ThH_2 ($L'2_b$) Structure: A2B_tI6_139_d_a-001

This structure originally had the label `A2B_tI6_139_d_a`. Calls to that address will be redirected here.

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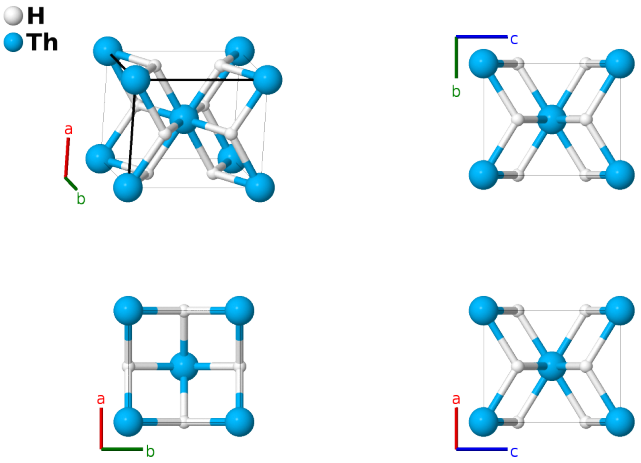
https://aflow.org/p/R0C0

https://aflow.org/p/A2B_tI6_139_d_a-001



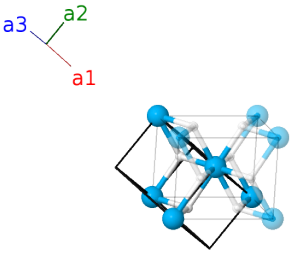
Prototype	H_2Th
AFLOW prototype label	A2B_tI6_139_d_a-001
***Strukturbericht* designation**	$L'2_b$
ICSD	24623
Pearson symbol	tI6
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2B_tI6_139_d_a-001 --params=`$a, c/a$

Other compounds with this structure
$SiPt_2$, TiH_2, ZrH_2, Pt_2Si (LT)

- This structure was given the extended *Strukturbericht* label $L'2_b$ by (Pearson, 1967). It did not appear in the original *Strukturbericht* volumes. We had previously followed (Villars, 1991) and (Westbrook, 1995) and gave it the label $L'2$, however this conflicts with the label for the $L'2_0$ "martensite" structure, so we will now use the original label.

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)	Th I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	H I

References

[1] R. E. Rundle, C. G. Shull, and E. O. Wollan, *The crystal structure of thorium and zirconium dihydrides by X-ray and neutron diffraction*, Acta Cryst. **5**, 22–26 (1952), doi:10.1107/S0365110X52000071.

[2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

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

[4] J. H. Westbrook and R. L. Fleischer, eds., *Intermetallic Compounds – Principles and Practice* (John Wiley & Sons, Ltd., Chichester, England, 1995). Two Volumes.