$BiGaO_3$ Structure: ABC3_oP20_54_e_d_cf-001

This structure originally had the label `ABC3_oP20_54_e_d_cf`. Calls to that address will be redirected here.

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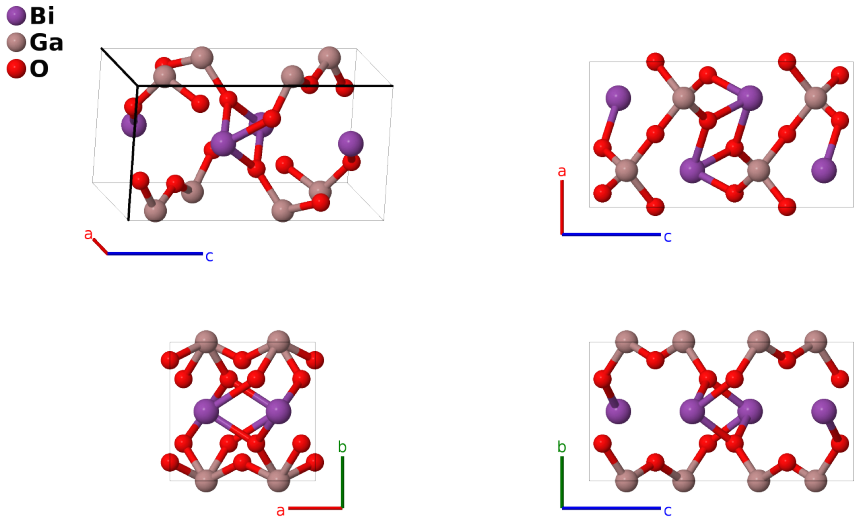
https://aflow.org/p/WWU9

https://aflow.org/p/ABC3_oP20_54_e_d_cf-001

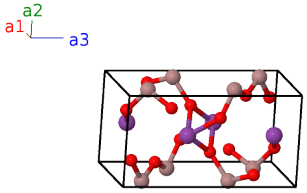


Prototype	$BiGaO_3$
AFLOW prototype label	ABC3_oP20_54_e_d_cf-001
ICSD	171709
Pearson symbol	oP20
Space group number	54
Space group symbol	*Pcca*
AFLOW prototype command	`aflow --proto=ABC3_oP20_54_e_d_cf-001 --params=`$a, b/a, c/a, y_1, z_2, z_3, x_4, y_4, z_4$

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{20}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II

References

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