$CaCu_5$ ($D2_d$) Structure: AB5_hP6_191_a_cg-001

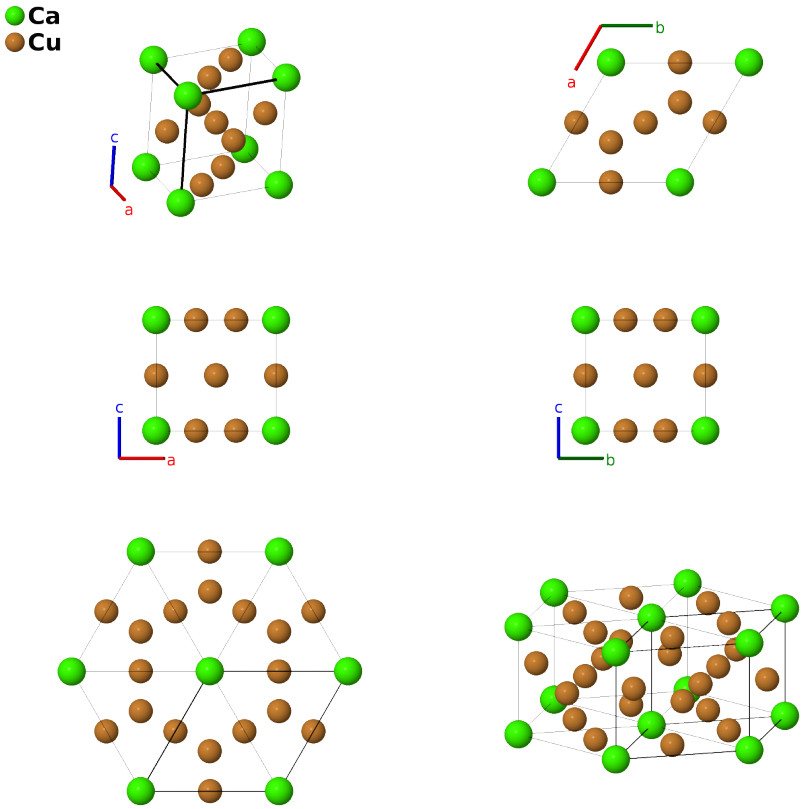
This structure originally had the label `AB5_hP6_191_a_cg`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. 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

---

https://aflow.org/p/F7Y6

https://aflow.org/p/AB5_hP6_191_a_cg-001



Prototype	$CaCu_5$
AFLOW prototype label	AB5_hP6_191_a_cg-001
***Strukturbericht* designation**	$D2_d$
ICSD	58882
Pearson symbol	hP6
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=AB5_hP6_191_a_cg-001 --params=`$a, c/a$

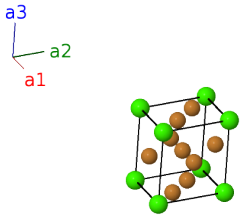
Other compounds with this structure

$BaAg_5$, $BaAu_5$, $BaPt_5$, $CaNi_5$, $CaPt_5$, $CaZn_5$, $CeCo_5$, $CeCu_5$, $CeFe_5$, $CeNi_5$, $CePt_5$, $CeZn_5$, $DyCo_5$, $DyFe_5$, $DyNi_5$, $ErCo_5$, $ErNi_5$, $GdCo_5$, $GdCu_5$, $GdFe_5$, $GdNi_5$, $HfBe_5$, $HoCo_5$, $HoCu_5$, $HoNi_5$, KAu_5, $LaCo_5$, $LaCu_5$, $LaNi_5$, $LaPt_5$, $LaZn_5$, $NdCo_5$, $NdCu_5$, $NdNi_5$, $NdPt_5$, $PrCo_5$, $PrCu_5$, $PrNi_5$, $PrPt_5$, $PrSr_5$, $PuNi_5$, $RbAu_5$, $ScBe_5$, $SmCo_5$, $SmCu_5$, $SmFe_5$, $SmNi_5$, $SrAg_5$, $SrAu_5$, $SrPd_5$, $TbCo_5$, $TbCu_5$, $TbNi_5$, $ThCo_5$, $ThFe_5$, $ThNi_5$, YCo_5, YCu_5, YFe_5, YNi_5

- The original version of this page inadvertantly used the lattice constants for $CaZn_5$ (a = 5.405Å, c = 4.183Å) rather than those for $CaCu_5$ (a = 5.082Å, c = 4.078Å). This has now been corrected.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ca I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Cu I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Cu I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Cu II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Cu II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Cu II

References

[1] W. Haucke, *Kristallstruktur von $CaZn_5$ und $CaCu_5$*, Z. Anorganische und Allgemeine Chemie **244**, 17–22 (1940), doi:10.1002/zaac.19402440103.

Found in

[1] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Tornoto, 1972).