α-$SrBr_2$ Structure: A2B_tP30_85_ab2g_cg-001

This structure originally had the label `A2B_tP30_85_ab2g_cg`. Calls to that address will be redirected here.

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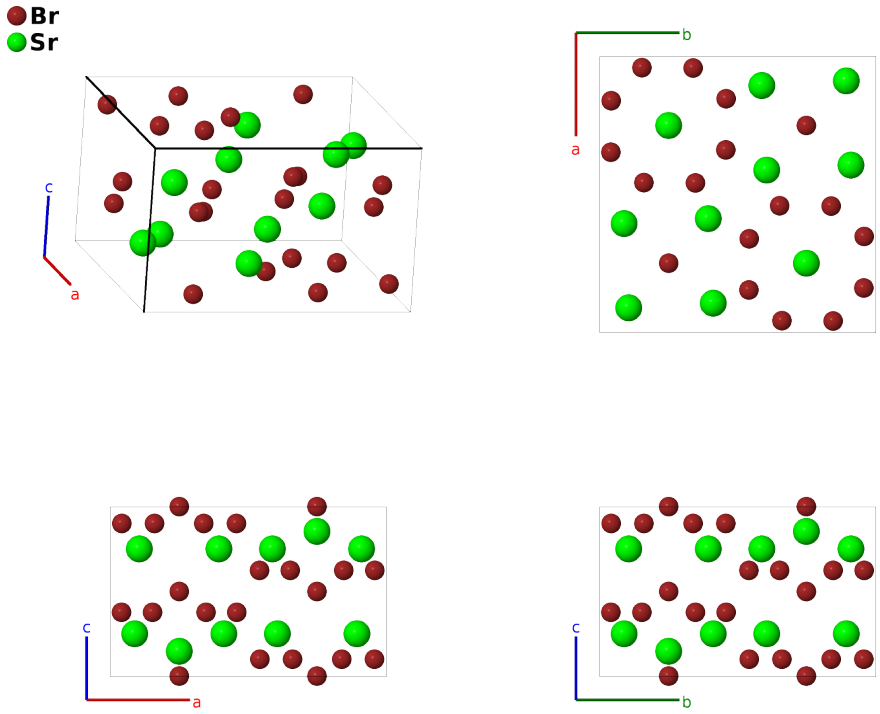
https://aflow.org/p/G8GD

https://aflow.org/p/A2B_tP30_85_ab2g_cg-001



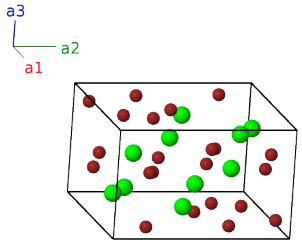
Prototype	Br_2Sr
AFLOW prototype label	A2B_tP30_85_ab2g_cg-001
ICSD	262673
Pearson symbol	tP30
Space group number	85
Space group symbol	$P4/n$
AFLOW prototype command	`aflow --proto=A2B_tP30_85_ab2g_cg-001 --params=`$a, c/a, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure
EuBr2, α-Se_2U

- (Hermann, 1943) originally assigned $SrBr_2$ to space group *Pnma* #62, and gave it the *Strukturbericht* designation *C*53. Subsequent investigation showed that the structure should be in space group $P4/n$ #85, but this structure was never given a *Strukturbericht* symbol, although (Parthé) does list it as *C*53.
- This compound can also be found as β-$SrBr_2$ in the fluorite ($C1$) structure.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	Br I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	Br I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Br II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Br II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	Sr I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	Sr I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_8}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_9}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_{12}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_{13}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	Br III
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{16}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{17}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{18}}$	=	$y_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{21}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{22}}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Br IV
$\mathbf{B_{23}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II

$\mathbf{B_{24}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II
$\mathbf{B_{25}}$	=	$-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1+x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II
$\mathbf{B_{26}}$	=	$y_6\,\mathbf{a}_1-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II
$\mathbf{B_{27}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II
$\mathbf{B_{28}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II
$\mathbf{B_{29}}$	=	$\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1-x_6\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II
$\mathbf{B_{30}}$	=	$-y_6\,\mathbf{a}_1+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	Sr II

References

[1] S. Hull, S. T. Norberg, I. Ahmed, S. G. Eriksson, and C. E. Mohn, *High temperature crystal structures and superionic properties of $SrCl_2$, $SrBr_2$, $BaCl_2$ and $BaBr_2$*, J. Solid State Chem. **184**, 2925–2935 (2011), doi:10.1016/j.jssc.2011.09.004.

[2] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).

[3] 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.