# Hexagonal Vaterite ($CaCO_3$) Structure: A3BC9_hP26_194_h_a_hk-001

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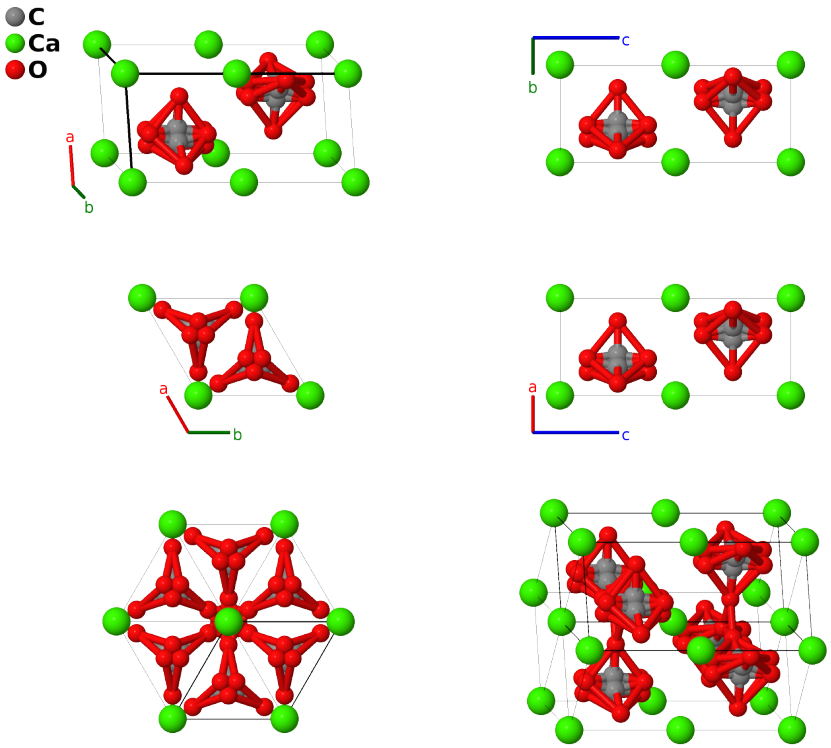
https://aflow.org/p/A3BC9_hP26_194_h_a_hk-001




| | |
|---|---|
| **Prototype** | $CCaO_3$ |
| **AFLOW prototype label** | A3BC9_hP26_194_h_a_hk-001 |
| **Mineral name** | vaterite |
| **ICSD** | 15879 |
| **Pearson symbol** | hP26 |
| **Space group number** | 194 |
| **Space group symbol** | $P6_3/mmc$ |
| **AFLOW prototype command** | `aflow --proto=A3BC9_hP26_194_h_a_hk-001 --params=`$a, c/a, x_2, x_3, x_4, z_4$ |

- Numerous structures have been proposed for vaterite: (Downs, 2003) lists fifteen. (Kabalah-Amitai, 2013) found that vaterite consists of at least two coexisting phases: this disordered hexagonal structure proposed by (Kamhi, 1963), and another orthorhombic but pseudo-hexagonal phase.
- $CaCO_3$ is also found as calcite ($G0_1$).

- The carbon and oxygen sites in this structure each have 1/3 occupation, giving the final $CaCO_3$ stoichiometry.

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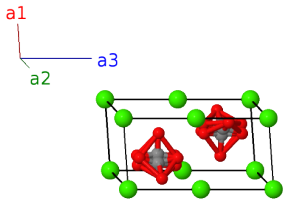
**Hexagonal primitive vectors**

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

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**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 |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | C I |
| $\mathbf{B_4}$ | = | $-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | C I |
| $\mathbf{B_5}$ | = | $x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | C I |
| $\mathbf{B_6}$ | = | $-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | C I |
| $\mathbf{B_7}$ | = | $2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | C I |
| $\mathbf{B_8}$ | = | $-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | C I |
| $\mathbf{B_9}$ | = | $x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | O I |
| $\mathbf{B_{10}}$ | = | $-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | O I |
| $\mathbf{B_{11}}$ | = | $x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | O I |
| $\mathbf{B_{12}}$ | = | $-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | O I |
| $\mathbf{B_{13}}$ | = | $2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | O I |
| $\mathbf{B_{14}}$ | = | $-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | O I |
| $\mathbf{B_{15}}$ | = | $x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{16}}$ | = | $-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{17}}$ | = | $x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{18}}$ | = | $-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{19}}$ | = | $2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{20}}$ | = | $-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\sqrt{3}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{21}}$ | = | $2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{22}}$ | = | $-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{23}}$ | = | $-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\sqrt{3}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{24}}$ | = | $-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{25}}$ | = | $x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12k) | O II |
| $\mathbf{B_{26}}$ | = | $x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12k) | O II |

**References**


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

**Found in**

[1] L. Kabalah-Amitai, B. Mayze, Y. Kauffmann, A. N. Fitch, L. Bloch, P. U. P. A. Gilbert, and B. Pokroy, *Vaterite Crystals Contain Two Interspersed Crystal Structures*, Science **340**, 454–457 (2013), doi:10.1126/science.1232139.