UTe_2 Structure: A2B_oI12_71_eh_f-001

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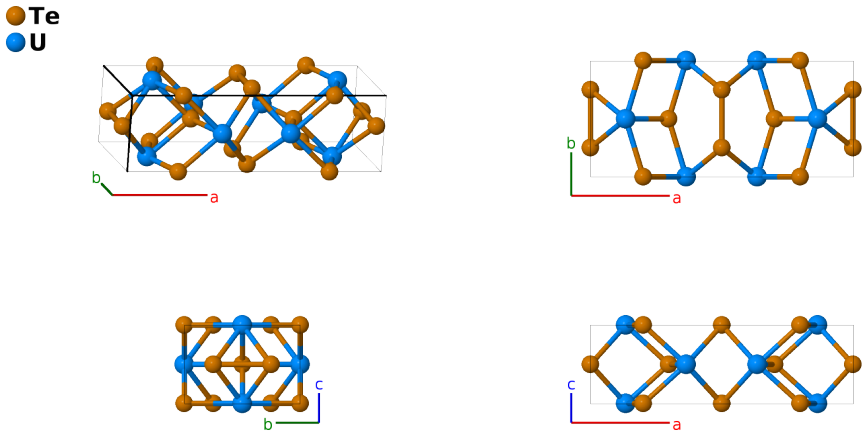
https://aflow.org/p/7HXW

https://aflow.org/p/A2B_oI12_71_eh_f-001

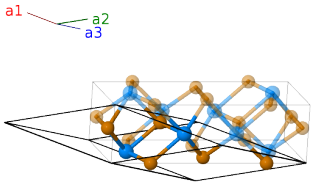


Prototype	Te_2U
AFLOW prototype label	A2B_oI12_71_eh_f-001
ICSD	403519
Pearson symbol	oI12
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A2B_oI12_71_eh_f-001 --params=`$a, b/a, c/a, x_1, x_2, y_3$

- Data for this structure was taken at 2.7K.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(4e)	Te I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Te I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	U I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	U I
$\mathbf{B_5}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B_6}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Te II

References

[1] V. Hutanu, H. Deng, S. Ran, W. T. Fuhrman, H. Thoma, and N. P. Butch, *Low-temperature crystal structure of the unconventional spin-triplet superconductor UTe_2 from single-crystal neutron diffraction*, Acta Crystallogr. Sect. B **76**, 137–143 (2020), doi:10.1107/S2052520619016950.