

ZrTe₃O₈ Structure:

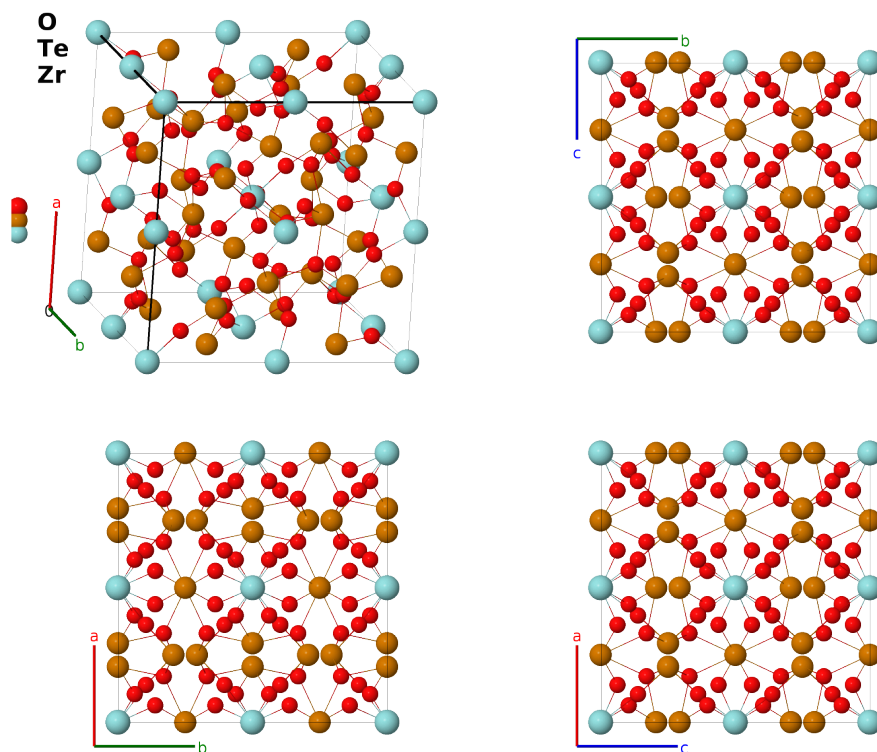
A8B3C_cI96_206_ce_d_a-001

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- 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/3HHF>

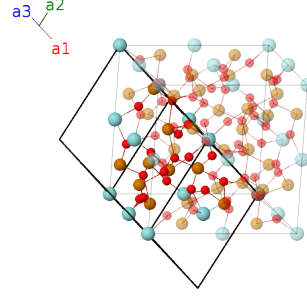
https://aflow.org/prototype-encyclopedia/A8B3C_cI96_206_ce_d_a-001



Prototype	O ₈ Te ₃ Zr
AFLOW prototype label	A8B3C_cI96_206_ce_d_a-001
ICSD	409713
CCDC	1726061
Pearson symbol	cI96
Space group number	206
Space group symbol	$Ia\bar{3}$
AFLOW prototype command	<pre>aflow --proto=A8B3C_cI96_206_ce_d_a-001 --params=a, x₂, x₃, x₄, y₄, z₄</pre>

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
$\mathbf{B}_1$	$= 0$	$=$	0	(8a)	Zr I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(8a)	Zr I
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(8a)	Zr I
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(8a)	Zr I
$\mathbf{B}_5$	$= 2x_2\mathbf{a}_1 + 2x_2\mathbf{a}_2 + 2x_2\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_1 - (2x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - a(x_2 - \frac{1}{2})\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_7$	$= -(2x_2 - \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2})\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_8$	$= -(2x_2 - \frac{1}{2})\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$ax_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - a(x_2 - \frac{1}{2})\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_9$	$= -2x_2\mathbf{a}_1 - 2x_2\mathbf{a}_2 - 2x_2\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_{10}$	$= \frac{1}{2}\mathbf{a}_1 + (2x_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + a(x_2 + \frac{1}{2})\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_{11}$	$= (2x_2 + \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2})\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_{12}$	$= (2x_2 + \frac{1}{2})\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$-ax_2\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} + a(x_2 + \frac{1}{2})\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B}_{13}$	$= \frac{1}{4}\mathbf{a}_1 + (x_3 + \frac{1}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{14}$	$= \frac{3}{4}\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{15}$	$= x_3\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_3 + \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}}$	(24d)	Te I
$\mathbf{B}_{16}$	$= -(x_3 - \frac{1}{2})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{17}$	$= (x_3 + \frac{1}{4})\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{18}$	$= -(x_3 - \frac{1}{4})\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{19}$	$= \frac{3}{4}\mathbf{a}_1 - (x_3 - \frac{3}{4})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{20}$	$= \frac{1}{4}\mathbf{a}_1 + (x_3 + \frac{3}{4})\mathbf{a}_2 + (x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{21}$	$= -x_3\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_3 - \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}}$	(24d)	Te I
$\mathbf{B}_{22}$	$= (x_3 + \frac{1}{2})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_3 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_3 + \frac{1}{2})\hat{\mathbf{y}}$	(24d)	Te I
$\mathbf{B}_{23}$	$= -(x_3 - \frac{3}{4})\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{24}$	$= (x_3 + \frac{3}{4})\mathbf{a}_1 + (x_3 + \frac{1}{2})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + a(x_3 + \frac{1}{2})\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B}_{25}$	$= (y_4 + z_4)\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + ay_4\hat{\mathbf{y}} + az_4\hat{\mathbf{z}}$	(48e)	O II

$\mathbf{B}_{26}$	$=$	$\begin{aligned} & - (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ & (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{27}$	$=$	$\begin{aligned} & (y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ & (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{28}$	$=$	$\begin{aligned} & - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + \\ & (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 \end{aligned}$	$=$	$ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{29}$	$=$	$\begin{aligned} & (x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + \\ & (x_4 + z_4) \mathbf{a}_3 \end{aligned}$	$=$	$az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{30}$	$=$	$\begin{aligned} & - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 + \\ & (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 \end{aligned}$	$=$	$az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{31}$	$=$	$\begin{aligned} & (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ & (y_4 - z_4) \mathbf{a}_2 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$-az_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{32}$	$=$	$\begin{aligned} & (x_4 - y_4) \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ & (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$-a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{33}$	$=$	$\begin{aligned} & (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \\ & (y_4 + z_4) \mathbf{a}_3 \end{aligned}$	$=$	$ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{34}$	$=$	$\begin{aligned} & - (x_4 - z_4) \mathbf{a}_1 - \\ & (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_2 + \\ & (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{35}$	$=$	$\begin{aligned} & - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + \\ & (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 \end{aligned}$	$=$	$ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{36}$	$=$	$\begin{aligned} & (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ & (x_4 - y_4) \mathbf{a}_2 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$-ay_4 \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{37}$	$=$	$\begin{aligned} & - (y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - \\ & (x_4 + y_4) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{38}$	$=$	$\begin{aligned} & (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ & (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{39}$	$=$	$\begin{aligned} & - (y_4 - z_4) \mathbf{a}_1 + \\ & (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ & (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{40}$	$=$	$\begin{aligned} & (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ & (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{41}$	$=$	$\begin{aligned} & - (x_4 + y_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - \\ & (x_4 + z_4) \mathbf{a}_3 \end{aligned}$	$=$	$-az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{42}$	$=$	$\begin{aligned} & (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ & (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 \end{aligned}$	$=$	$-az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{43}$	$=$	$\begin{aligned} & (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 - \\ & (y_4 - z_4) \mathbf{a}_2 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$az_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{44}$	$=$	$\begin{aligned} & - (x_4 - y_4) \mathbf{a}_1 + \\ & (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ & (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned}$	$=$	$a(z_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{45}$	$=$	$\begin{aligned} & - (x_4 + z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - \\ & (y_4 + z_4) \mathbf{a}_3 \end{aligned}$	$=$	$-ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B}_{46}$	$=$	<				

$$\mathbf{B}_{48} = \begin{pmatrix} -x_4 + z_4 + \frac{1}{2} \\ x_4 - y_4 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_4 + z_4 + \frac{1}{2} \\ \end{pmatrix} \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{2} \right) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} \quad (48e) \quad \text{O II}$$

References

- [1] O. Noguera, P. Thomas, O. Masson, and J.-C. Champarnaud-Mesjard, *Refinement of the crystal structure of zirconium tritellurate(IV), ZrTe_3O_8* , Z. Kristallogr. NCS **218**, 293–294 (2003), doi:10.1524/ncrs.2003.218.jg.315.

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