

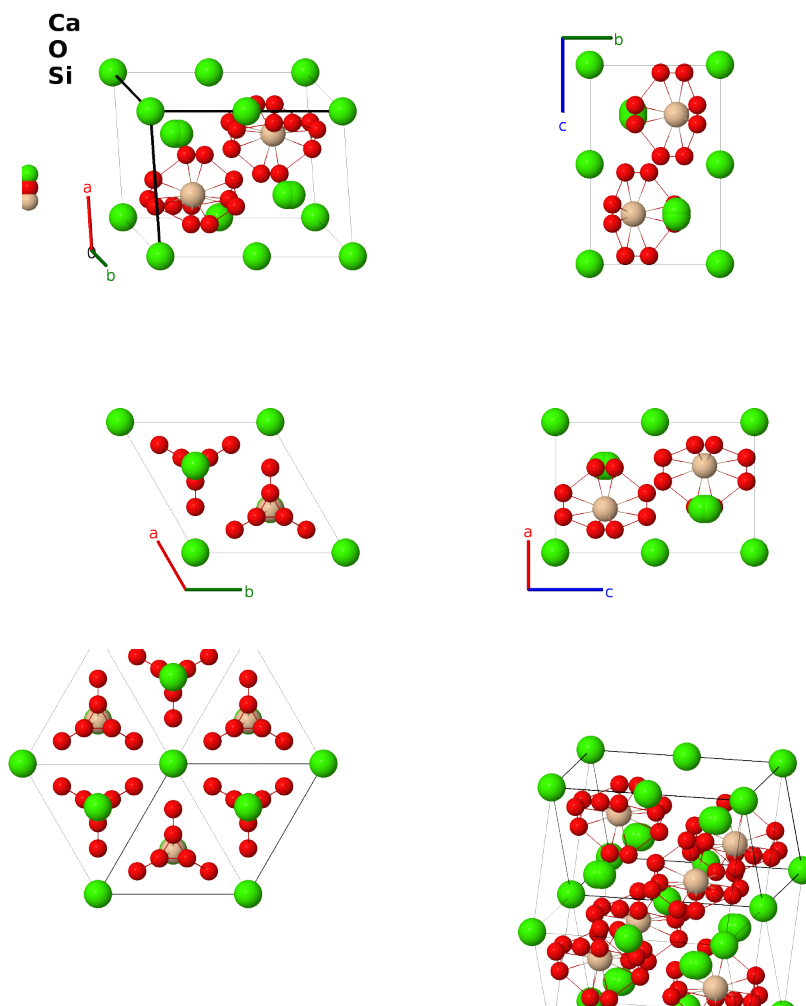
Hexagonal α -Ca₂SiO₄ Structure: A3B12C_hP32_194_af_2k_c-001

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<https://aflow.org/prototype-encyclopedia/CEQR>

https://aflow.org/prototype-encyclopedia/A3B12C_hP32_194_af_2k_c-001



Prototype	Ca ₂ O ₄ Si
AFLOW prototype label	A3B12C_hP32_194_af_2k_c-001
ICSD	82998
CCDC	1643050
Pearson symbol	hP32
Space group number	194

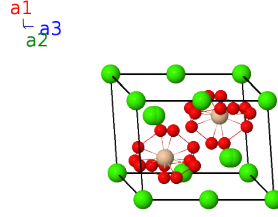
Space group symbol $P6_3/mmc$

AFLOW prototype command `aflow --proto=A3B12C_hP32_194_af_2k_c-001`
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- Ca_2SiO_4 exists in a variety of structures (Mumme, 1996; Yamnova, 2011):
 - hexagonal $\alpha\text{-Ca}_2\text{SiO}_4$, stable above 1445°C. There is some dispute as to whether this occurs in a
 - * trigonal, space group $P\bar{3}m1$ #164 structure or a
 - * disordered hexagonal, space group $P6_3/mmc$ #194 structure, as shown here.
 - orthorhombic $\alpha_H'\text{-Ca}_2\text{SiO}_4$, stable in the range 1160 – 1425°C,
 - orthorhombic $\alpha_L'\text{-Ca}_2\text{SiO}_4$, stable in the range 690 – 1160°C,
 - monoclinic $\beta\text{-Ca}_2\text{SiO}_4$, stable in the range 500 – 690°C and found in nature as the metastable mineral larnite, and
 - $\gamma\text{-Ca}_2\text{SiO}_4$, stable below 500°C, in the olivine ($S1_2$) structure.
- There is considerable disorder in this structure: the Ca-II (4f) site is half-filled, and both the oxygen sites are 1/3 filled. Presumably this means that four oxygen atoms surround each silicon atom.

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
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Ca I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f)	Ca II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ca II
$\mathbf{B}_7$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f)	Ca II
$\mathbf{B}_8$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ca II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{10}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{13}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	O I

$$\begin{aligned}
\mathbf{B}_{15} &= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\text{O I} \\
\mathbf{B}_{16} &= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\text{O I} \\
\mathbf{B}_{17} &= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \sqrt{3}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\text{O I} \\
\mathbf{B}_{18} &= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{O I} \\
\mathbf{B}_{19} &= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{O I} \\
\mathbf{B}_{20} &= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -\sqrt{3}ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) &\text{O I} \\
\mathbf{B}_{21} &= 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}} &(12k) &\text{O II} \\
\mathbf{B}_{22} &= -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}} &(12k) &\text{O II} \\
\mathbf{B}_{23} &= 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}} &(12k) &\text{O II} \\
\mathbf{B}_{24} &= -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}} &(12k) &\text{O II} \\
\mathbf{B}_{25} &= 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}} &(12k) &\text{O II} \\
\mathbf{B}_{26} &= -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}} &(12k) &\text{O II} \\
\mathbf{B}_{27} &= 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}} &(12k) &\text{O II} \\
\mathbf{B}_{28} &= -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}} &(12k) &\text{O II} \\
\mathbf{B}_{29} &= -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}} &(12k) &\text{O II} \\
\mathbf{B}_{30} &= -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}} &(12k) &\text{O II} \\
\mathbf{B}_{31} &= 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}} &(12k) &\text{O II} \\
\mathbf{B}_{32} &= 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}} &(12k) &\text{O II}
\end{aligned}$$

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