ThB$_2$C Structure:
A2BC_hR12_166_g_d_ac-001

https://aflow.org/p/AFH9

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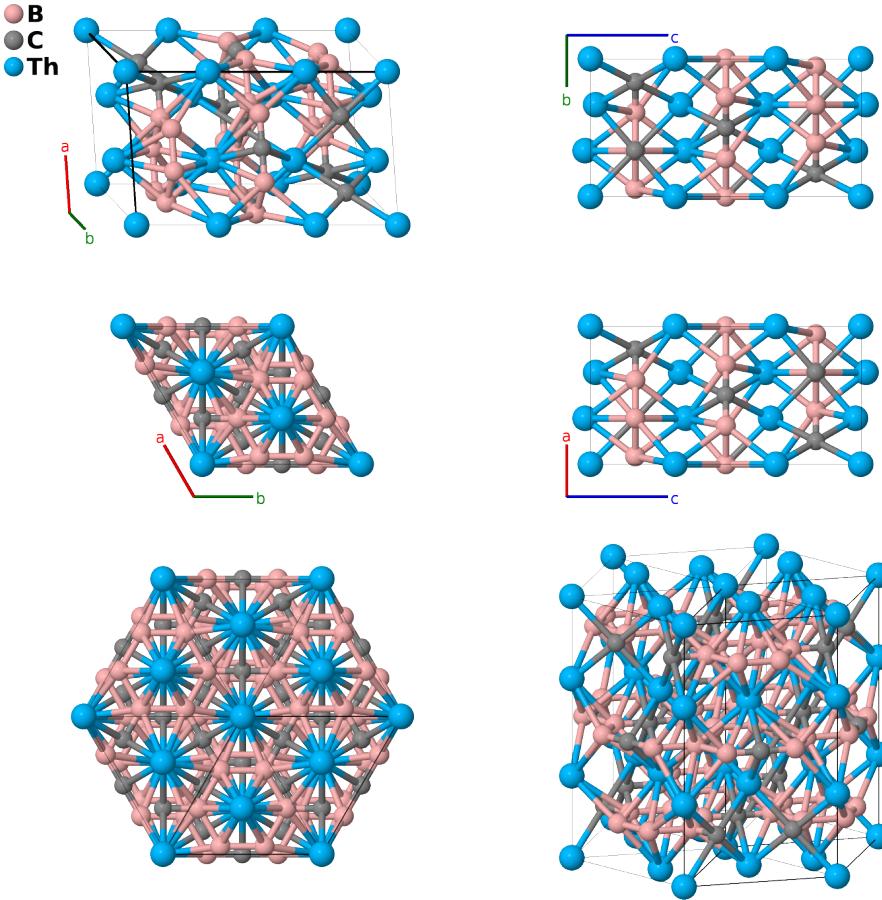
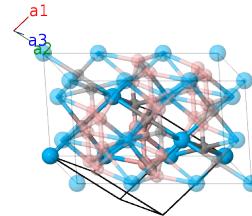|	
Prototype	BCTh$_2$
AFLOW prototype label	A2BC_hR12_166_g_d_ac-001
ICSD	68414
Pearson symbol	hR12
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	aflow --proto=A2BC_hR12_166_g_d_ac-001 --params=$a, c/a, x_2, x_4$

Other compounds with this structure

β-UB$_2$C (HT)

- We take the coordinates from the neutron powder diffraction data at 298K.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Th I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + x_2\,\mathbf{a_3}$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Th II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} - x_2\,\mathbf{a_3}$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Th II
$\mathbf{B_4}$	=	$\tfrac{1}{2}\,\mathbf{a_1}$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	C I
$\mathbf{B_5}$	=	$\tfrac{1}{2}\,\mathbf{a_2}$	=	$\tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	C I
$\mathbf{B_6}$	=	$\tfrac{1}{2}\,\mathbf{a_3}$	=	$-\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	C I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	=	$\tfrac{1}{4}a\,(2x_4-1)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,(6x_4+1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_8}$	=	$\tfrac{1}{2}\,\mathbf{a_1} + x_4\,\mathbf{a_2} - x_4\,\mathbf{a_3}$	=	$\tfrac{1}{4}a\,(2x_4+1)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{12}a\,(6x_4-1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a_1} + \tfrac{1}{2}\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	=	$-ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	=	$-\tfrac{1}{4}a\,(2x_4+1)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{12}a\,(6x_4-1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{11}}$	=	$\tfrac{1}{2}\,\mathbf{a_1} - x_4\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	=	$-\tfrac{1}{4}a\,(2x_4-1)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,(6x_4+1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a_1} + \tfrac{1}{2}\,\mathbf{a_2} - x_4\,\mathbf{a_3}$	=	$ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I

References

[1] P. Rogl and P. Fischer, *Single-crystal X-ray and powder neutron diffraction of ThB$_2$C (ThB$_2$C-type)*, J. Solid State Chem. **78**, 294–300 (1989), doi:10.1016/0022-4596(89)90110-2.

Found in

[1] P. Rogl and P. Fischer, *Powder neutron diffraction of αUB$_2$C (αUB$_2$C-type)*, J. Solid State Chem. **90**, 285–290 (1991), doi:10.1016/0022-4596(91)90144-7.