

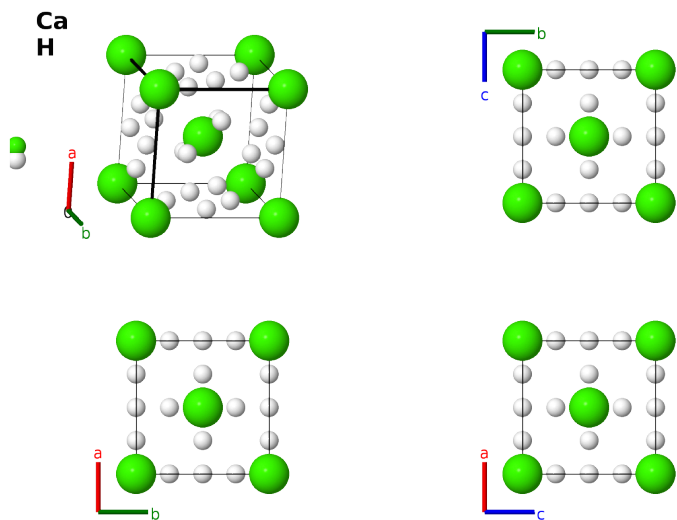
High Pressure Cubic CaH_6 Structure: AB6_cI14_229_a_d-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/N2LT>

https://aflow.org/prototype-encyclopedia/AB6_cI14_229_a_d-001



Prototype	CaH_6
AFLOW prototype label	AB6_cI14_229_a_d-001
Pearson symbol	cI14
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB6_cI14_229_a_d-001 --params=a</code>

Other compounds with this structure

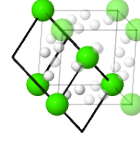
YH_6

- (Wang, 2012) predict this structure to become superconducting with a critical temperature of 220-235K at 150 GPa. (Ma, 2022) later synthesized the material and found $T_c = 215\text{K}$ at 172 GPa. We show the structure at the lattice constant predicted by (Wang, 2012) at the pressure 150 GPa.

Body-centered Cubic primitive vectors

a3
a2
a1

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	Ca I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12d) H I
$\mathbf{B}_3$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$	(12d) H I
$\mathbf{B}_4$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(12d) H I
$\mathbf{B}_5$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12d) H I
$\mathbf{B}_6$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(12d) H I
$\mathbf{B}_7$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(12d) H I

References

- [1] H. Wang, J. S. Tse, K. Tanaka, T. Iitaka, and Y. Ma, *Superconductive sodalite-like clathrate calcium hydride at high pressures*, Proc. Natl. Acad. Sci. **109**, 6463–6466 (2012), doi:10.1073/pnas.1118168109.
- [2] L. Ma, K. Wang, Y. Xie, X. Yang, Y. Wang, M. Zhou, H. Liu, X. Yu, Y. Zhao, H. Wang, G. Liu, and Y. Ma, *High-Temperature Superconducting Phase in Clathrate Calcium Hydride CaH_6 up to 215 K at a Pressure of 172 GPa*, Phys. Rev. Lett. **128**, 167001 (2022), doi:10.1103/PhysRevLett.128.167001.

First cited in

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