Monoclinic Vaterite ($CaCO_3$) Structure: ABC3_oP20_62_c_a_cd-001

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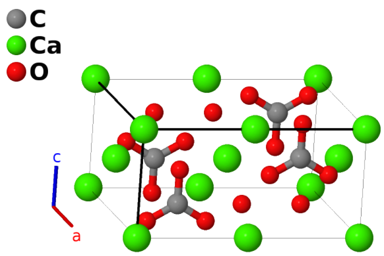
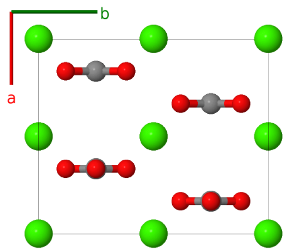
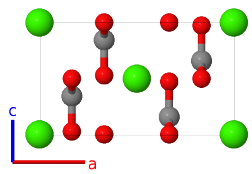
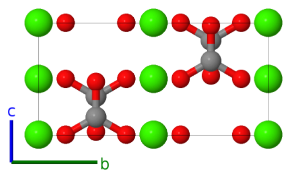
https://aflow.org/p/RGRE

https://aflow.org/p/ABC3_oP20_62_c_a_cd-001







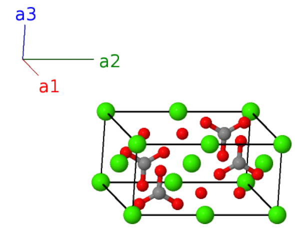


Prototype	$CCaO_3$
AFLOW prototype label	ABC3_oP20_62_c_a_cd-001
Mineral name	vaterite
ICSD	27827
Pearson symbol	oP20
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	`aflow --proto=ABC3_oP20_62_c_a_cd-001` `--params=`$a, b/a, c/a, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

- Numerous structures have been proposed for vaterite: (Downs, 2003) lists fifteen. (Kabalah-Amitai, 2013) found that vaterite consists of at least two coexisting phases: a disordered hexagonal structure proposed by (Kamhi, 1963), and another monoclinic but pseudo-hexagonal phase, shown here.
- (Meyer, 1960) gave the positions in this structure in the $Pbnm$ setting of space group #62. We used FINDSYM to transform this to the standard $Pnma$ setting. This rotates the coordinate axes around the (111) axis.
- $CaCO_3$ is also found as calcite ($G0_1$).

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\mathbf{\hat{x}}$$
$$\mathbf{a_2} = b\,\mathbf{\hat{y}}$$
$$\mathbf{a_3} = c\,\mathbf{\hat{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Ca I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(4a)	Ca I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\mathbf{\hat{y}}$	(4a)	Ca I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}b\,\mathbf{\hat{y}} + \frac{1}{2}c\,\mathbf{\hat{z}}$	(4a)	Ca I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(4c)	C I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	C I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(4c)	C I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	C I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + cz_3\,\mathbf{\hat{z}}$	(4c)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} - cz_3\,\mathbf{\hat{z}}$	(4c)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + b\left(y_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{18}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{20}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O II

References

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[3] 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.

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