

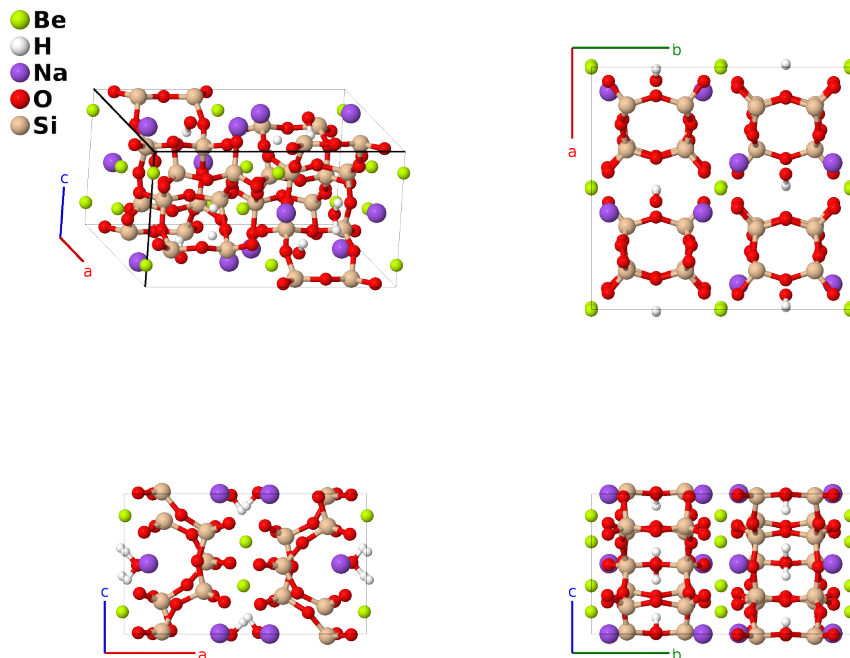
Epididymite ($\text{BeHNaO}_8\text{Si}_3$, $S4_7$) Structure: ABCD8E3_oP112_62_d_2c_d_4c6d_3d-001

This structure originally had the label ABCD8E3_oP112_62_d_2c_d_4c6d_3d. Calls to that address will be redirected here.

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<https://aflow.org/p/QQ21>

https://aflow.org/p/ABCD8E3_oP112_62_d_2c_d_4c6d_3d-001

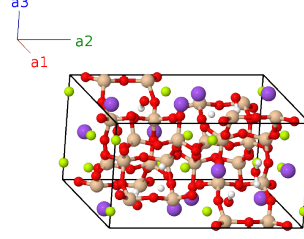


Prototype	$\text{BeHNaO}_8\text{Si}_3$
AFLOW prototype label	ABCD8E3_oP112_62_d_2c_d_4c6d_3d-001
<i>Strukturbericht</i> designation	$S4_7$
Mineral name	epididymite
ICSD	160817
Pearson symbol	oP112
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<pre>aflow --proto=ABCD8E3_oP112_62_d_2c_d_4c6d_3d-001 --params=a,b/a,c/a,x1,z1,x2,z2,x3,z3,x4,z4,x5,z5,x6,z6,x7,y7,z7,x8,y8,z8,x9, y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16, x17,y17,z17</pre>

- (Ito, 1934)'s original determination of the epididymite structure, designated as $S4_7$ by (Gottfried, 1937), was flawed, even in the author's estimation. In particular, both the Si-O and Si-Be distances are very small, with Si-Be less than 1 Å.
- Ito and many later authors assumed that the hydrogen atoms formed OH radicals, but (Gatta, 2008) found that the hydrogen atoms were actually a part of a water molecule.
- Since the (Ito, 1934) structure is not even suitable for starting first-principles calculations and the (Gatta, 2008) structure maintains the $Pnma$ #62 space group, we have dropped the former and designate the later as $S4_7$.
- Epididymite and its diomorph, eudidymite, are two forms of hydrated sodium beryllium silicate which are stable under ambient conditions. (Gatta, 2008)

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_2	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_3	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_4	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_6	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_7	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_8	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_9	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{10}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{11}	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{12}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{14}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{15}	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{16}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{17}	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	O III

$$\mathbf{B}_{110} = \begin{pmatrix} (x_{17} + \frac{1}{2}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 - \\ (z_{17} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} \quad (8d) \quad \text{Si III}$$

$$\mathbf{B}_{111} = x_{17} \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = ax_{17} \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} \quad (8d) \quad \text{Si III}$$

$$\mathbf{B}_{112} = -\begin{pmatrix} (x_{17} - \frac{1}{2}) \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{17} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} \quad (8d) \quad \text{Si III}$$

References

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- [2] T. Ito, *The Structure of Epididymite (HNaBeSi3O8)*, *Z. Kristallogr.* **88**, 142–149 (1934), doi:10.1524/zkri.1934.88.1.142.
- [3] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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