ZnTe (high-pressure) Structure: AB_hP6_144_a_a-001

This structure originally had the label `AB_hP6_144_a_a`. Calls to that address will be redirected here.

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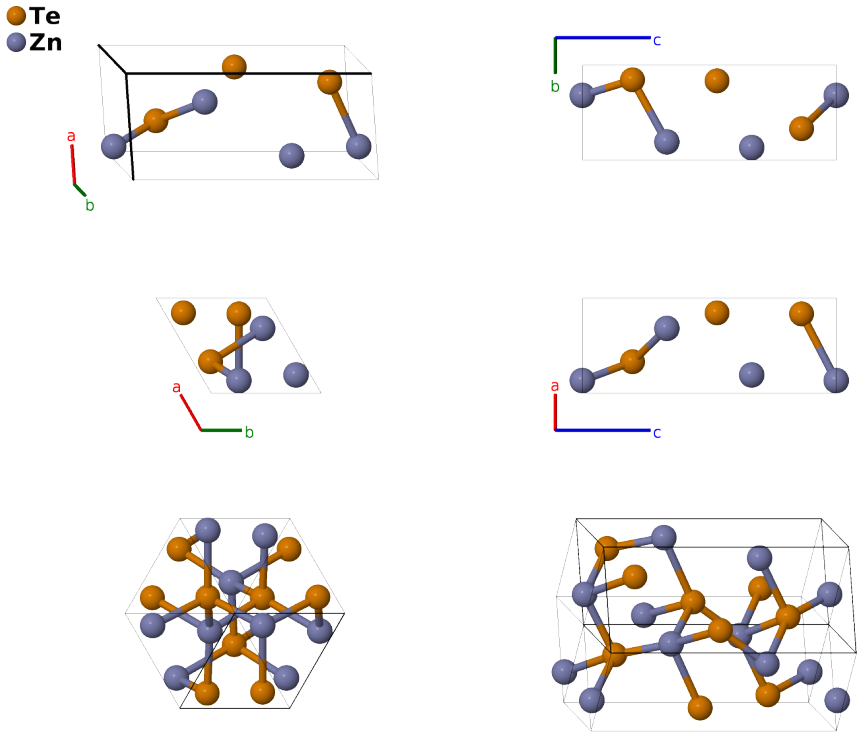
https://aflow.org/p/LX4R

https://aflow.org/p/AB_hP6_144_a_a-001

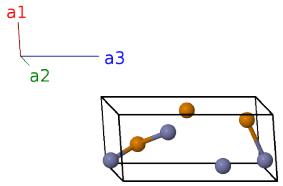


Prototype	TeZn
AFLOW prototype label	AB_hP6_144_a_a-001
ICSD	80076
Pearson symbol	hP6
Space group number	144
Space group symbol	$P3_1$
AFLOW prototype command	`aflow --proto=AB_hP6_144_a_a-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2$

- This structure was determined at 11.5 GPa.
- This structure can also be found in the enantiomorphic space group $P3_2$ #145.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1+y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_1-y_1)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(3a)	Te I
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_1 + (x_1-y_1)\,\mathbf{a}_2 + \left(z_1+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1-2y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Te I
$\mathbf{B_3}$	=	$-(x_1-y_1)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_1-y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_1+2)\,\hat{\mathbf{z}}$	(3a)	Te I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(3a)	Zn I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + (x_2-y_2)\,\mathbf{a}_2 + \left(z_2+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2-2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Zn I
$\mathbf{B_6}$	=	$-(x_2-y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2+2)\,\hat{\mathbf{z}}$	(3a)	Zn I

References

[1] K. Kusaba and D. J. Weidner, *Structure of high pressure phase I in ZnTe*, AIP Conference Proceedings **309**, 553 (1994), doi:10.1063/1.46096.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.