ThB_2C Structure: A2BC_hR12_166_g_d_ac-001

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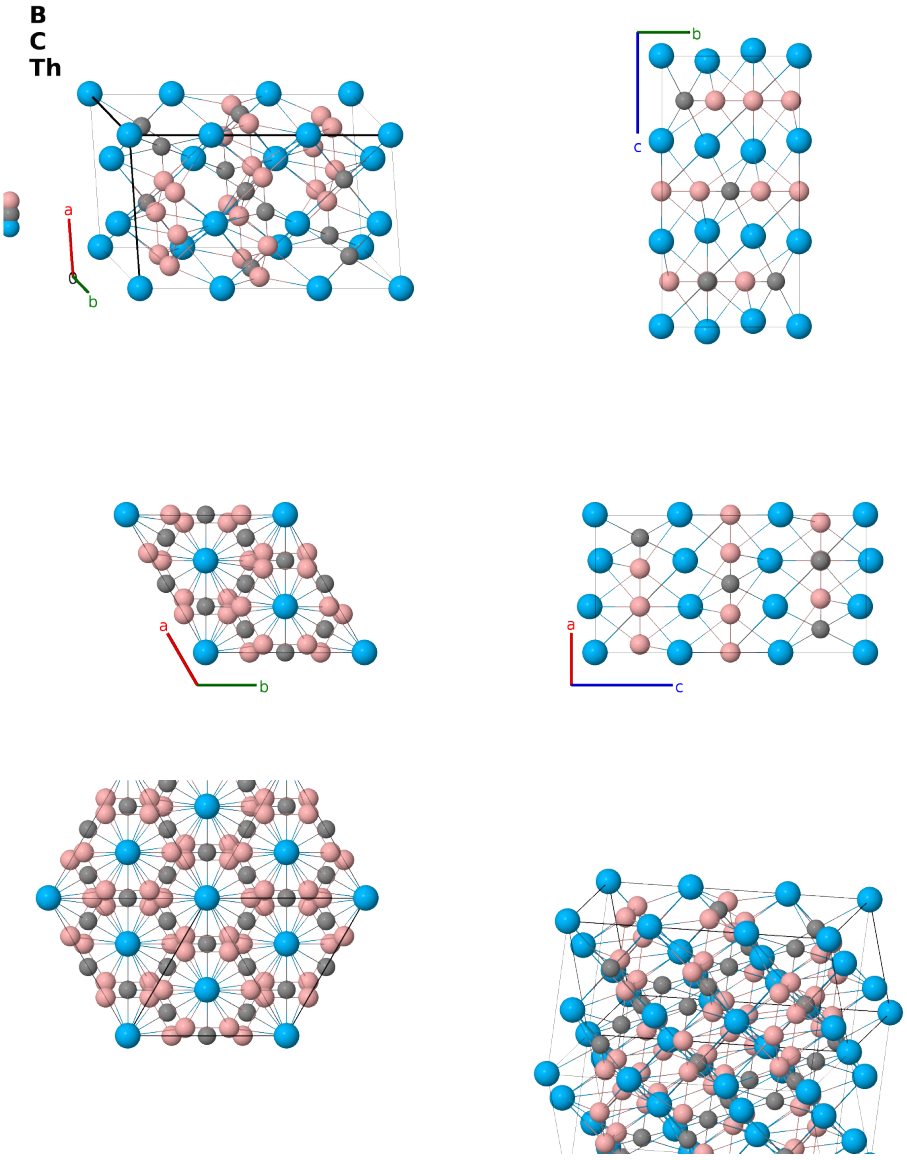
https://aflow.org/prototype-encyclopedia/AFH9

https://aflow.org/prototype-encyclopedia/A2BC_hR12_166_g_d_ac-001



Prototype	$BCTh_2$
AFLOW prototype label	A2BC_hR12_166_g_d_ac-001
ICSD	68414

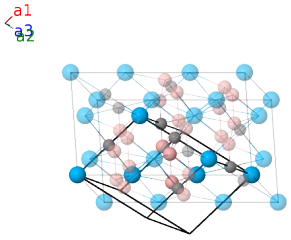
CCDC	1630337
Pearson symbol	hR12
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A2BC_hR12_166_g_d_ac-001 --params=`$a, c/a, x_2, x_4$

Other compounds with this structure
β-UB_2C (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

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



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
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	C I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	C I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	C I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2x_4 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6x_4 + 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2x_4 + 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6x_4 - 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,(2x_4 + 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6x_4 - 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,(2x_4 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6x_4 + 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	B I

References

[1] P. Rogl and P. Fischer, *Single-crystal X-ray and powder neutron diffraction of ThB_2C (ThB_2C-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_2C (αUB_2C-type)*, J. Solid State Chem. **90**, 285–290 (1991), doi:10.1016/0022-4596(91)90144-7.

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