Swedenborgite ($NaBe_4SbO_7$, $E9_2$) Structure: A4BC7D_hP26_186_ac_b_a2c_b-001

This structure originally had the label `A4BC7D_hP26_186_ac_b_a2c_b`. Calls to that address will be redirected here.

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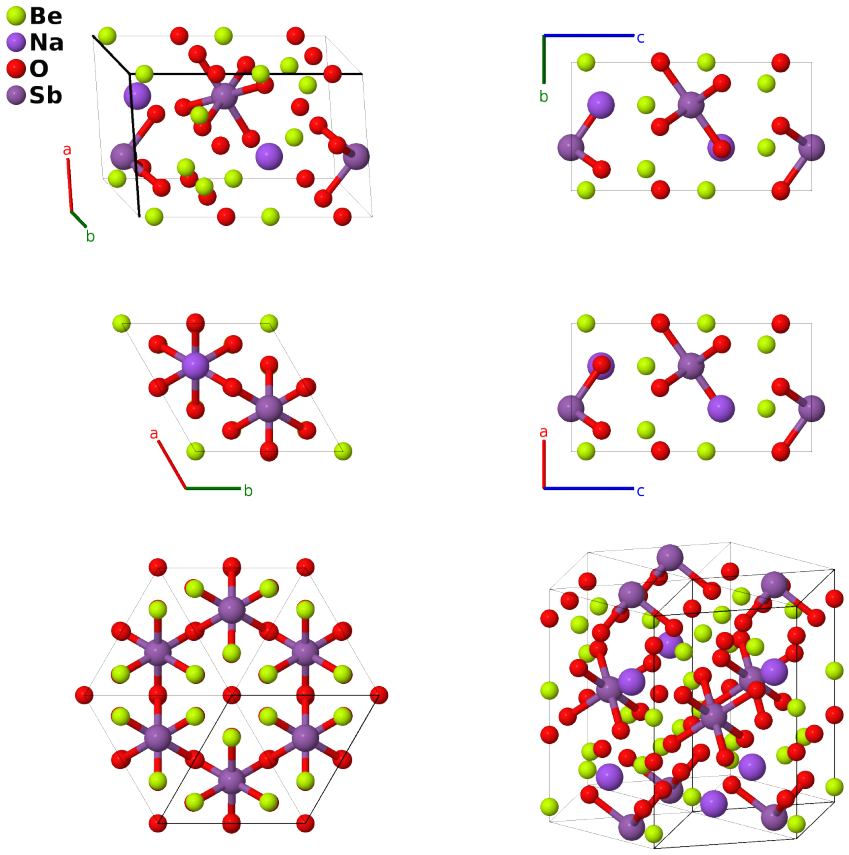
https://aflow.org/p/QF4S

https://aflow.org/p/A4BC7D_hP26_186_ac_b_a2c_b-001



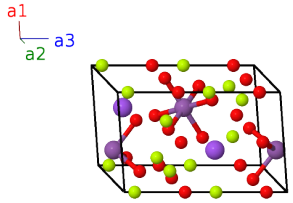
Prototype	Be_4NaSbO_7
AFLOW prototype label	A4BC7D_hP26_186_ac_b_a2c_b-001
***Strukturbericht* designation**	$E9_2$
Mineral name	swedenborgite
ICSD	27599
Pearson symbol	hP26
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A4BC7D_hP26_186_ac_b_a2c_b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, x_5, z_5, x_6, z_6, x_7, z_7$

Other compounds with this structure
$CaBa(Fe_2Mn_2)O_7$, $CaBaCo_3AlO_7$, $CaBaCo_3FeO_7$, $CaBaCo_3ZnO_7$, $CaBaCo_4O_7$, $CaBaFe_4O_7$, $Er_2Si_4N_6C$, $Ho_2Si_4N_6C$, $Tb_2Si_4N_6C$, $Y_2Si_4N_6C$, $YBaCo_3AlO_7$, $YBaCo_3FeO_7$, $YBaCo_4O_7$, $YBaMn_3AlO_7$, $Yb_2Si_4N_6C$, $YbBaSi_4N_7$

- The actual composition of the studied sample is $(Na_{0.89}Ca_{0.04})Be_4SbO_7$, with the sodium (Na-I) site containing 89% sodium, 4% calcium, and 7% vacancies.
- Space group $P6_3mc$ #186 does not fix the origin of the z-coordinate. Here the position of the antimony atom (Sb-I) is set so that $z_4 = 0$.
- The ICSD entry is from (Pauling, 1935).

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Be I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Be I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(2b)	Sb I
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Sb I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Be II
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1+2x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Be II
$\mathbf{B_{11}}$	=	$-2x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Be II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Be II
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1-2x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Be II
$\mathbf{B_{14}}$	=	$2x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Be II
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{16}}$	=	$x_6\,\mathbf{a}_1+2x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{17}}$	=	$-2x_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1-2x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{20}}$	=	$2x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-\sqrt{3}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O III

$\mathbf{B_{22}}$	=	$x_7\,\mathbf{a}_1 + 2x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{23}}$	=	$-2x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{24}}$	=	$-x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{25}}$	=	$-x_7\,\mathbf{a}_1 - 2x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{26}}$	=	$2x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III

References

[1] D. M. C. Huminicki and F. C. Hawthorne, *Refinement of the Crystal Structure of Swedenborgite*, Can. Mineral. **39**, 153–158 (2001), doi:10.2113/gscanmin.39.1.153.

[2] L. Pauling, H. P. Klug, and A. N. Winchell, *The Crystal Structure of Swedenborgite, $NaBe_4SbO_7$*, Am. Mineral. **20**, 492–501 (1935).