$HfCuSi_2$ Structure: ABC2_tP8_129_a_c_bc-002

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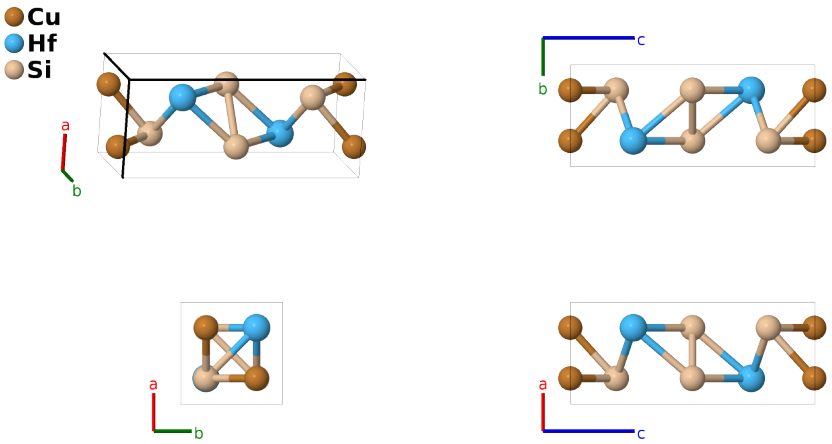
https://aflow.org/p/3Z42

https://aflow.org/p/ABC2_tP8_129_a_c_bc-002



Prototype	$CuHfSi_2$
AFLOW prototype label	ABC2_tP8_129_a_c_bc-002
ICSD	87174
Pearson symbol	tP8
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=ABC2_tP8_129_a_c_bc-002 --params=`$a, c/a, z_3, z_4$

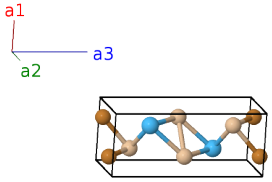
Other compounds with this structure

$CeAsSb_2$, $DyZnSn_2$, $ErZnSn_2$, $GdZnSn_2$, $HfCuGe_2$, $HfCuSi_2$, $HoZnSn_2$, $LaAsSb_2$, $LuSn_2$, $TmZnSn_2$, $YZnSn_2$, $YbMnBi_2$, $YbMnSb_2$, $ZrCuGe_2$, $ZrCuSi_2$

- This is a ternary form of AsCuSiZr and LaOAgS.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Si I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Si I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	Hf I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	Hf I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	Si II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2c)	Si II

References

[1] L. S. Andrukhiv, L. A. Lysenko, Y. P. Yarmolyuk, and E. I. Gladyshevskii, *On structure of the compounds HfCuSi$_2$, HfCuGe$_2$, ZrCuSi$_2$ and ZrCuGe$_2$*, Dopov. Akad. Nauk Ukr. RSR, Ser. A pp. 645–648 (1975).

Found in

[1] M. W. Pohlkamp and W. Jeitschko, *Preparation, Properties, and Crystal Structure of Quaternary Silicide Carbides RCr$_2$Si$_2$C (R = Y, La-Nd, Sm, Gd-Ho)*, Z. Naturforsch. B **56**, 1143–1148 (2001), doi:10.1515/znb-2001-1108.