# Paralstonite ($BaCa(CO_3)_2$) Structure: AB2CD6_hP30_150_e_c2d_f_3g-001

This structure originally had the label `AB2CD6_hP30_150_e_c2d_f_3g`. Calls to that address will be redirected here.

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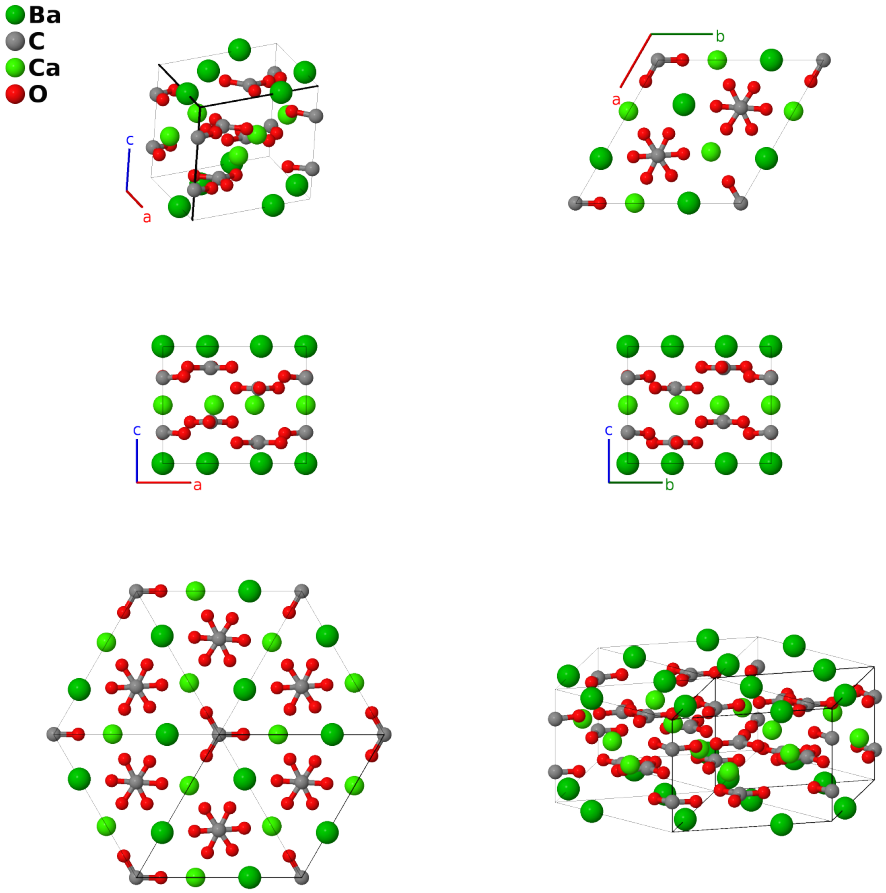
https://aflow.org/p/FL2F

https://aflow.org/p/AB2CD6_hP30_150_e_c2d_f_3g-001

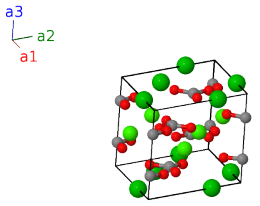



| | |
|---|---|
| **Prototype** | $BaC_2CaO_6$ |
| **AFLOW prototype label** | AB2CD6_hP30_150_e_c2d_f_3g-001 |
| **Mineral name** | paralstonite |
| **ICSD** | 100477 |
| **Pearson symbol** | hP30 |
| **Space group number** | 150 |
| **Space group symbol** | $P321$ |
| **AFLOW prototype command** | `aflow --proto=AB2CD6_hP30_150_e_c2d_f_3g-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, x_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$ |

- $BaCa(CO_3)_2$ comes in a variety of crystal structures (Spahr, 2019):
  - monoclinic barytocalcite, space group $P2_1/m$ #11,
  - trigonal paralstonite, space group $P321$ #150 (the current structure),
  - 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.
- We were unable to obtain a copy of (Effenberger, 1980), so we use the data provided by (Downs, 2003).

**Trigonal (Hexagonal) primitive vectors**

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




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_3$ | = | $cz_1\,\hat{\mathbf{z}}$ | (2c) | C I |
| $\mathbf{B_2}$ | = | $-z_1\,\mathbf{a}_3$ | = | $-cz_1\,\hat{\mathbf{z}}$ | (2c) | C I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2d) | C II |
| $\mathbf{B_4}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (2d) | C II |
| $\mathbf{B_5}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2d) | C III |
| $\mathbf{B_6}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2d) | C III |
| $\mathbf{B_7}$ | = | $x_4\,\mathbf{a}_1$ | = | $\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$ | (3e) | Ba I |
| $\mathbf{B_8}$ | = | $x_4\,\mathbf{a}_2$ | = | $\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$ | (3e) | Ba I |
| $\mathbf{B_9}$ | = | $-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$ | = | $-ax_4\,\hat{\mathbf{x}}$ | (3e) | Ba I |
| $\mathbf{B_{10}}$ | = | $x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (3f) | Ca I |
| $\mathbf{B_{11}}$ | = | $x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (3f) | Ca I |
| $\mathbf{B_{12}}$ | = | $-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (3f) | Ca I |
| $\mathbf{B_{13}}$ | = | $x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (6g) | O I |
| $\mathbf{B_{14}}$ | = | $-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (6g) | O I |
| $\mathbf{B_{15}}$ | = | $-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (6g) | O I |
| $\mathbf{B_{16}}$ | = | $y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (6g) | O I |
| $\mathbf{B_{17}}$ | = | $(x_6 - y_6)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (6g) | O I |
| $\mathbf{B_{18}}$ | = | $-x_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (6g) | O I |
| $\mathbf{B_{19}}$ | = | $x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (6g) | O II |
| $\mathbf{B_{20}}$ | = | $-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (6g) | O II |
| $\mathbf{B_{21}}$ | = | $-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (6g) | O II |
| $\mathbf{B_{22}}$ | = | $y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$ | (6g) | O II |

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| $\mathbf{B_{23}}$ | = | $(x_7 - y_7)\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$ | (6g) | O II |
| $\mathbf{B_{24}}$ | = | $-x_7\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$ | (6g) | O II |
| $\mathbf{B_{25}}$ | = | $x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (6g) | O III |
| $\mathbf{B_{26}}$ | = | $-y_8\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (6g) | O III |
| $\mathbf{B_{27}}$ | = | $-(x_8 - y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (6g) | O III |
| $\mathbf{B_{28}}$ | = | $y_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (6g) | O III |
| $\mathbf{B_{29}}$ | = | $(x_8 - y_8)\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (6g) | O III |
| $\mathbf{B_{30}}$ | = | $-x_8\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (6g) | O III |

## References


[1] H. Effenberger, *Die kristallstruktur des minerals paralstonite, $BaCa(CO_3)_2$*, Neues Jahrb. Mineral. Monatsh. **1980**, 353–363 (1980).

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

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


## Found in


[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.