$B_{13}C_2$ "B_4C" ($D1_g$) Structure: A13B2_hR15_166_a2h_c-001

This structure originally had the label `A13B2_hR15_166_b2h_c`. Calls to that address will be redirected here.

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https://aflow.org/p/PZDF

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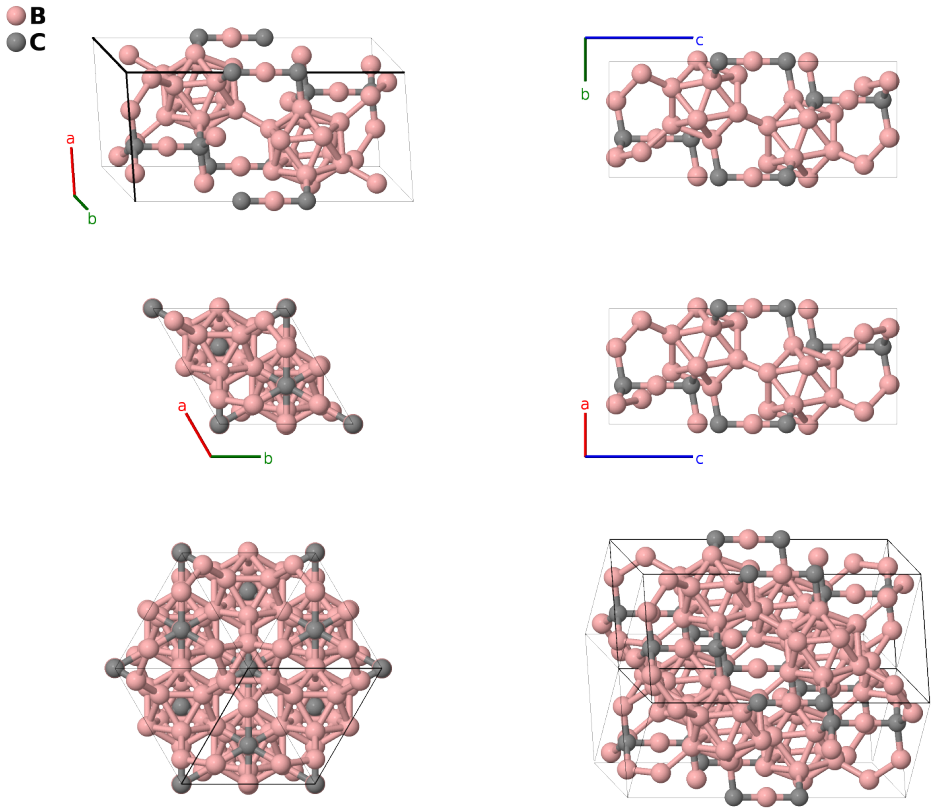


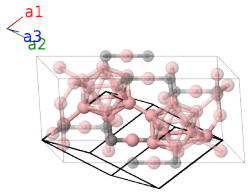
Prototype	$B_{13}C_2$
AFLOW prototype label	A13B2_hR15_166_a2h_c-001
***Strukturbericht* designation**	$D1_g$
ICSD	612566
Pearson symbol	hR15
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A13B2_hR15_166_a2h_c-001 --params=`$a, c/a, x_2, x_3, z_3, x_4, z_4$

Other compounds with this structure
$B_{1-x}C_x$, $B_{13}P_2$, B_4Si, B_6O

- This structure has a rather complicated history:
- It is difficult to determine the species of atoms at a given site because of the similar electronic and nuclear cross sections of ^{11}B and ^{12}C (Domnich, 2011).
- Early investigations (Clark, 1943) assumed the structure was B_4C, with the extra carbon atom replacing the boron on the (1b) site. [Note that Clark has an error in the coordinates of one set of boron atoms, giving a boron-boron distance of less that 1Å. This error is repeated in (Brandes, 1992) and (Wykcoff, 1964).]
- In reality, concentrations can range from 8-20% carbon (Domnich, 2011).
- (Larson, 1986) states that in $B_{13}C_2$ the (1b) site is boron and as the structure becomes more carbon rich the carbon atoms replace borons in the iscosahedra. We follow this and use the structure determined by (Will, 1976) as our reference.
- (Lazzari, 1999) states that excess electrons go on the "polar" sites of the icosahedron, *i.e.* the sites closest to the carbon atoms on the chains (the B III atoms in our notation).
- The original version of this page (Hicks, 2021) listed $a = 6.617$Å rather than $a = 5.617$Å. This has now been corrected.

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)	B 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)	C I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	C I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\,\hat{\mathbf{z}}$	(6h)	B III
$\mathbf{B_{11}}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\,\hat{\mathbf{z}}$	(6h)	B III

$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$	(6h)	B III
$\mathbf{B_{13}}$	=	$-z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$	(6h)	B III
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$	(6h)	B III
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_4 - z_4)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$	(6h)	B III

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