

ThH₂ ($L'2_b$) Structure: A2B_tI6_139_d_a-001

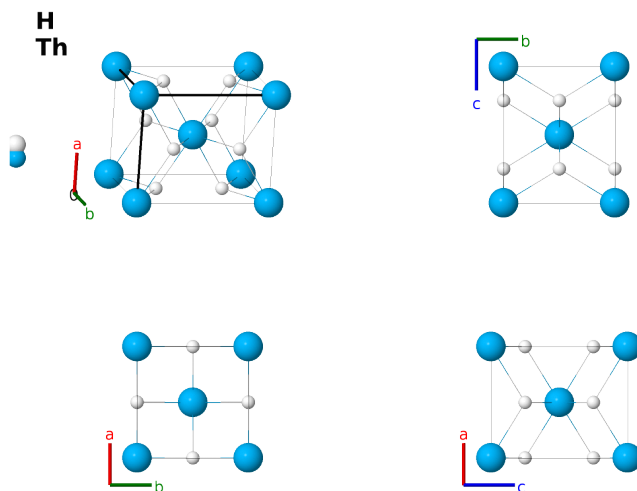
This structure previously used the label(s) **A2B_tI6_139_d_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/R0C0>

https://aflow.org/prototype-encyclopedia/A2B_tI6_139_d_a-001



Prototype	H ₂ Th
AFLOW prototype label	A2B_tI6_139_d_a-001
<i>Strukturbericht</i> designation	$L'2_b$
ICSD	24623
CCDC	1600642
Pearson symbol	tI6
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=A2B_tI6_139_d_a-001 --params=a, c/a</code>

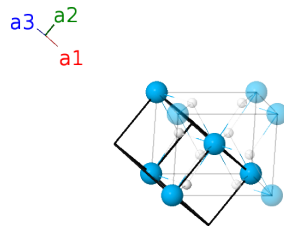
Other compounds with this structure

SiPt₂, TiH₂, ZrH₂, Pt₂Si (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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	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.

First cited in

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