

UTe₂ Structure:

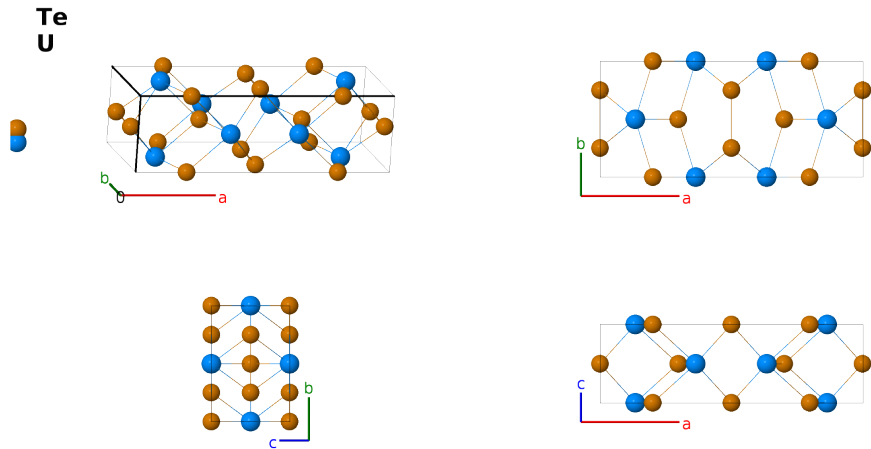
A2B_oI12_71_eh_f-001

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<https://aflow.org/prototype-encyclopedia/7HXW>

https://aflow.org/prototype-encyclopedia/A2B_oI12_71_eh_f-001

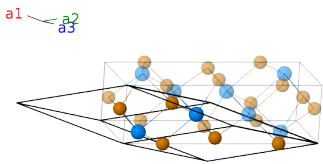


Prototype	Te ₂ U
AFLOW prototype label	A2B_oI12_71_eh_f-001
ICSD	403519
CCDC	1919708
Pearson symbol	oI12
Space group number	71
Space group symbol	<i>Immm</i>
AFLOW prototype command	<code>aflow --proto=A2B_oI12_71_eh_f-001</code> <code>--params=a, b/a, c/a, x₁, x₂, y₃</code>

- Data for this structure was taken at 2.7K.

Body-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}} \end{aligned}$$



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
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(4f) U I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(4f) U I
$\mathbf{B}_5$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h) Te II
$\mathbf{B}_6$	$=$	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(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 UTe₂ from single-crystal neutron diffraction*, Acta Crystallogr. Sect. B **76**, 137–143 (2020), doi:10.1107/S2052520619016950.

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