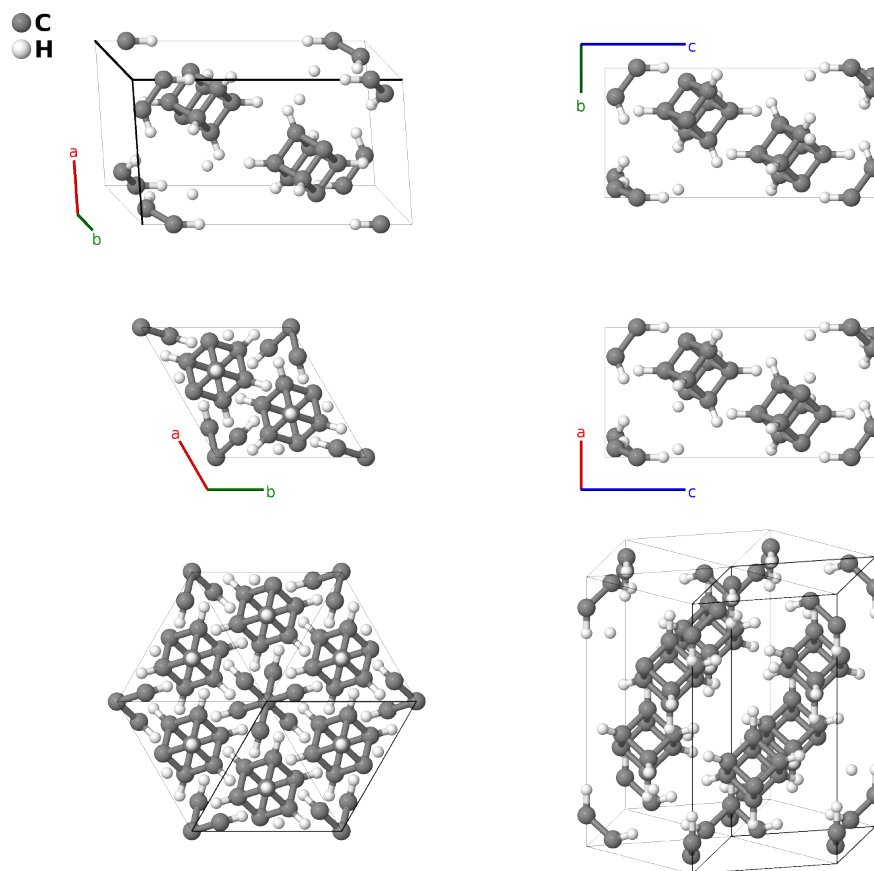# Solid Cubane (C$_8$H$_8$) Structure: AB_hR16_148_cf_cf-001

This structure originally had the label `AB_hR16_148_cf_cf`. Calls to that address will be redirected here.

https://aflow.org/p/8Z24

https://aflow.org/p/AB_hR16_148_cf_cf-001

Prototype	C$_8$H$_8$
AFLOW prototype label	AB_hR16_148_cf_cf-001
Mineral name	cubane
ICSD	none
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 --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

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

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

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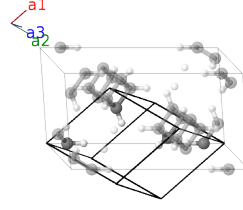
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + x_1\,\mathbf{a_3}$	$=$	$cx_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 - z_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_3 - 2y_3 + z_3\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	C II
$\mathbf{B_6}$	$=$	$z_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + y_3\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(y_3 - z_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_3 - y_3 - z_3\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	C II
$\mathbf{B_7}$	$=$	$y_3\,\mathbf{a_1} + z_3\,\mathbf{a_2} + x_3\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_3 - y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_3 + y_3 - 2z_3\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	C II
$\mathbf{B_8}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_3 - z_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_3 - 2y_3 + z_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	C II
$\mathbf{B_9}$	$=$	$-z_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - y_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(y_3 - z_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_3 - y_3 - z_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	C II
$\mathbf{B_{10}}$	$=$	$-y_3\,\mathbf{a_1} - z_3\,\mathbf{a_2} - x_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 - y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_3 + y_3 - 2z_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6f)	C II
$\mathbf{B_{11}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{12}}$	$=$	$z_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{13}}$	$=$	$y_4\,\mathbf{a_1} + z_4\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{14}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{15}}$	$=$	$-z_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - y_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	H II
$\mathbf{B_{16}}$	$=$	$-y_4\,\mathbf{a_1} - z_4\,\mathbf{a_2} - x_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(x_4 + y_4 - 2z_4\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(6f)	H II

References

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