

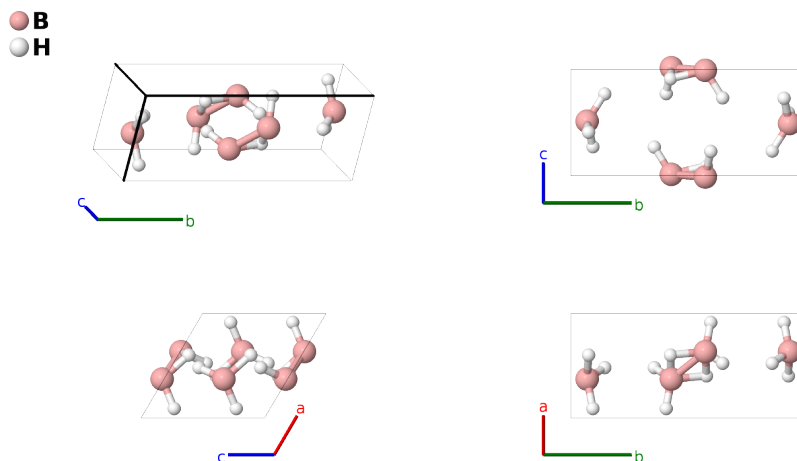
“ $P2_1/c$ ”- B_2H_6 Structure: AB3_mP16_14_e_3e-002

This structure originally had the label AB3_mP16_14_e_3e. Calls to that address will be redirected here.

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<https://aflow.org/p/3XCA>

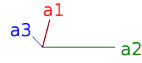
https://aflow.org/p/AB3_mP16_14_e_3e-002



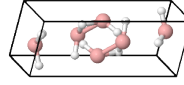
Prototype	B_2H_6
AFLOW prototype label	AB3_mP16_14_e_3e-002
ICSD	none
Pearson symbol	mP16
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=AB3_mP16_14_e_3e-002 --params=a, b/a, c/a, β, $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$</pre>

- (Mark, 1925) studied a variety of B_2H_6 structures, including the one given *Strukturbericht* designation $D4_1$ by (Ewald, 1931). Very little information was given about this structure, other than Ewald's statement "The position of the boron atoms is exactly the same as that of the Hg atoms in the A10 (α -Hg) structure." (Yao, 2011) found the current structure computationally, and note that it is likely the structure found by (Mark, 1925).
- This structure shares the same AFLOW designation, AB3_mP16_14_e_3e, as the β - B_2H_6 structure described by (Smith, 1965). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Monoclinic primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	B I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	B I
\mathbf{B}_3	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	B I
\mathbf{B}_4	$x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	B I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	H I
\mathbf{B}_6	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H I
\mathbf{B}_7	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	H I
\mathbf{B}_8	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H I
\mathbf{B}_9	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	H II
\mathbf{B}_{10}	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H II
\mathbf{B}_{11}	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	H II
\mathbf{B}_{12}	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H II
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	H III
\mathbf{B}_{14}	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H III
\mathbf{B}_{15}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	H III
\mathbf{B}_{16}	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H III

References

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