(Ba,Ca)CO_3 ("$C2$") Structure: ABC3_mC10_5_b_a_ac-001

This structure originally had the label `ABC3_mC10_5_b_a_ac`. Calls to that address will be redirected here.

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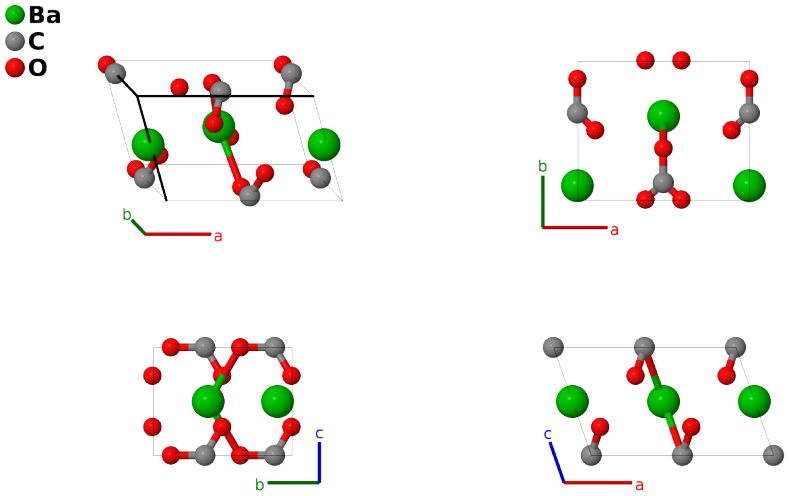
https://aflow.org/p/6HGL

https://aflow.org/p/ABC3_mC10_5_b_a_ac-001

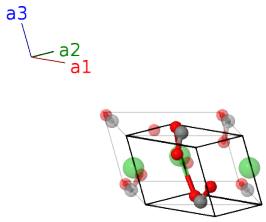


Prototype	$BaCCaO_3$
AFLOW prototype label	ABC3_mC10_5_b_a_ac-001
ICSD	403432
Pearson symbol	mC10
Space group number	5
Space group symbol	$C2$
AFLOW prototype command	`aflow --proto=ABC3_mC10_5_b_a_ac-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, y_3, x_4, y_4, z_4$

- (Ba,Ca)$(CO_3)_2$ comes in a variety of crystal structures (Spahr, 2019):
  - monoclinic barytocalcite, space group $P2_1/m$ #11
  - trigonal paralstonite, space group $P321$ #150,
  - triclinic alstonite (space group $P1$ #1 or $P\bar{1}$ #2) (Sartori, 1975), and
  - a new monoclinic structure, space group $C2$ #5, synthesized by (Spahr, 2019), and lacking the centrosymmetric character of barytocalcite (the current structure).
- We used the data using the "HT synthesis" results of (Spahr, 2019) while the ICSD entry uses the "precipitation syntheis" results. This makes the two CIF files slightly different.
- The site we have labeled Ba is actually a mixture of barium and calcium atoms.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(2a)	C I
$\mathbf{B_2}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$by_2\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_3}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B_4}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_5}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4c)	O II

References

[1] D. Spahr, L. Bayarjargal, V. Vinograd, R. Luchitskaia, V. Milman, and B. Winkler, *A new $BaCa(CO_3)_2$ polymorph*, Acta Crystallogr. Sect. B **75**, 291–300 (2019), doi:10.1107/S2052520619003238.

[2] F. Sartori, *New data on alstonite*, Lithos **8**, 199–207 (1975).