

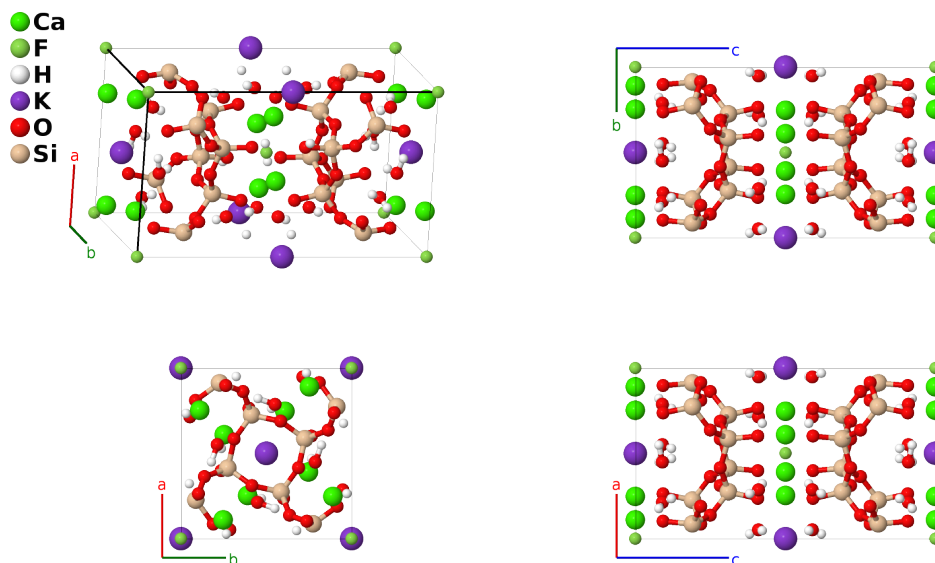
# Apophyllite ( $\text{KCa}_4\text{Si}_8\text{O}_{20}\text{F}\cdot 8\text{H}_2\text{O}$ , $S5_2$ ) Structure: A4BC16DE28F8\_tP116\_128\_h\_a\_2i\_b\_g3i\_i-001

This structure originally had the label A4BC16DE28F8\_tP116\_128\_h\_a\_2i\_b\_g3i\_i. Calls to that address will be redirected here.

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

[https://aflow.org/p/A4BC16DE28F8\\_tP116\\_128\\_h\\_a\\_2i\\_b\\_g3i\\_i-001](https://aflow.org/p/A4BC16DE28F8_tP116_128_h_a_2i_b_g3i_i-001)

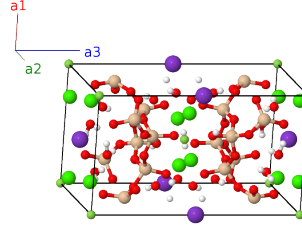


Prototype	$\text{Ca}_4\text{FH}_{16}\text{KO}_{28}\text{Si}_8$
AFLOW prototype label	A4BC16DE28F8_tP116_128_h_a_2i_b_g3i_i-001
<i>Strukturbericht</i> designation	$S5_2$
Mineral name	apophyllite
ICSD	24954
Pearson symbol	tP116
Space group number	128
Space group symbol	$P4/mnc$
AFLOW prototype command	<pre>aflow --proto=A4BC16DE28F8_tP116_128_h_a_2i_b_g3i_i-001       --params=a, c/a, x3, x4, y4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10,       z10</pre>

- Although we use the structure found by (Chao, 1971), we should note that there is some disagreement between the Chao's X-ray diffraction data and the neutron diffraction data taken by (Prince, 1971): while both agree on the positions of the heavy atoms, Prince's work suggests that some of the hydrogens may form OH radicals rather than water molecules.
- In any case, the fluorine set atoms are usually partially replaced by OH radicals. This sample, which is predominantly fluorine, is technically labeled apophyllite-(KF).

## Simple Tetragonal primitive vectors

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



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	$0$	(2a)	F I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	F I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b)	K I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2b)	K I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_7$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_8$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{11}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{12}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	(8h)	Ca I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	(8h)	Ca I
$\mathbf{B}_{15}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(8h)	Ca I
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(8h)	Ca I
$\mathbf{B}_{17}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Ca I
$\mathbf{B}_{18}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Ca I
$\mathbf{B}_{19}$	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Ca I
$\mathbf{B}_{20}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Ca I
$\mathbf{B}_{21}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B}_{23}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B}_{24}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B}_{25}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B}_{26}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16i)	H I







$$\mathbf{B}_{116} = \begin{pmatrix} (y_{10} + \frac{1}{2}) \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a (y_{10} + \frac{1}{2}) \hat{\mathbf{x}} + a (x_{10} + \frac{1}{2}) \hat{\mathbf{y}} + \\ c (z_{10} + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} \quad (16i) \quad \text{Si I}$$

## References

- [1] G. Y. Chao, *The refinement of the crystal structure of apophyllite: II. Determination of the hydrogen positions by X-ray diffraction*, Am. Mineral. **56**, 1234–1242 (1971).
- [2] E. Prince, *The refinement of the crystal structure of apophyllite: III. Determination of the hydrogen positions by neutron diffraction*, Am. Mineral. **56**, 1243–1251 (1971).