

# Solid Cubane ( $\text{C}_8\text{H}_8$ ) Structure: AB\_hR16\_148\_cf\_cf-001

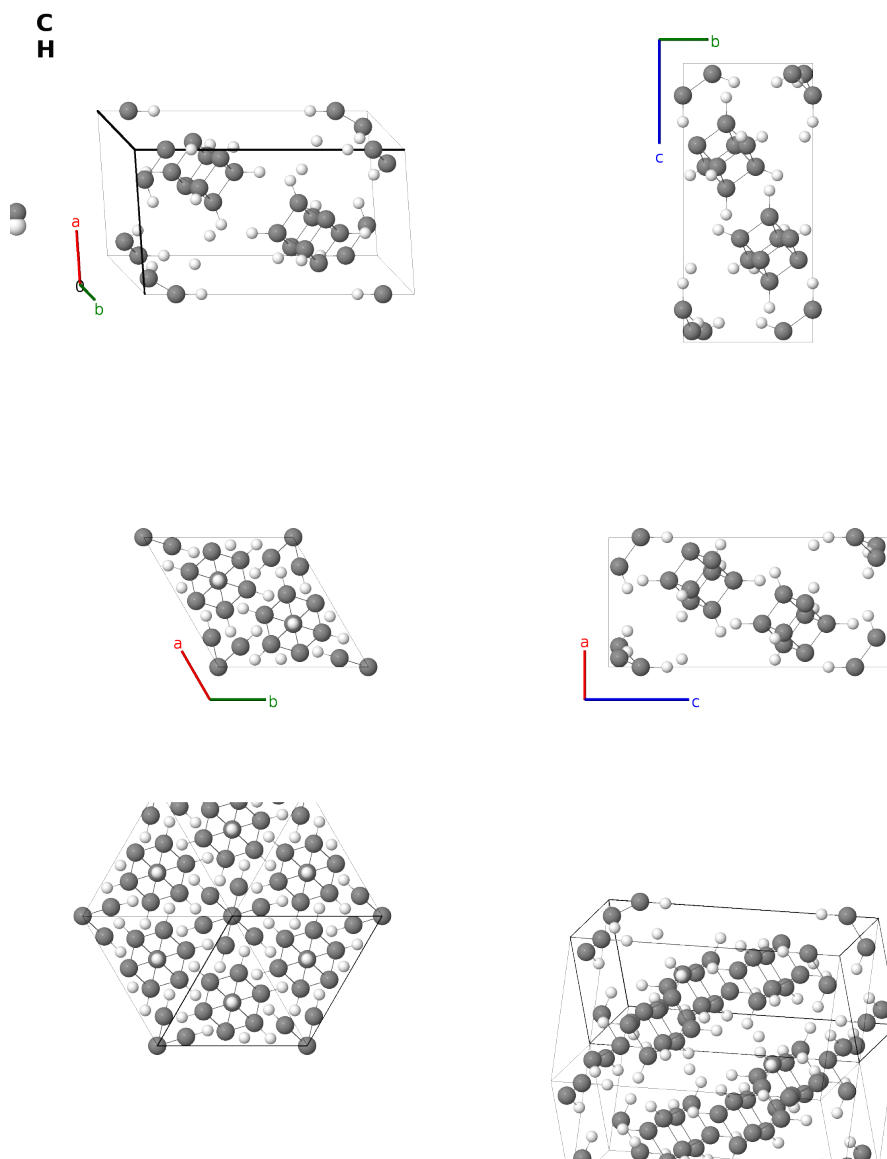
This structure previously used the label(s) **AB\_hR16\_148\_cf\_cf**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/8Z24>

[https://aflow.org/prototype-encyclopedia/AB\\_hR16\\_148\\_cf\\_cf-001](https://aflow.org/prototype-encyclopedia/AB_hR16_148_cf_cf-001)



Prototype

$\text{C}_8\text{H}_8$

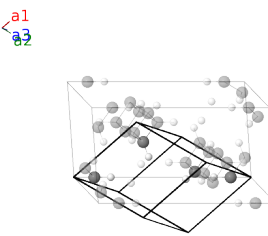
AFLOW prototype label

AB\_hR16\_148\_cf\_cf-001

|                         |                                                                                                   |
|-------------------------|---------------------------------------------------------------------------------------------------|
| Mineral name            | cubane                                                                                            |
| CCDC                    | 1132082                                                                                           |
| Pearson symbol          | hR16                                                                                              |
| Space group number      | 148                                                                                               |
| Space group symbol      | $R\bar{3}$                                                                                        |
| AFLOW prototype command | aflow --proto=AB_hR16_148_cf_cf-001<br>--params= $a, c/a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4$ |

- Hexagonal settings of this structure can be obtained with the option `--hex`.

### Rhombohedral primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
 \end{aligned}$$


### Basis vectors

|                   | Lattice coordinates                                       |   | Cartesian coordinates                                                                                                                                 | Wyckoff position | Atom type |
|-------------------|-----------------------------------------------------------|---|-------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$  | = | $cx_1 \hat{\mathbf{z}}$                                                                                                                               | (2c)             | C I       |
| $\mathbf{B}_2$    | $-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$ | = | $-cx_1 \hat{\mathbf{z}}$                                                                                                                              | (2c)             | C I       |
| $\mathbf{B}_3$    | $x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$  | = | $cx_2 \hat{\mathbf{z}}$                                                                                                                               | (2c)             | H I       |
| $\mathbf{B}_4$    | $-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$ | = | $-cx_2 \hat{\mathbf{z}}$                                                                                                                              | (2c)             | H I       |
| $\mathbf{B}_5$    | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$  | = | $\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$  | (6f)             | C II      |
| $\mathbf{B}_6$    | $z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$  | = | $-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$ | (6f)             | C II      |
| $\mathbf{B}_7$    | $y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$  | = | $-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$ | (6f)             | C II      |
| $\mathbf{B}_8$    | $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ | = | $-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$ | (6f)             | C II      |
| $\mathbf{B}_9$    | $-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$ | = | $\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$  | (6f)             | C II      |
| $\mathbf{B}_{10}$ | $-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$ | = | $\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$  | (6f)             | C II      |
| $\mathbf{B}_{11}$ | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$  | = | $\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$  | (6f)             | H II      |
| $\mathbf{B}_{12}$ | $z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$  | = | $-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$ | (6f)             | H II      |

$$\begin{aligned}
\mathbf{B}_{13} &= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= -\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} &(6f) &\text{H II} \\
\mathbf{B}_{14} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} &(6f) &\text{H II} \\
\mathbf{B}_{15} &= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 &= \frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} &(6f) &\text{H II} \\
\mathbf{B}_{16} &= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} &(6f) &\text{H II}
\end{aligned}$$

## References

- [1] E. B. Fleischer, *X-Ray Structure Determination of Cubane*, J. Am. Chem. Soc. **86**, 3889–3890 (1964), doi:10.1021/ja01072a069.

## First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017