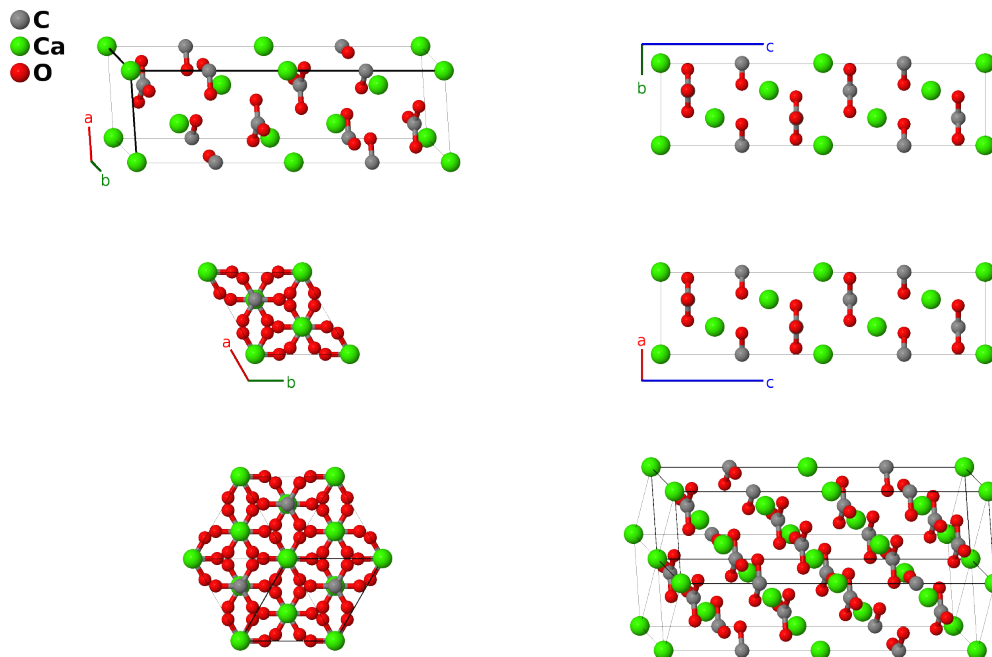# Calcite (CaCO$_3$, $G0_1$) Structure: ABC3_hR10_167_a_b_e-002

This structure originally had the label `ABC3_hR10_167_a_b_e.CaCO3`. Calls to that address will be redirected here.

https://aflow.org/p/UVUF

https://aflow.org/p/ABC3_hR10_167_a_b_e-002

Prototype	CCaO$_3$
AFLOW prototype label	ABC3_hR10_167_a_b_e-002
***Strukturbericht* designation**	$G0_1$
Mineral name	calcite
ICSD	40107
Pearson symbol	hR10
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	aflow --proto=ABC3_hR10_167_a_b_e-002 --params=$a, c/a, x_3$

Other compounds with this structure

AlBO$_3$, (Ca, Mn)CO$_3$ (kutnohorite, rhodocrosite), CdCO$_3$ (otavite), (Cd, Mg)CO$_3$ (otavite), CoCO$_3$ (spherocobaltite), CuCO$_3$, FeCO$_3$ (siderite), InBO$_3$, (La, Na)O$_3$ (loparite), LaNiO$_3$, MgCO$_3$ (magnesite), MnCO$_3$ (rhodochrosite), NaNO$_3$ (nitratine), NiCO$_3$ (gaspeite), ZnCO$_3$ (smithsonite)

- *Strukturbericht Band* I, (Ewald, 1931) pp.292-295, gives this the designation $G1$, but the index in *Band* II (Hermann, 1937) lists this as $G0_1$.

- $CaCO_3$ can also be found in the form of monoclinic or hexagonal vaterite. These two structures can coexist.

- Paraelectric $LiNbO_3$ and calcite $CaCO_3$ have the same AFLOW prototype label, ABC3_hR10_167_a_b_e. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

- Hexagonal settings rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
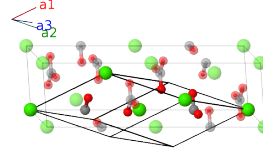
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + \tfrac{1}{4}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_2}$	$=$	$\tfrac{3}{4}\mathbf{a_1} + \tfrac{3}{4}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_3}$	$=$	0	$=$	0	(2b)	Ca I
$\mathbf{B_4}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a_1} - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{8}a\left(4x_3 - 1\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{8}a\left(4x_3 - 1\right)\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_6}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + x_3\,\mathbf{a_2} - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{8}a\left(4x_3 - 1\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{8}a\left(4x_3 - 1\right)\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_7}$	$=$	$-\left(x_3 - \tfrac{1}{2}\right)\mathbf{a_1} + \tfrac{1}{4}\mathbf{a_2} + x_3\,\mathbf{a_3}$	$=$	$-a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_8}$	$=$	$-x_3\,\mathbf{a_1} + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{8}a\left(4x_3 + 3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{24}a\left(12x_3 + 1\right)\hat{\mathbf{y}} + \tfrac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_9}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - x_3\,\mathbf{a_2} + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{8}a\left(4x_3 - 1\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{24}a\left(12x_3 + 5\right)\hat{\mathbf{y}} + \tfrac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{10}}$	$=$	$\left(x_3 + \tfrac{1}{2}\right)\mathbf{a_1} + \tfrac{3}{4}\mathbf{a_2} - x_3\,\mathbf{a_3}$	$=$	$a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I

References

[1] S. A. Markgraf and R. J. Reeder, *High-temperature structure refinements of calcite and magnesite*, Am. Mineral. **70**, 590–600 (1985).

[2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

[3] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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