Sr_2Bi_3 Structure: A3B2_oP20_52_de_cd-001

This structure originally had the label `A3B2_oP20_52_de_cd`. Calls to that address will be redirected here.

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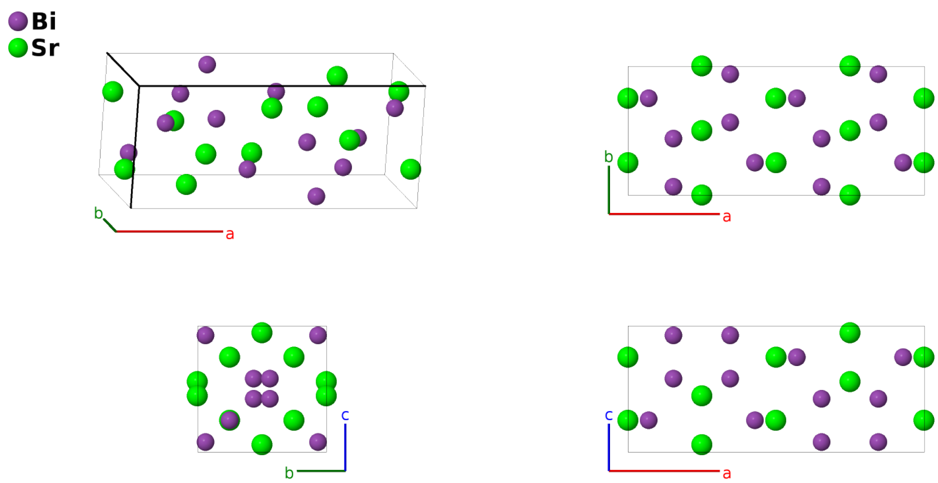
https://aflow.org/p/12L3

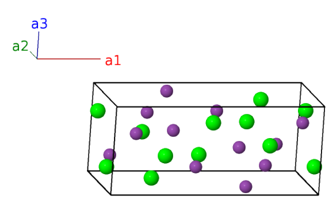
https://aflow.org/p/A3B2_oP20_52_de_cd-001



Prototype	Bi_3Sr_2
AFLOW prototype label	A3B2_oP20_52_de_cd-001
ICSD	164987
Pearson symbol	oP20
Space group number	52
Space group symbol	$Pnna$
AFLOW prototype command	`aflow --proto=A3B2_oP20_52_de_cd-001 --params=`$a, b/a, c/a, z_1, x_2, x_3, x_4, y_4, z_4$

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + cz_1\,\mathbf{\hat{z}}$	(4c)	Sr I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + \frac{1}{2}b\,\mathbf{\hat{y}} - c\left(z_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Sr I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\mathbf{\hat{x}} - cz_1\,\mathbf{\hat{z}}$	(4c)	Sr I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\mathbf{\hat{x}} + \frac{1}{2}b\,\mathbf{\hat{y}} + c\left(z_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Sr I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4d)	Bi I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4d)	Bi I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(4d)	Bi I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(4d)	Bi I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4d)	Sr II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4d)	Sr II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(4d)	Sr II
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(4d)	Sr II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{15}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{18}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{19}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8e)	Bi II
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + b\left(y_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8e)	Bi II

References

[1] F. Merlo and M. L. Fornasini, *Crystal structure of some phases and alloying behaviour in alkaline earths, europium and ytterbium pnictides*, Mater. Res. Bull. **29**, 149–154 (1994), doi:10.1016/0025-5408(94)90135-X.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.