Pt_8Ti Structure: A8B_tI18_139_hi_a-001

This structure originally had the label `A8B_tI18_139_hi_a`. Calls to that address will be redirected here.

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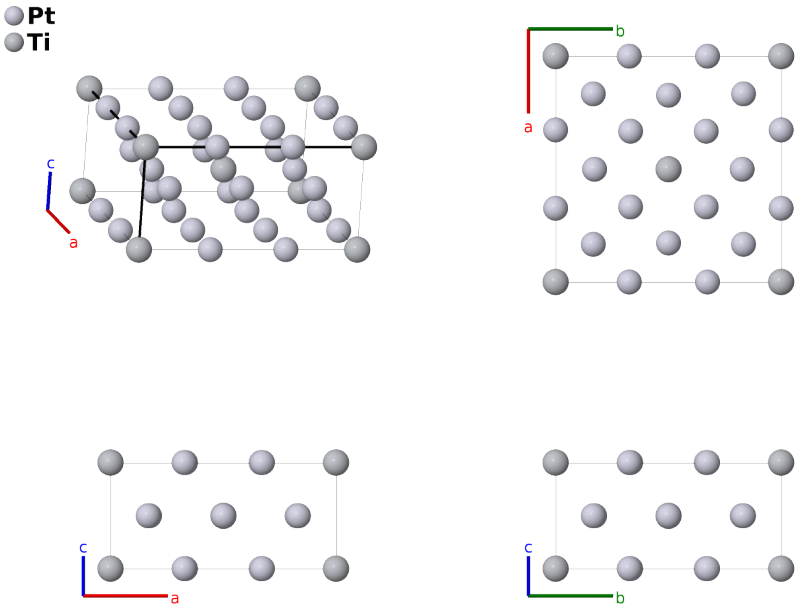
https://aflow.org/p/XTZU

https://aflow.org/p/A8B_tI18_139_hi_a-001



Prototype	Pt_8Ti
AFLOW prototype label	A8B_tI18_139_hi_a-001
ICSD	105818
Pearson symbol	tI18
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A8B_tI18_139_hi_a-001 --params=`$a, c/a, x_2, x_3$

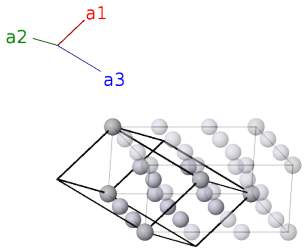
Other compounds with this structure

Ni_8Mo, Ni_8Nb, Ni_8Ta, Ni_8V, Pd_8Mo, Pd_8V, Pd_8W, Pt_8Ce, Pt_8Ti, Pt_8V, Pt_8Zr

- When $a = 3/(\sqrt{2})a_{fcc}$, $c = a_{fcc}$, $x_2 = 1/3$, and $x_3 = 1/3$ the atoms are on the sites of the fcc lattice. Compare this structure to the very similar V_4Zn_5.

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
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Pt I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - 2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Pt I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Pt I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Pt I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8i)	Pt II
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8i)	Pt II
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(8i)	Pt II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(8i)	Pt II

References

[1] P. Pietrokowsky, *Novel Ordered Phase, Pt_8Ti*, Nature **206**, 291 (1965), doi:10.1038/206291a0.

[2] R. H. Taylor, S. Curtarolo, and G. L. W. Hart, *Predictions of the Pt_8Ti Phase in Unexpected Systems*, Journal of the American Chemical Society **132**, 6851–6854 (2010), doi:10.1021/ja101890k.

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.