# Trigonal $\alpha$-$Ca_2SiO_4$ Structure: A2B4C_hP14_164_abd_di_d-001

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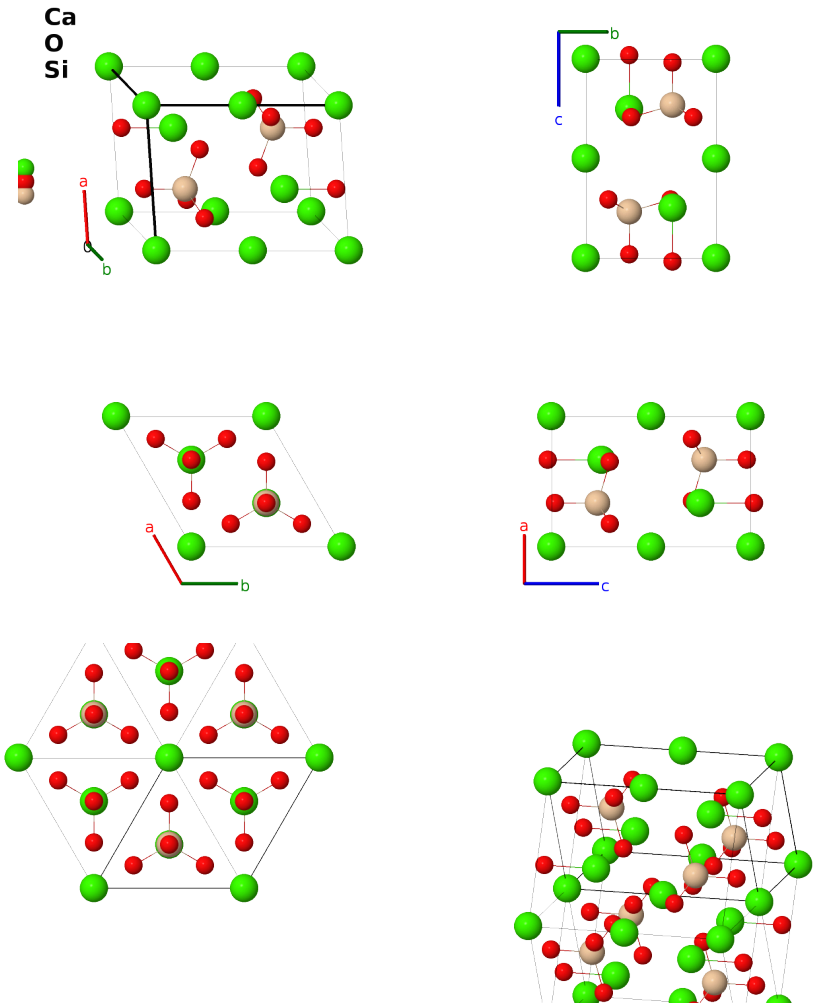
https://aflow.org/prototype-encyclopedia/DBUP

https://aflow.org/prototype-encyclopedia/A2B4C_hP14_164_abd_di_d-001




| | |
|---|---|
| **Prototype** | $Ca_2O_4Si$ |
| **AFLOW prototype label** | A2B4C_hP14_164_abd_di_d-001 |
| **ICSD** | 182052 |
| **CCDC** | 1691448 |
| **Pearson symbol** | hP14 |
| **Space group number** | 164 |

**Space group symbol** $P\bar{3}m1$

**AFLOW prototype command** `aflow --proto=A2B4C_hP14_164_abd_di_d-001 --params=`$a, c/a, z_3, z_4, z_5, x_6, z_6$

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- $Ca_2SiO_4$ exists in a variety of structures (Mumme, 1996; Yamnova, 2011):
  - hexagonal $\alpha$-$Ca_2SiO_4$, stable above 1445°C. There is some dispute as to whether this occurs in a
    - trigonal, space group $P\bar{3}m1$ #164 structure (shown here) or a
    - disordered hexagonal, space group $P6_3/mmc$ #194 structure.
  - orthorhombic $\alpha_H$'-$Ca_2SiO_4$, stable in the range 1160 – 1425°C,
  - orthorhombic $\alpha_L$'-$Ca_2SiO_4$, stable in the range 690 – 1160°C,
  - monoclinic $\beta$-$Ca_2SiO_4$, stable in the range 500 – 690°C and found in nature as the metastable mineral larnite, and
  - $\gamma$-$Ca_2SiO_4$, stable below 500°C, in the olivine ($S1_2$) structure.
- The ICSD entry for this structure is from (Eysel, 1970). The atomic positions are significantly different than those given in (Mumme, 1996), but we have no ICSD entry from that paper.

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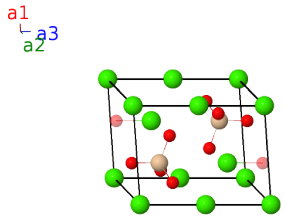
**Trigonal (Hexagonal) primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | Ca I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (1b) | Ca II |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2d) | Ca III |
| $\mathbf{B_4}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2d) | Ca III |
| $\mathbf{B_5}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (2d) | O I |
| $\mathbf{B_6}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (2d) | O I |
| $\mathbf{B_7}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (2d) | Si I |
| $\mathbf{B_8}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (2d) | Si I |
| $\mathbf{B_9}$ | = | $x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (6i) | O II |
| $\mathbf{B_{10}}$ | = | $x_6\,\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (6i) | O II |
| $\mathbf{B_{11}}$ | = | $-2x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (6i) | O II |
| $\mathbf{B_{12}}$ | = | $-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $\sqrt{3}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (6i) | O II |
| $\mathbf{B_{13}}$ | = | $2x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (6i) | O II |
| $\mathbf{B_{14}}$ | = | $-x_6\,\mathbf{a}_1 - 2x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (6i) | O II |

## References


[1] W. Mumme, L. Cranswick, and B. Chakoumakos, *Rietveld crystal structure refinements from high temperature neutron powder diffraction data for the polymorphs of dicalcium silicate*, Neues mineral. Abhandlungen **170**, 171–188 (1996), doi:10.1134/S1063774511020209.

[2] W. Eysel and T. Hahn, *Polymorphism and solid solution of $Ca_2(GeO_4)$ and $Ca_2(SiO_4)$*, Z. Krystallogr. **131**, 322–341 (1970), doi:10.1524/zkri.1970.131.16.322.


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[1] N. A. Yamnova, N. V. Zubkova, N. N. Eremin, A. E. Zadov, and V. M. Gazeev, *Crystal structure of larnite $\beta$-$Ca_2SiO_4$ and specific features of polymorphic transitions in dicalcium orthosilicate*, Crystallogr. Rep. **56**, 210–220 (2011), doi:10.1134/S1063774511020209.


## First cited in


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