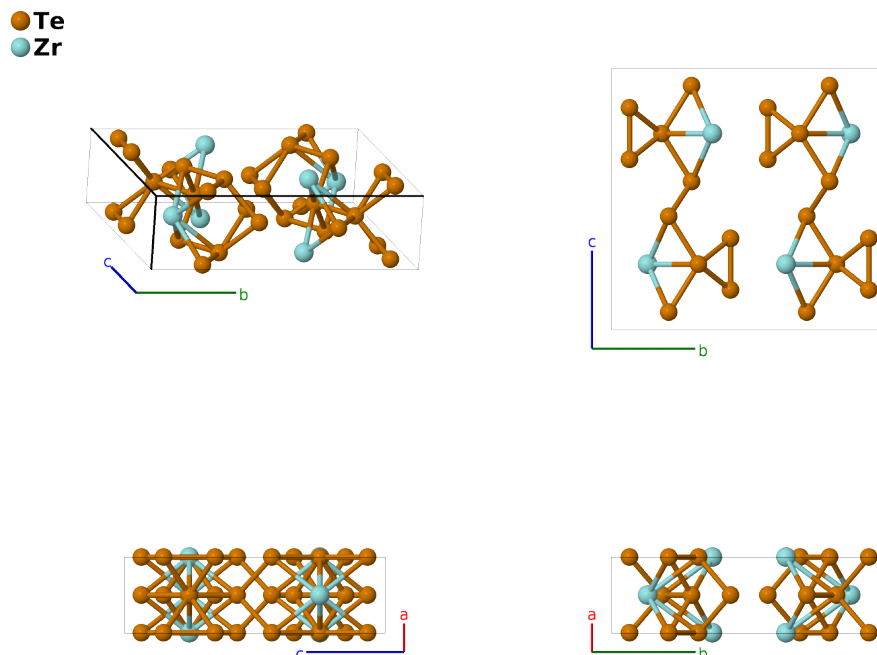# ZrTe$_5$ Structure: A5B_oC24_63_c2f_c-001

This structure originally had the label `A5B_oC24_63_c2f_c`. Calls to that address will be redirected here.

https://aflow.org/p/EE51

https://aflow.org/p/A5B_oC24_63_c2f_c-001

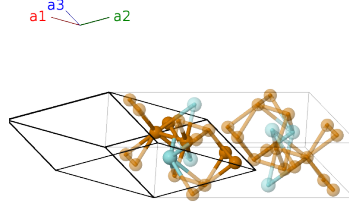|	
Prototype	Te$_5$Zr
AFLOW prototype label	A5B_oC24_63_c2f_c-001
ICSD	85506
Pearson symbol	oC24
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A5B_oC24_63_c2f_c-001` `--params=`$a, b/a, c/a, y_1, y_2, y_3, z_3, y_4, z_4$

Other compounds with this structure

HfTe$_5$

- We use the data taken at room temperature.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$-y_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$by_1\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B_2}$	$=$	$y_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$-by_1\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B_3}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$by_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Zr I
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$-by_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Zr I
$\mathbf{B_5}$	$=$	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Te II
$\mathbf{B_6}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Te II
$\mathbf{B_7}$	$=$	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Te II
$\mathbf{B_8}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Te II
$\mathbf{B_9}$	$=$	$-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Te III
$\mathbf{B_{10}}$	$=$	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Te III
$\mathbf{B_{11}}$	$=$	$-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Te III
$\mathbf{B_{12}}$	$=$	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Te III

References

[1] H. Fjellvåg and A. Kjekshus, *Structural Properties of ZrTe$_5$ and HfTe$_5$ as Seen by Power Diffraction*, Solid State Commun. **60**, 91–93 (1986), doi:10.1016/0038-1098(86)90536-3.