Predicted High-Pressure $YCaH_{12}$ Structure: AB12C_cP14_221_a_h_b-001

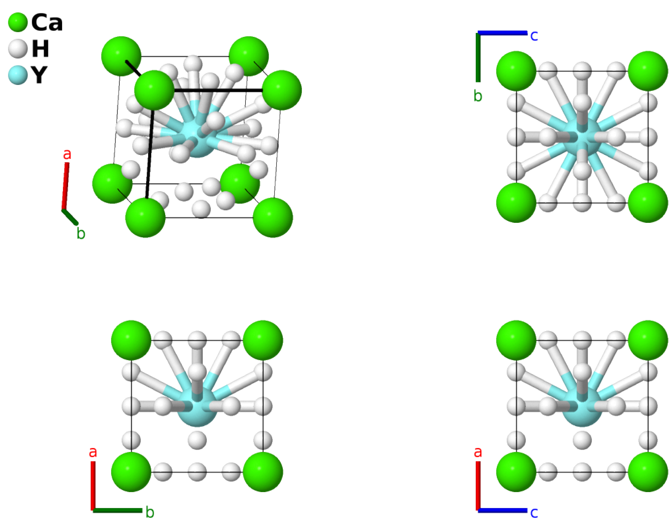
This structure originally had the label `AB12C_cP14_221_a_h_b`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/p/SQ16

https://aflow.org/p/AB12C_cP14_221_a_h_b-001



Prototype $CaH_{12}Y$

AFLOW prototype label AB12C_cP14_221_a_h_b-001

ICSD 686726

Pearson symbol cP14

Space group number 221

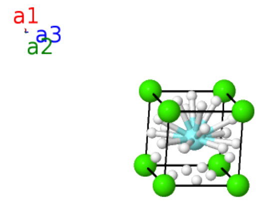
Space group symbol $Pm\bar{3}m$

AFLOW prototype command `aflow --proto=AB12C_cP14_221_a_h_b-001`
`--params=`a, x_3

- This structure was determined by *ab initio* methods and is predicted to be stable in the pressure range 180-257GPa, with $T_c = 230$K at 180GPa. We show the predicted structure at 200GPa.
- The ICSD entry is from the calculations of (Liang, 2019).

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ca I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Y I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12h)	H I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12h)	H I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(12h)	H I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(12h)	H I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(12h)	H I
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(12h)	H I

References

[1] H. Xie, D. Duan, Z. Shao, H. Song, Y. Wang, X. Xiao, D. Li, F. Tian, B. Liu, and T. Cui, *High-temperature superconductivity in ternary clathrate $YCaH_{12}$ under high pressures*, J. Phys.: Condens. Matter **31**, 245404 (2019), doi:10.1088/1361-648X/ab09b4.

[2] X. Liang, A. Bergara, L. Wang, B. Wen, Z. Zhao, X.-F. Zhou, J. He, G. Gao, and Y. Tian, *Potential high-T_c superconductivity in $CaYH_{12}$ under pressure*, Phys. Rev. B **99**, 100505(R) (2019), doi:10.1103/PhysRevB.99.100505.