

BiGaO₃ Structure:

ABC3_oP20_54_e_d_cf-001

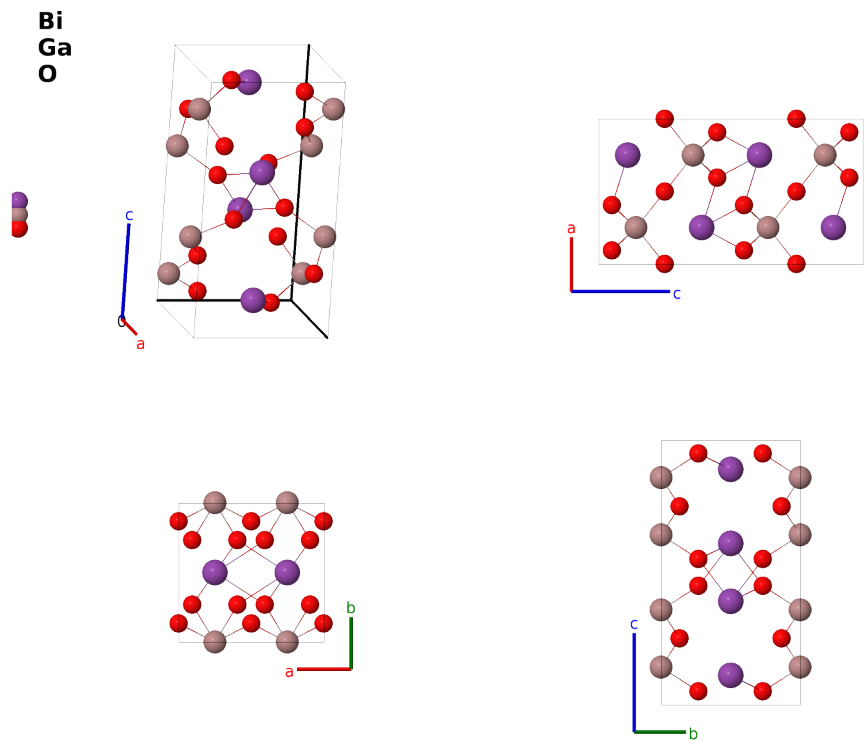
This structure previously used the label(s) **ABC3_oP20_54_e_d_cf**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/WWU9>

https://aflow.org/prototype-encyclopedia/ABC3_oP20_54_e_d_cf-001

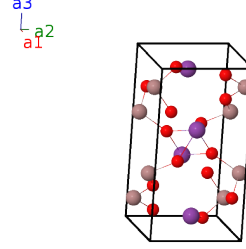


Prototype	BiGaO ₃
AFLOW prototype label	ABC3_oP20_54_e_d_cf-001
ICSD	171709
CCDC	1686909
Pearson symbol	oP20
Space group number	54
Space group symbol	<i>Pcca</i>
AFLOW prototype command	<code>aflow --proto=ABC3_oP20_54_e_d_cf-001</code> <code>--params=a, b/a, c/a, y₁, z₂, z₃, x₄, y₄, z₄</code>

- The lattice constants for this structure are from (Yusa, 2009), measured at 3.2 GPa. The authors did not give the atomic positions. These are taken from (Belik, 2006) at ambient pressure and temperature and are assumed to be similar to those at higher pressure.
- The ICSD entry is from (Belik, 2006).

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
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + cz_2 \hat{\mathbf{z}}$	(4d)	Ga I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ga I
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(4d)	Ga I
$\mathbf{B}_8$	$= \frac{1}{4} \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ga I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	Bi I
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Bi I
$\mathbf{B}_{11}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4e)	Bi I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Bi I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{14}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{18}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{20}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O II

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- [1] P. Villars, *BiGaO_3 (GaBiO_3 orth) Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

First cited in

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