

BaS₃ (original $D0_{17}$) Structure: AB3_oP16_18_ab_3c-001

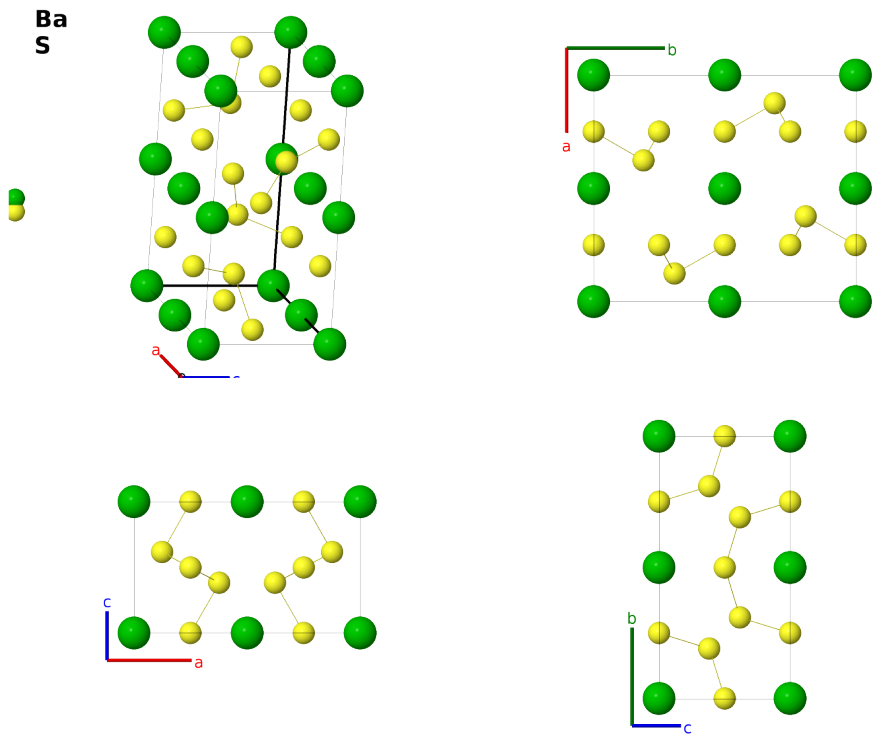
This structure previously used the label(s) **AB3_oP16_18_ab_3c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/69TS>

https://aflow.org/prototype-encyclopedia/AB3_oP16_18_ab_3c-001

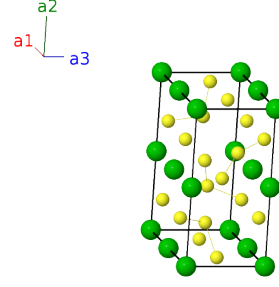


Prototype	BaS ₃
AFLOW prototype label	AB3_oP16_18_ab_3c-001
ICSD	26765
CCDC	1602149
Pearson symbol	oP16
Space group number	18
Space group symbol	$P2_12_12$
AFLOW prototype command	<code>aflow --proto=AB3_oP16_18_ab_3c-001</code> <code>--params=$a, b/a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$</code>

- (Gottfried, 1938) identified this as the $D0_{17}$ structure, but (Parthé, 1993) gave that designation to $P\bar{4}2_1m$ #113 BaS₃.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2b)	Ba II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c z_2 \hat{\mathbf{z}}$	(2b)	Ba II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B}_7$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B}_8$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B}_{11}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B}_{12}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B}_{15}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B}_{16}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(4c)	S III

References

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- [2] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.
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Found in

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First cited in

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