Calcite ($CaCO_3$, $G0_1$) Structure: ABC3_hR10_167_a_b_e-002

This structure previously used the label(s) `ABC3_hR10_167_a_b_e.CaCO3`. Calls to these addresses will be redirected here.

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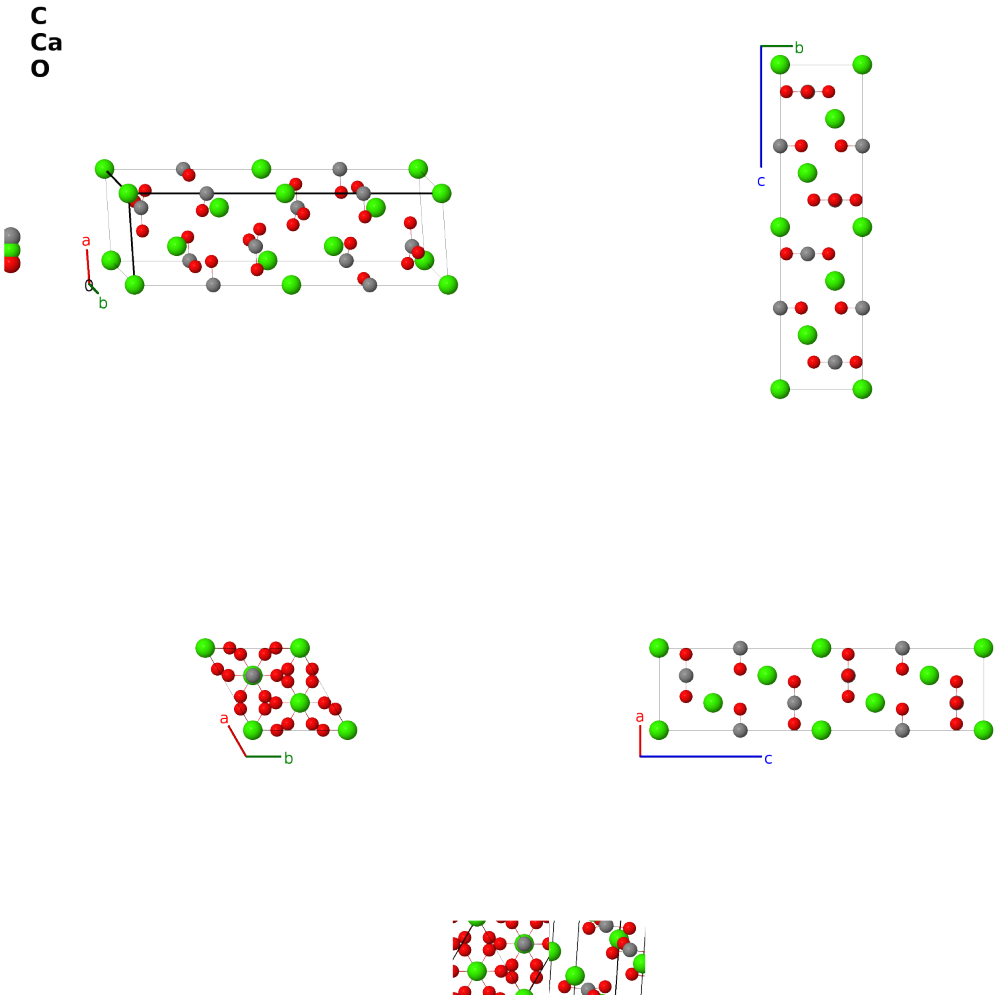
https://aflow.org/prototype-encyclopedia/UVUF

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

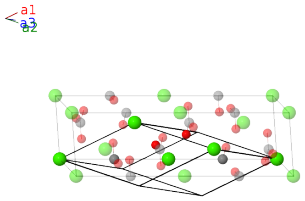
CCDC	1610021
Pearson symbol	hR10
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=ABC3_hR10_167_a_b_e-002 --params=`$a, c/a, x_3$

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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_3}$	=	0	=	0	(2b)	Ca I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_3 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_3 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I

$$\mathbf{B_{10}} = \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - x_3\,\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{5}{12}c\,\hat{\mathbf{z}} \quad \text{(6e)} \quad \text{O I}$$

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).

Found in

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