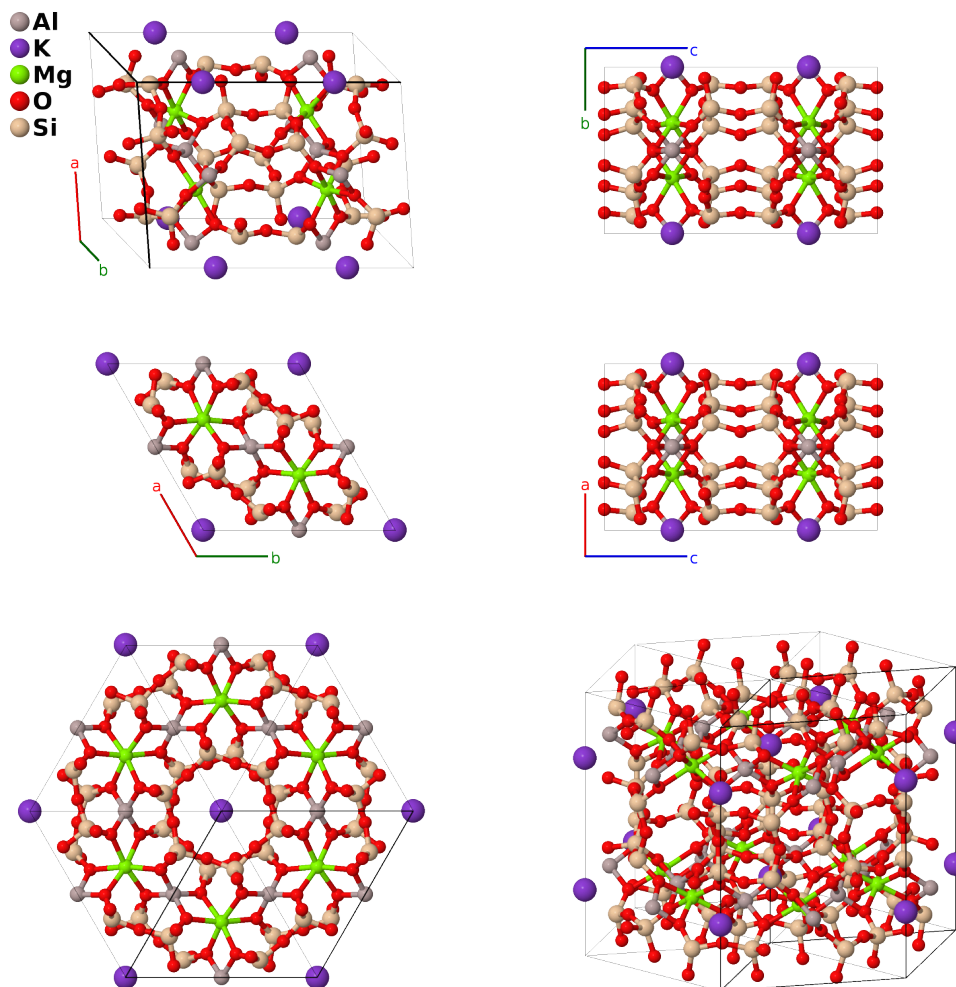


Osumilite ($\text{KMg}_2\text{Al}_3\text{Si}_{12}\text{O}_{30}$) Structure: A3BC2D30E12_hP96_192_f_a_c_l2m_m-001

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<https://aflow.org/p/FPN8>

https://aflow.org/p/A3BC2D30E12_hP96_192_f_a_c_l2m_m-001

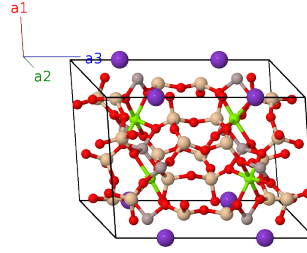


Prototype	$\text{Al}_3\text{KMg}_2\text{O}_{15}\text{Si}_{12}$
AFLOW prototype label	A3BC2D30E12_hP96_192_f_a_c_l2m_m-001
Mineral name	osumilite
ICSD	202731
Pearson symbol	hP96
Space group number	192
Space group symbol	$P6/mcc$
AFLOW prototype command	<code>aflow --proto=A3BC2D30E12_hP96_192_f_a_c_l2m_m-001 --params=a, c/a, x4, y4, x5, y5, z5, x6, y6, z6, x7, y7, z7</code>

- We use the data from the Antarctica sample of (Armbruster, 1988). As with most minerals, some of the sites contain mixtures of elements and vacancies. We use the compositions in the American Mineralogist Crystal Structure Database (Downs, 2003):
 - The K (2a) site is 91% potassium and 1% iron, with the remainder of the sites vacant.
 - The Mg (4c) site is 99% magnesium/aluminum and 1% iron.
 - The Al (6f) site is mostly aluminum/magnesium with a trace of iron/manganese/titanium, even though in Table 4 they call it an Fe site.
 - The Si (24m) site is 86% silicon and 14% magnesium.
 - The oxygen sites are all filled.
- These compositions are very dependent upon where the sample was found. See Table 5 in (Armbruster, 1988) for more details.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2a)	K I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2a)	K I
\mathbf{B}_3	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_4	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_5	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_6	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_9	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{10}	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{11}	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}}$	(12l)	O I
\mathbf{B}_{14}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(12l)	O I
\mathbf{B}_{15}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(12l)	O I
\mathbf{B}_{16}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}}$	(12l)	O I
\mathbf{B}_{17}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(12l)	O I
\mathbf{B}_{18}	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(12l)	O I
\mathbf{B}_{19}	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(12l)	O I

$$\begin{aligned}
\mathbf{B}_{88} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (24m) & \text{Si I} \\
\mathbf{B}_{89} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (24m) & \text{Si I} \\
\mathbf{B}_{90} &= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (24m) & \text{Si I} \\
\mathbf{B}_{91} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + & (24m) & \text{Si I} \\
&&& c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} \\
\mathbf{B}_{92} &= -(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 + &= \frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (24m) & \text{Si I} \\
&& (z_7 + \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{93} &= x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (24m) & \text{Si I} \\
\mathbf{B}_{94} &= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + & (24m) & \text{Si I} \\
&&& c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} \\
\mathbf{B}_{95} &= (x_7 - y_7) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (24m) & \text{Si I} \\
\mathbf{B}_{96} &= -x_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + &= -\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (24m) & \text{Si I} \\
&& (z_7 + \frac{1}{2}) \mathbf{a}_3
\end{aligned}$$

References

- [1] T. Armbruster and R. Oberhänsli, *Crystal chemistry of double-ring silicates: Structural, chemical, and optical variation in osumilites*, Am. Mineral. **73**, 585–594 (1988).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).