Bertrandite ($Be_4Si_2O_7(OH)_2$, $S4_6$) Structure: A4B7C2D2_oC60_36_2b_a3b_2a_b-001

This structure previously used the label(s) `A4B7C2D2_oC60_36_2b_a3b_2a_b`. Calls to these addresses will be redirected here.

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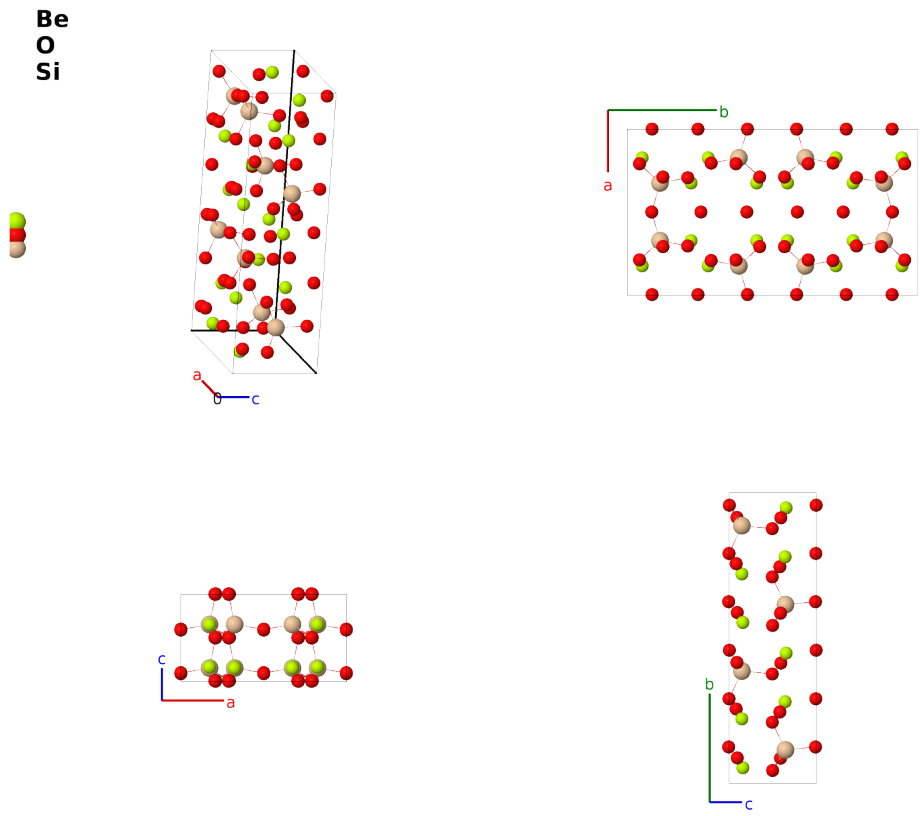
https://aflow.org/prototype-encyclopedia/NZ59

https://aflow.org/prototype-encyclopedia/A4B7C2D2_oC60_36_2b_a3b_2a_b-001



Prototype	$Be_4Si_2O_7(OH)_2$
AFLOW prototype label	A4B7C2D2_oC60_36_2b_a3b_2a_b-001
***Strukturbericht* designation**	$S4_6$
Mineral name	bertrandite
ICSD	64946
CCDC	1627104
Pearson symbol	oC60
Space group number	36

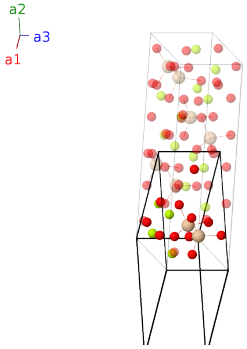
Space group symbol $Cmc2_1$

AFLOW prototype command `aflow --proto=A4B7C2D2_oC60_36_2b_a3b_2a_b-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- All sources agree that the space group for Bertrandite is $Cmc2_1$ #36 but differ slightly in details. We have chosen to use (Hazen, 1986) as the prototype over (Ito, 1932), which was originally designated $S4_6$, and (Solov'eva, 1965), which has unrealistically large Be-O distances.
- No paper locates the hydrogen atoms in the hydroxide ions, which may indicate that these ions can freely rotate. The ICSD entry lists the the OH radicals as O4 and O5. We instead label them OH.
- We use the data taken at 1 atmosphere.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	OH I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	OH I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	OH II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	OH II
$\mathbf{B_7}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Be I
$\mathbf{B_8}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Be I
$\mathbf{B_9}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Be I
$\mathbf{B_{10}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Be I
$\mathbf{B_{11}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	Be II
$\mathbf{B_{12}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Be II

$$\mathbf{B_{13}} = (x_5+y_5)\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{Be II}$$

$$\mathbf{B_{14}} = -(x_5+y_5)\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} \quad (8b) \quad \text{Be II}$$

$$\mathbf{B_{15}} = (x_6-y_6)\,\mathbf{a}_1+(x_6+y_6)\,\mathbf{a}_2+z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{16}} = -(x_6-y_6)\,\mathbf{a}_1-(x_6+y_6)\,\mathbf{a}_2+\left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{17}} = (x_6+y_6)\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+\left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{18}} = -(x_6+y_6)\,\mathbf{a}_1-(x_6-y_6)\,\mathbf{a}_2+z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{19}} = (x_7-y_7)\,\mathbf{a}_1+(x_7+y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{20}} = -(x_7-y_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{21}} = (x_7+y_7)\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{22}} = -(x_7+y_7)\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{23}} = (x_8-y_8)\,\mathbf{a}_1+(x_8+y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{24}} = -(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2+\left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{25}} = (x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{26}} = -(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{27}} = (x_9-y_9)\,\mathbf{a}_1+(x_9+y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (8b) \quad \text{Si I}$$

$$\mathbf{B_{28}} = -(x_9-y_9)\,\mathbf{a}_1-(x_9+y_9)\,\mathbf{a}_2+\left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{Si I}$$

$$\mathbf{B_{29}} = (x_9+y_9)\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{Si I}$$

$$\mathbf{B_{30}} = -(x_9+y_9)\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (8b) \quad \text{Si I}$$

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