Huntite [$CaMg_3(CO_3)_4$] Structure: A4BC3D12_hR20_155_ad_b_e_2df-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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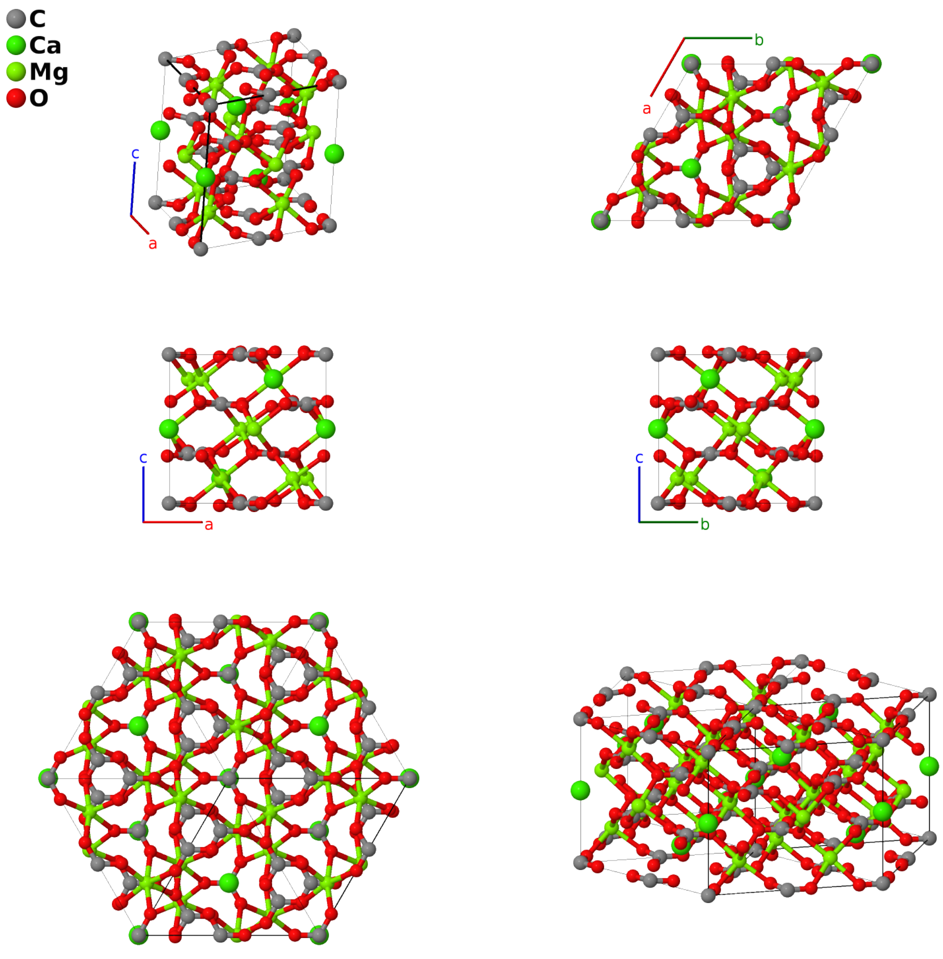
https://aflow.org/p/1B5F

https://aflow.org/p/A4BC3D12_hR20_155_ad_b_e_2df-001



Prototype	$C_3CaMg_3O_{12}$
AFLOW prototype label	A4BC3D12_hR20_155_ad_b_e_2df-001
Mineral name	huntite
ICSD	201729
Pearson symbol	hR20
Space group number	155
Space group symbol	$R32$
AFLOW prototype command	`aflow --proto=A4BC3D12_hR20_155_ad_b_e_2df-001` `--params=`$a, c/a, y_3, y_4, y_5, y_6, x_7, y_7, z_7$

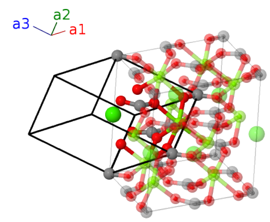
Other compounds with this structure

$EuAl_3(BO_3)_4$, $GdAl_3(BO_3)_4$, $HoAl_3(BO_3)_4$, $LaAl_3(BO_3)_4$, $NdAl_3(BO_3)_4$, $PrAl_3(BO_3)_4$, $SmAl_3(BO_3)_4$, $TbAl_3(BO_3)_4$, $TmAl_3(BO_3)_4$, $YAl_3(BO_3)_4$, $YbAl_3(BO_3)_4$

- We have shifted the origin away from that used by (Dollase, 1986): the C-I atom is now on the (1a) Wyckoff position.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + \tfrac{1}{3}c\,\mathbf{\hat{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\mathbf{\hat{y}} + \tfrac{1}{3}c\,\mathbf{\hat{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + \tfrac{1}{3}c\,\mathbf{\hat{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\mathbf{\hat{z}}$	(1b)	Ca I
$\mathbf{B_3}$	=	$y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{1}{2}ay_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_3\,\mathbf{\hat{y}}$	(3d)	C II
$\mathbf{B_4}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$-ay_3\,\mathbf{\hat{x}}$	(3d)	C II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$\frac{1}{2}ay_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_3\,\mathbf{\hat{y}}$	(3d)	C II
$\mathbf{B_6}$	=	$y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$\frac{1}{2}ay_4\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}}$	(3d)	O I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{x}}$	(3d)	O I
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$\frac{1}{2}ay_4\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}}$	(3d)	O I
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$\frac{1}{2}ay_5\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}}$	(3d)	O II
$\mathbf{B_{10}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_3$	=	$-ay_5\,\mathbf{\hat{x}}$	(3d)	O II
$\mathbf{B_{11}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$\frac{1}{2}ay_5\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}}$	(3d)	O II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2y_6+1)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{12}a\,(6y_6-1)\,\mathbf{\hat{y}} + \frac{1}{6}c\,\mathbf{\hat{z}}$	(3e)	Mg I
$\mathbf{B_{13}}$	=	$-y_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-ay_6\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + \frac{1}{6}c\,\mathbf{\hat{z}}$	(3e)	Mg I
$\mathbf{B_{14}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2y_6-1)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{12}a\,(6y_6+1)\,\mathbf{\hat{y}} + \frac{1}{6}c\,\mathbf{\hat{z}}$	(3e)	Mg I
$\mathbf{B_{15}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7-z_7)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_7-2y_7+z_7)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_7+y_7+z_7)\,\mathbf{\hat{z}}$	(6f)	O III
$\mathbf{B_{16}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7-z_7)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(2x_7-y_7-z_7)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_7+y_7+z_7)\,\mathbf{\hat{z}}$	(6f)	O III
$\mathbf{B_{17}}$	=	$y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7-y_7)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(x_7+y_7-2z_7)\,\mathbf{\hat{y}} + \frac{1}{3}c\,(x_7+y_7+z_7)\,\mathbf{\hat{z}}$	(6f)	O III
$\mathbf{B_{18}}$	=	$-z_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7-z_7)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(x_7-2y_7+z_7)\,\mathbf{\hat{y}} - \frac{1}{3}c\,(x_7+y_7+z_7)\,\mathbf{\hat{z}}$	(6f)	O III
$\mathbf{B_{19}}$	=	$-y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_7-z_7)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,(2x_7-y_7-z_7)\,\mathbf{\hat{y}} - \frac{1}{3}c\,(x_7+y_7+z_7)\,\mathbf{\hat{z}}$	(6f)	O III
$\mathbf{B_{20}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7-y_7)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,(x_7+y_7-2z_7)\,\mathbf{\hat{y}} - \frac{1}{3}c\,(x_7+y_7+z_7)\,\mathbf{\hat{z}}$	(6f)	O III

References

[1] W. A. Dollase and R. J. Reeder, *Crystal structure refinement of huntite, $CaMg_3(CO_3)_4$, with X-ray powder data*, Am. Mineral. **71**, 163–166 (1986).