

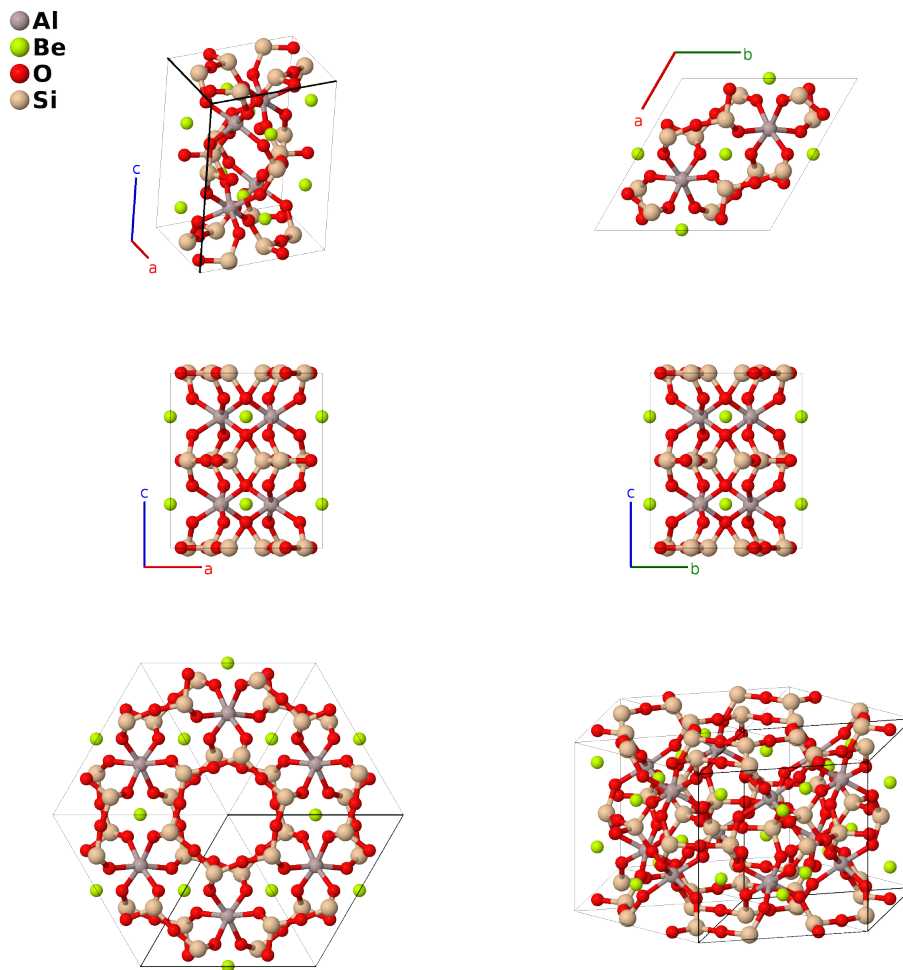
Beryl ($\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$, $S3_1$) Structure: A2B3C18D6_hP58_192_c_f_lm_l-001

This structure originally had the label A2B3C18D6_hP58_192_c_f_lm_l. Calls to that address will be redirected here.

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<https://aflow.org/p/52T5>

https://aflow.org/p/A2B3C18D6_hP58_192_c_f_lm_l-001



Prototype	$\text{Al}_2\text{Be}_3\text{O}_{18}\text{Si}_6$
AFLOW prototype label	A2B3C18D6_hP58_192_c_f_lm_l-001
<i>Strukturbericht</i> designation	$S3_1$
Mineral name	beryl
ICSD	202090
Pearson symbol	hP58
Space group number	192

Space group symbol

$P6/mcc$

AFLOW prototype command

aflow --proto=A2B3C18D6_hP58_192_c_f_lm_l-001
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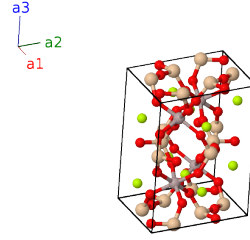
Other compounds with this structure

$Mg_2Al_3Si_6O_{18}$ (indialite)

- (Morosin, 1972) places oxygen atoms on the (2a) Wyckoff site, with lattice coordinates $(0, 0, \pm\frac{1}{4})$ and an occupation of (0.0991). We follow (Hazen, 1986) and ignore this small contribution to the structure.
- We originally followed (Ewald, 1931) and gave this the *Strukturbericht* designation $G3_1$. However, (Hermann, 1937) relabeled it as $S3_1$ to keep it with the rest of the silicate structures.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{2}a\hat{y} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \\ \mathbf{a}_3 &= c\hat{z}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{4}c\hat{z}$	(4c)	Al I
\mathbf{B}_2	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{4}c\hat{z}$	(4c)	Al I
\mathbf{B}_3	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} + \frac{3}{4}c\hat{z}$	(4c)	Al I
\mathbf{B}_4	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{6}a\hat{y} + \frac{3}{4}c\hat{z}$	(4c)	Al I
\mathbf{B}_5	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} - \frac{\sqrt{3}}{4}a\hat{y} + \frac{1}{4}c\hat{z}$	(6f)	Be I
\mathbf{B}_6	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{\sqrt{3}}{4}a\hat{y} + \frac{1}{4}c\hat{z}$	(6f)	Be I
\mathbf{B}_7	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{4}c\hat{z}$	(6f)	Be I
\mathbf{B}_8	$= \frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} - \frac{\sqrt{3}}{4}a\hat{y} + \frac{3}{4}c\hat{z}$	(6f)	Be I
\mathbf{B}_9	$= \frac{1}{2}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{\sqrt{3}}{4}a\hat{y} + \frac{3}{4}c\hat{z}$	(6f)	Be I
\mathbf{B}_{10}	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{3}{4}c\hat{z}$	(6f)	Be I
\mathbf{B}_{11}	$= x_3\mathbf{a}_1 + y_3\mathbf{a}_2$	$=$	$\frac{1}{2}a(x_3 + y_3)\hat{x} - \frac{\sqrt{3}}{2}a(x_3 - y_3)\hat{y}$	(12l)	O I
\mathbf{B}_{12}	$= -y_3\mathbf{a}_1 + (x_3 - y_3)\mathbf{a}_2$	$=$	$\frac{1}{2}a(x_3 - 2y_3)\hat{x} + \frac{\sqrt{3}}{2}ax_3\hat{y}$	(12l)	O I
\mathbf{B}_{13}	$= -(x_3 - y_3)\mathbf{a}_1 - x_3\mathbf{a}_2$	$=$	$-\frac{1}{2}a(2x_3 - y_3)\hat{x} - \frac{\sqrt{3}}{2}ay_3\hat{y}$	(12l)	O I
\mathbf{B}_{14}	$= -x_3\mathbf{a}_1 - y_3\mathbf{a}_2$	$=$	$-\frac{1}{2}a(x_3 + y_3)\hat{x} + \frac{\sqrt{3}}{2}a(x_3 - y_3)\hat{y}$	(12l)	O I
\mathbf{B}_{15}	$= y_3\mathbf{a}_1 - (x_3 - y_3)\mathbf{a}_2$	$=$	$\frac{1}{2}a(-x_3 + 2y_3)\hat{x} - \frac{\sqrt{3}}{2}ax_3\hat{y}$	(12l)	O I
\mathbf{B}_{16}	$= (x_3 - y_3)\mathbf{a}_1 + x_3\mathbf{a}_2$	$=$	$\frac{1}{2}a(2x_3 - y_3)\hat{x} + \frac{\sqrt{3}}{2}ay_3\hat{y}$	(12l)	O I
\mathbf{B}_{17}	$= y_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3)\hat{x} + \frac{\sqrt{3}}{2}a(x_3 - y_3)\hat{y} + \frac{1}{2}c\hat{z}$	(12l)	O I
\mathbf{B}_{18}	$= (x_3 - y_3)\mathbf{a}_1 - y_3\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3)\hat{x} - \frac{\sqrt{3}}{2}ax_3\hat{y} + \frac{1}{2}c\hat{z}$	(12l)	O I
\mathbf{B}_{19}	$= -x_3\mathbf{a}_1 - (x_3 - y_3)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3)\hat{x} + \frac{\sqrt{3}}{2}ay_3\hat{y} + \frac{1}{2}c\hat{z}$	(12l)	O I

$$\mathbf{B}_{56} = y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

$$\mathbf{B}_{57} = (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

$$\mathbf{B}_{58} = -x_5 \mathbf{a}_1 - \left(x_5 - y_5\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (24m) \quad \text{O II}$$

References

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