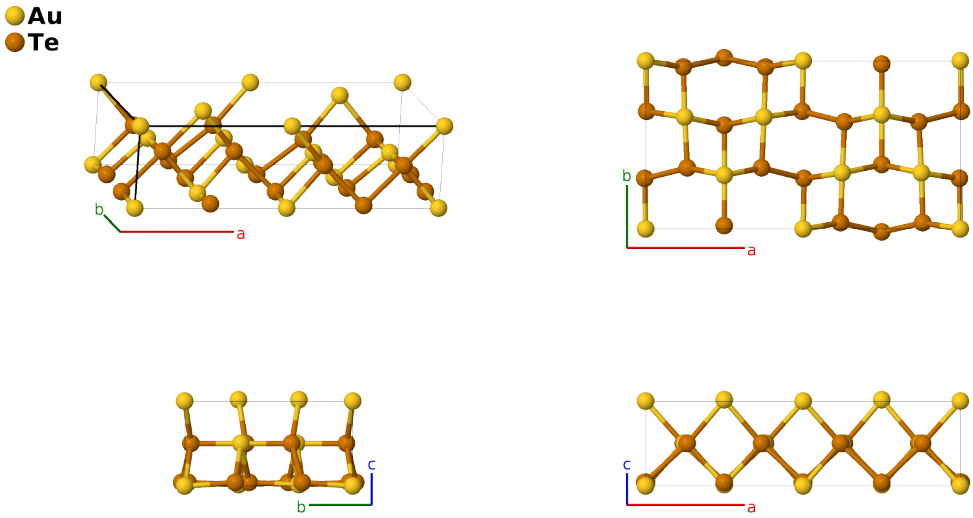
https://aflow.org/p/A9SX

https://aflow.org/p/AB2_oP24_28_acd_2c3d-001



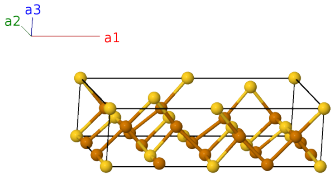
Prototype	$AuTe_2$
AFLOW prototype label	AB2_oP24_28_acd_2c3d-001
Mineral name	krennerite
ICSD	612391
Pearson symbol	oP24
Space group number	28
Space group symbol	$Pma2$
AFLOW prototype command	`aflow --proto=AB2_oP24_28_acd_2c3d-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- The ICSD entry is from the much earlier work of (Tunnell, 1936).
- The current sample (Tunnell, 1950) has composition $(Au_{0.88}Ag_{0.12})Te_2$. 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Au I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Au I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Au II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Au II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B_{11}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B_{12}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Au III
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B_{15}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B_{16}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Te III
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B_{18}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B_{19}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B_{20}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	Te IV
$\mathbf{B_{21}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	Te V
$\mathbf{B_{22}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	Te V
$\mathbf{B_{23}}$	=	$\left(x_8 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$a\left(x_8 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	Te V
$\mathbf{B_{24}}$	=	$-\left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-a\left(x_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	Te V

References

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[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, Tornoto, 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.