$Sr_2Be_2B_2O_7$ Structure: A2B2C7D2_hP26_188_i_h_cl_ab-001

https://aflow.org/p/FFAL

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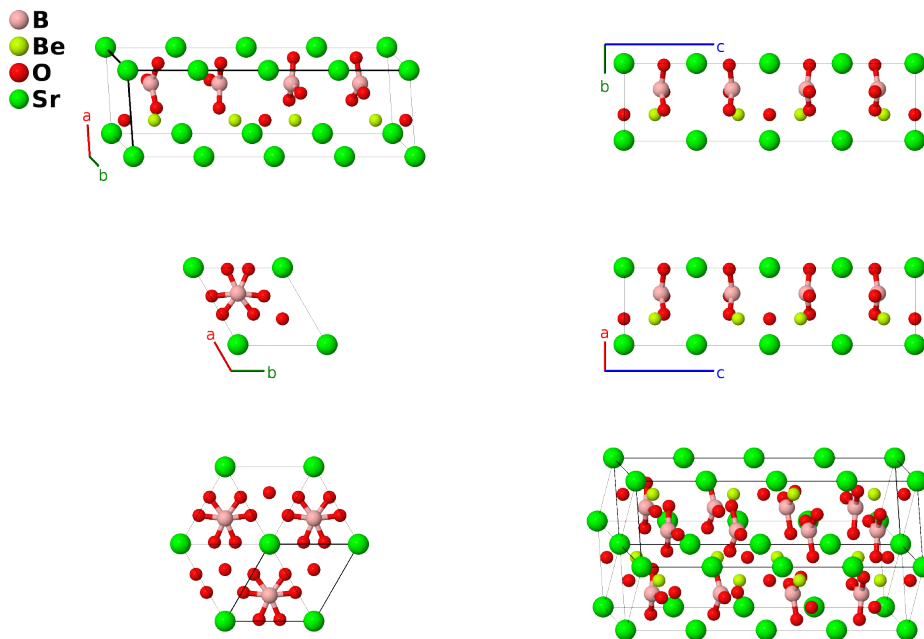
Prototype	$B_2Be_2O_7Sr_2$
AFLOW prototype label	A2B2C7D2_hP26_188_i_h_cl_ab-001
ICSD	79025
Pearson symbol	hP26
Space group number	188
Space group symbol	$P\bar{6}c2$
AFLOW prototype command	aflow --proto=A2B2C7D2_hP26_188_i_h_cl_ab-001
	--params=$a, c/a, z_4, z_5, x_6, y_6, z_6$

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
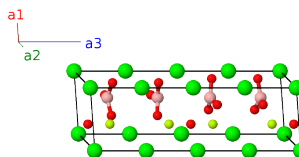
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Sr I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Sr I
$\mathbf{B_3}$	$=$	$\frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Sr II
$\mathbf{B_4}$	$=$	$\frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Sr II
$\mathbf{B_5}$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	O I
$\mathbf{B_6}$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_7}$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4h)	Be I
$\mathbf{B_8}$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4h)	Be I
$\mathbf{B_9}$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4h)	Be I
$\mathbf{B_{10}}$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4h)	Be I
$\mathbf{B_{11}}$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_{12}}$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_{13}}$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_{14}}$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_{15}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_6 + y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_6 - y_6\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{16}}$	$=$	$-y_6\,\mathbf{a}_1 + \left(x_6 - y_6\right)\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_6 - 2y_6\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{17}}$	$=$	$-\left(x_6 - y_6\right)\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(2x_6 - y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{18}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_6 + y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_6 - y_6\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{19}}$	$=$	$-y_6\,\mathbf{a}_1 + \left(x_6 - y_6\right)\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_6 - 2y_6\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{20}}$	$=$	$-\left(x_6 - y_6\right)\mathbf{a}_1 - x_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(2x_6 - y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{21}}$	$=$	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_6 + y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_6 - y_6\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{22}}$	$=$	$-\left(x_6 - y_6\right)\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(-x_6 + 2y_6\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{23}}$	$=$	$x_6\,\mathbf{a}_1 + \left(x_6 - y_6\right)\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(2x_6 - y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{24}}$	$=$	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_6 + y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_6 - y_6\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{25}}$	$=$	$-\left(x_6 - y_6\right)\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(-x_6 + 2y_6\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12l)	O II
$\mathbf{B_{26}}$	$=$	$x_6\,\mathbf{a}_1 + \left(x_6 - y_6\right)\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(2x_6 - y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12l)	O II

References

[1] C. Chen, Y. Wang, B. Wu, K. Wu, W. Zeng, and L. Yu, *Design and synthesis of an ultraviolet-transparent nonlinear optical crystal $Sr_2Be_2B_2O_7$*, Nature **373**, 322–323 (1995), doi:10.1038/373322a0.

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[1] Z. Lin, Z. Wang, and C. Chen, *Mechanism for linear and nonlinear optical effects in crystals of the $Sr_2Be_2B_2O_7$ family*, J. Appl. Phys. **93**, 9717–9723 (2003), doi:10.1063/1.1577816.