Ti_5Te_4 Structure: A4B5_tI18_87_h_ah-001

This structure previously used the label(s) `A4B5_tI18_87_h_ah`. Calls to these addresses will be redirected here.

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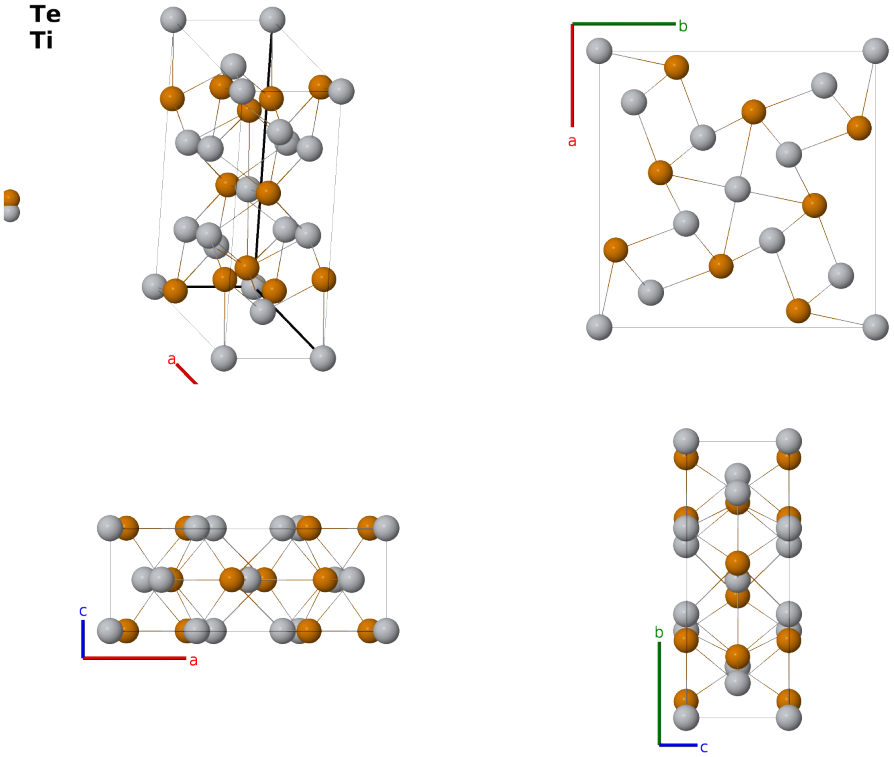
https://aflow.org/prototype-encyclopedia/E7DL

https://aflow.org/prototype-encyclopedia/A4B5_tI18_87_h_ah-001



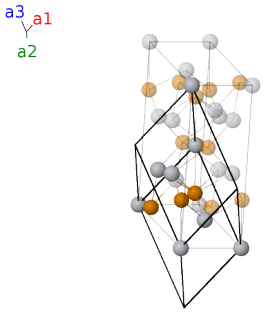
Prototype	Te_4Ti_5
AFLOW prototype label	A4B5_tI18_87_h_ah-001
ICSD	15451
CCDC	1596196
Pearson symbol	tI18
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=A4B5_tI18_87_h_ah-001 --params=`$a, c/a, x_2, y_2, x_3, y_3$

Other compounds with this structure

Mo_5As_4, Nb_5Sb_4, Nb_5Se_4, Nb_5Te_4, Ta_5Sb_4, V_5S_4, V_5Se_4

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ti I
$\mathbf{B_2}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + (x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(8h)	Te I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - (x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(8h)	Te I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + (x_2-y_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Te I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - (x_2-y_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Te I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	Ti II
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	Ti II
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Ti II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Ti II

References

[1] F. Gr, A. Kjekshus, and F. Raaum, *The crystal structure of Ti_5Te_4*, Acta Cryst. **14**, 930–934 (1961), doi:10.1107/S0365110X61002722.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

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