

α -SrBr₂ Structure:

A2B_tP30_85_ab2g_cg-001

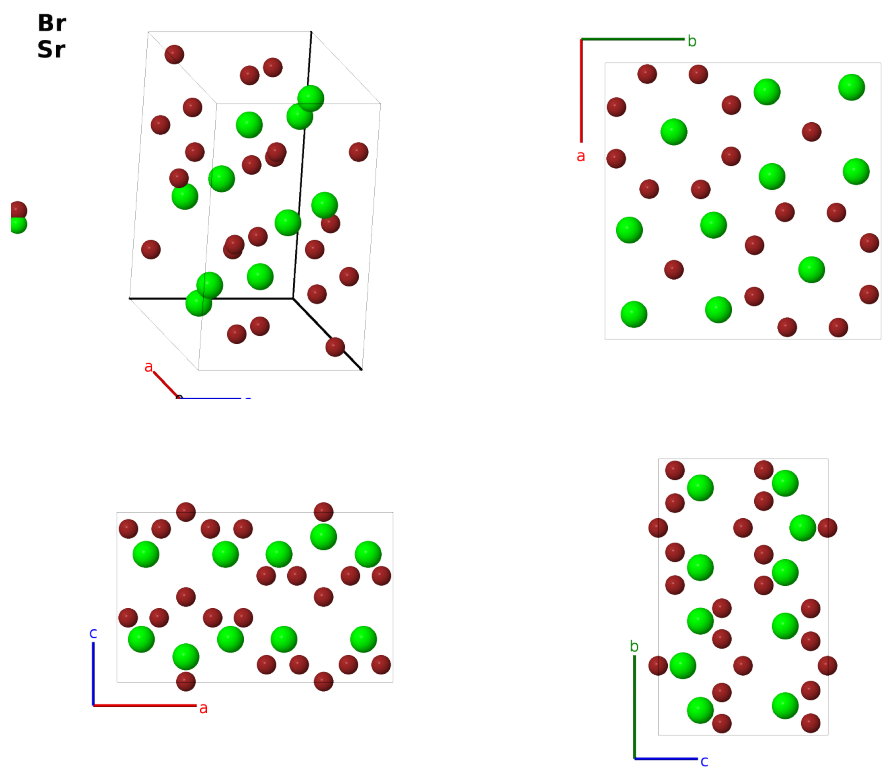
This structure previously used the label(s) **A2B_tP30_85_ab2g_cg**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/G8GD>

https://aflow.org/prototype-encyclopedia/A2B_tP30_85_ab2g_cg-001



Prototype	Br ₂ Sr
AFLOW prototype label	A2B_tP30_85_ab2g_cg-001
ICSD	262673
CCDC	1720273
Pearson symbol	tP30
Space group number	85
Space group symbol	$P4/n$
AFLOW prototype command	<code>aflow --proto=A2B_tP30_85_ab2g_cg-001</code> <code>--params=$a, c/a, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$</code>

Other compounds with this structure

EuBr₂, α -Se₂U

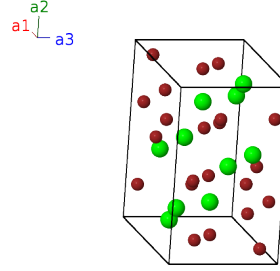
- (Hermann, 1943) originally assigned SrBr₂ to space group $Pnma$ #62, and gave it the *Strukturbericht* designation $C53$. Subsequent investigation showed that the structure should be in space group $P4/n$ #85, but this structure was never given a *Strukturbericht* symbol, although (Parthé) does list it as $C53$.
- This compound can also be found as β -SrBr₂ 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

$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{Sr II}
\end{aligned}$$

References

- [1] S. Hull, S. T. Norberg, I. Ahmed, S. G. Eriksson, and C. E. Mohn, *High temperature crystal structures and superionic properties of SrCl₂, SrBr₂, BaCl₂ and BaBr₂*, 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.

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