$ZrTe_3O_8$ Structure: A8B3C_cI96_206_ce_d_a-001

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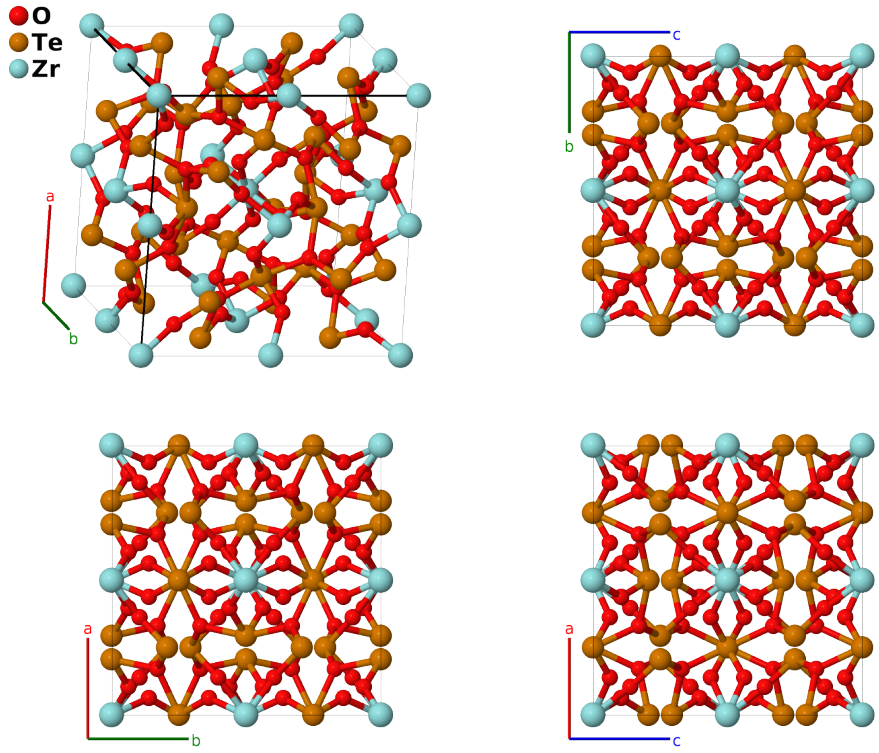
https://aflow.org/p/3HHF

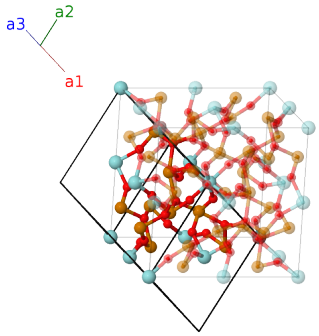
https://aflow.org/p/A8B3C_cI96_206_ce_d_a-001



Prototype	O_8Te_3Zr
AFLOW prototype label	A8B3C_cI96_206_ce_d_a-001
ICSD	409713
Pearson symbol	cI96
Space group number	206
Space group symbol	$Ia\bar{3}$
AFLOW prototype command	`aflow --proto=A8B3C_cI96_206_ce_d_a-001 --params=`$a, x_2, x_3, x_4, y_4, z_4$

Body-centered Cubic primitive vectors

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



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
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B_7}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B_8}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B_{11}}$	=	$\left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B_{12}}$	=	$\left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B_{13}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{14}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{15}}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(24d)	Te I
$\mathbf{B_{16}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{17}}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{18}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{19}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{20}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(24d)	Te I
$\mathbf{B_{22}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(24d)	Te I
$\mathbf{B_{23}}$	=	$-\left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24d)	Te I
$\mathbf{B_{24}}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{26}}$	=	$\left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - \left(x_4 + y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(48e)	O II

$\mathbf{B_{27}}$	$=$	$(y_4 - z_4)\ \mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{2}\right)\ \mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\ \hat{\mathbf{x}} + a y_4\ \hat{\mathbf{y}} - a z_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{28}}$	$=$	$-\left(y_4 + z_4 - \frac{1}{2}\right)\ \mathbf{a}_1 + \left(x_4 - z_4 + \frac{1}{2}\right)\ \mathbf{a}_2 + (x_4 - y_4)\ \mathbf{a}_3$	$=$	$a x_4\ \hat{\mathbf{x}} - a y_4\ \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{29}}$	$=$	$(x_4 + y_4)\ \mathbf{a}_1 + (y_4 + z_4)\ \mathbf{a}_2 + (x_4 + z_4)\ \mathbf{a}_3$	$=$	$a z_4\ \hat{\mathbf{x}} + a x_4\ \hat{\mathbf{y}} + a y_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{30}}$	$=$	$-\left(x_4 + y_4 - \frac{1}{2}\right)\ \mathbf{a}_1 + \left(-y_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_2 - (x_4 - z_4)\ \mathbf{a}_3$	$=$	$a z_4\ \hat{\mathbf{x}} - a x_4\ \hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{31}}$	$=$	$\left(-x_4 + y_4 + \frac{1}{2}\right)\ \mathbf{a}_1 + (y_4 - z_4)\ \mathbf{a}_2 - \left(x_4 + z_4 - \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a z_4\ \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\ \hat{\mathbf{y}} + a y_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{32}}$	$=$	$(x_4 - y_4)\ \mathbf{a}_1 - \left(y_4 + z_4 - \frac{1}{2}\right)\ \mathbf{a}_2 + \left(x_4 - z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a\left(z_4 - \frac{1}{2}\right)\ \hat{\mathbf{x}} + a x_4\ \hat{\mathbf{y}} - a y_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{33}}$	$=$	$(x_4 + z_4)\ \mathbf{a}_1 + (x_4 + y_4)\ \mathbf{a}_2 + (y_4 + z_4)\ \mathbf{a}_3$	$=$	$a y_4\ \hat{\mathbf{x}} + a z_4\ \hat{\mathbf{y}} + a x_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{34}}$	$=$	$-(x_4 - z_4)\ \mathbf{a}_1 - \left(x_4 + y_4 - \frac{1}{2}\right)\ \mathbf{a}_2 + \left(-y_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a\left(y_4 - \frac{1}{2}\right)\ \hat{\mathbf{x}} + a z_4\ \hat{\mathbf{y}} - a x_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{35}}$	$=$	$-\left(x_4 + z_4 - \frac{1}{2}\right)\ \mathbf{a}_1 + \left(-x_4 + y_4 + \frac{1}{2}\right)\ \mathbf{a}_2 + (y_4 - z_4)\ \mathbf{a}_3$	$=$	$a y_4\ \hat{\mathbf{x}} - a z_4\ \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{36}}$	$=$	$\left(x_4 - z_4 + \frac{1}{2}\right)\ \mathbf{a}_1 + (x_4 - y_4)\ \mathbf{a}_2 - \left(y_4 + z_4 - \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a y_4\ \hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right)\ \hat{\mathbf{y}} + a x_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{37}}$	$=$	$-(y_4 + z_4)\ \mathbf{a}_1 - (x_4 + z_4)\ \mathbf{a}_2 - (x_4 + y_4)\ \mathbf{a}_3$	$=$	$-a x_4\ \hat{\mathbf{x}} - a y_4\ \hat{\mathbf{y}} - a z_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{38}}$	$=$	$\left(y_4 - z_4 + \frac{1}{2}\right)\ \mathbf{a}_1 + (x_4 - z_4)\ \mathbf{a}_2 + \left(x_4 + y_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a x_4\ \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\ \hat{\mathbf{y}} - a z_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{39}}$	$=$	$-(y_4 - z_4)\ \mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(x_4 - y_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right)\ \hat{\mathbf{x}} - a y_4\ \hat{\mathbf{y}} + a z_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{40}}$	$=$	$\left(y_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_2 - (x_4 - y_4)\ \mathbf{a}_3$	$=$	$-a x_4\ \hat{\mathbf{x}} + a y_4\ \hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{41}}$	$=$	$-(x_4 + y_4)\ \mathbf{a}_1 - (y_4 + z_4)\ \mathbf{a}_2 - (x_4 + z_4)\ \mathbf{a}_3$	$=$	$-a z_4\ \hat{\mathbf{x}} - a x_4\ \hat{\mathbf{y}} - a y_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{42}}$	$=$	$\left(x_4 + y_4 + \frac{1}{2}\right)\ \mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\ \mathbf{a}_2 + (x_4 - z_4)\ \mathbf{a}_3$	$=$	$-a z_4\ \hat{\mathbf{x}} + a x_4\ \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{43}}$	$=$	$\left(x_4 - y_4 + \frac{1}{2}\right)\ \mathbf{a}_1 - (y_4 - z_4)\ \mathbf{a}_2 + \left(x_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a z_4\ \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\ \hat{\mathbf{y}} - a y_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{44}}$	$=$	$-(x_4 - y_4)\ \mathbf{a}_1 + \left(y_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(-x_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a\left(z_4 + \frac{1}{2}\right)\ \hat{\mathbf{x}} - a x_4\ \hat{\mathbf{y}} + a y_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{45}}$	$=$	$-(x_4 + z_4)\ \mathbf{a}_1 - (x_4 + y_4)\ \mathbf{a}_2 - (y_4 + z_4)\ \mathbf{a}_3$	$=$	$-a y_4\ \hat{\mathbf{x}} - a z_4\ \hat{\mathbf{y}} - a x_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{46}}$	$=$	$(x_4 - z_4)\ \mathbf{a}_1 + \left(x_4 + y_4 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(y_4 - z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right)\ \hat{\mathbf{x}} - a z_4\ \hat{\mathbf{y}} + a x_4\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{47}}$	$=$	$\left(x_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_1 + \left(x_4 - y_4 + \frac{1}{2}\right)\ \mathbf{a}_2 - (y_4 - z_4)\ \mathbf{a}_3$	$=$	$-a y_4\ \hat{\mathbf{x}} + a z_4\ \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(48e)	O II
$\mathbf{B_{48}}$	$=$	$\left(-x_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_1 - (x_4 - y_4)\ \mathbf{a}_2 + \left(y_4 + z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a y_4\ \hat{\mathbf{x}} + a\left(z_4 + \frac{1}{2}\right)\ \hat{\mathbf{y}} - a x_4\ \hat{\mathbf{z}}$	(48e)	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.