WTe_2 Structure: A2B_oP12_31_4a_2a-001

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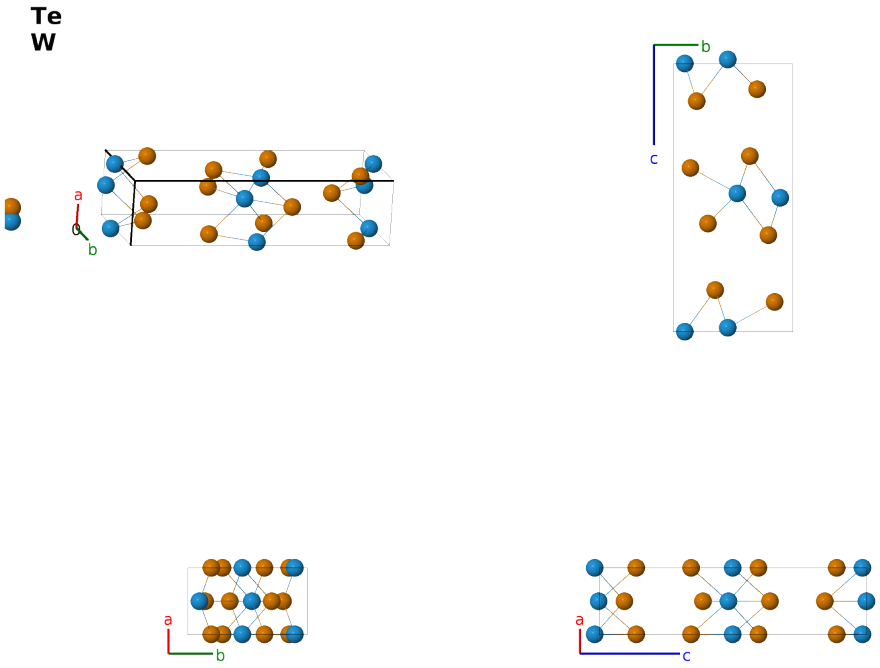
https://aflow.org/prototype-encyclopedia/ZLWB

https://aflow.org/prototype-encyclopedia/A2B_oP12_31_4a_2a-001

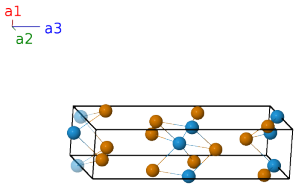


Prototype	Te_2W
AFLOW prototype label	A2B_oP12_31_4a_2a-001
ICSD	14348
CCDC	1595734
Pearson symbol	oP12
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	`aflow --proto=A2B_oP12_31_4a_2a-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6$

- (Brown, 1966) gives this structure in the $Pnm2_1$ setting of space group #31. We used FINDSYM to transform this to the standard $Pmn2_1$ setting.
- Space group $Pmn2_1$ allows an arbitrary choice of origin for the z-axis. We set $z_5 = 1/2$ for the W-I atom.

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
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Te I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te I
$\mathbf{B_3}$	=	$y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2a)	Te II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2a)	Te III
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te III
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2a)	Te IV
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te IV
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2a)	W I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	W I
$\mathbf{B_{11}}$	=	$y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2a)	W II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	W II

References

[1] B. E. Brown, *The crystal structures of WTe_2 and high-temperature $MoTe_2$*, Acta Cryst. **20**, 268–274 (1966), doi:10.1107/S0365110X66000513.

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