$NbIrTe_4$ Structure: ABC4_oP24_31_2a_2a_8a-001

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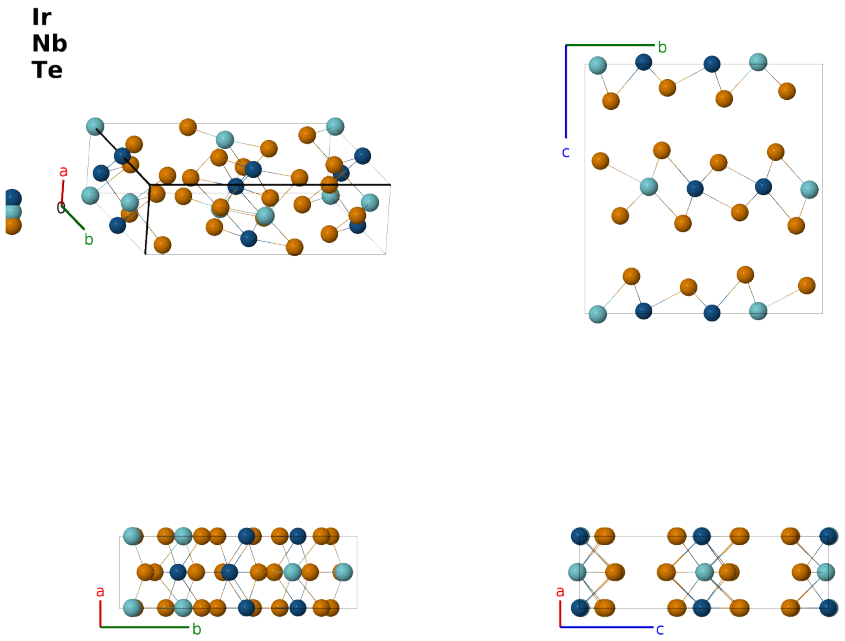
https://aflow.org/prototype-encyclopedia/H22P

https://aflow.org/prototype-encyclopedia/ABC4_oP24_31_2a_2a_8a-001



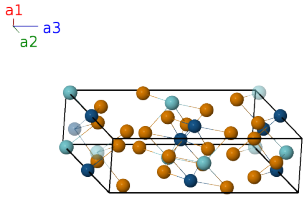
Prototype	$IrNbTe_4$
AFLOW prototype label	ABC4_oP24_31_2a_2a_8a-001
ICSD	73690
CCDC	1634457
Pearson symbol	oP24
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	`aflow --proto=ABC4_oP24_31_2a_2a_8a-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, y_7, z_7, y_8, z_8, y_9, z_9, y_{10}, z_{10}, y_{11}, z_{11}, y_{12}, z_{12}$

Other compounds with this structure
$NbOsTe_4$, $TaIrTe_4$, $TaOsTe_4$, $TaRhTe_4$, $TaRuTe_4$

- Space group $Pmn2_1$ #31 allows an arbitrary placement of the origin of the z-axis. Here we set $z_1 = 0$ for the first iridium Wyckoff position.

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)	Ir 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)	Ir 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)	Ir 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)	Ir 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)	Nb I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2a)	Nb II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Nb II
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2a)	Te 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)	Te 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)	Te 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)	Te II
$\mathbf{B_{13}}$	=	$y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2a)	Te III
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te III
$\mathbf{B_{15}}$	=	$y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(2a)	Te IV
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te IV
$\mathbf{B_{17}}$	=	$y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(2a)	Te V
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te V
$\mathbf{B_{19}}$	=	$y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(2a)	Te VI
$\mathbf{B_{20}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te VI
$\mathbf{B_{21}}$	=	$y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(2a)	Te VII
$\mathbf{B_{22}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Te VII
$\mathbf{B_{23}}$	=	$y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(2a)	Te VIII

$$\mathbf{B_{24}} = \tfrac{1}{2}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(2a)} \quad \text{Te VIII}$$

References

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