$HfFe_6Ge_6$ Structure: A6B6C_hP13_191_i_cde_a-002

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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.

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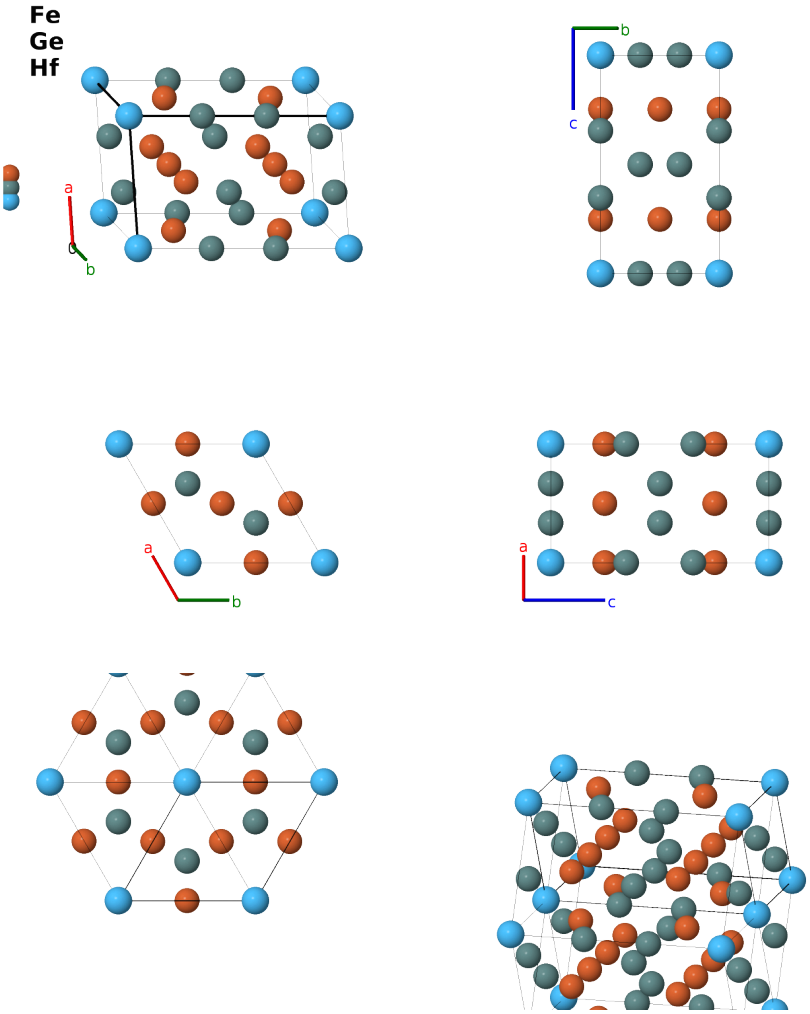
https://aflow.org/prototype-encyclopedia/4E59

https://aflow.org/prototype-encyclopedia/A6B6C_hP13_191_i_cde_a-002



Prototype	Fe_6Ge_6Hf
AFLOW prototype label	A6B6C_hP13_191_i_cde_a-002
ICSD	632038
CCDC	1754769
Pearson symbol	hP13
Space group number	191

Space group symbol $P6/mmm$

AFLOW prototype command `aflow --proto=A6B6C_hP13_191_i_cde_a-002 --params=`$a, c/a, z_4, z_5$

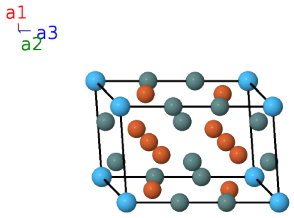
Other compounds with this structure

$DyCr_6Ge_6$, $DyCo_6Ge_6$, $DyFe_6Ge_6$, $DyMn_6Ge_6$, DyV_6Sn_6, $ErCo_6Ge_6$, $ErCr_6Ge_6$, $ErFe_6Ge_6$, $ErMn_6Ge_6$, ErV_6Sn_6, $GdCo_6Ge_6$, $GdCr_6Ge_6$, $GdFe_6Ge_6$, $GdMn_6Ge_6$, GdV_6Sn_6, $HfCo_6Ge_6$, $HfFe_6Ge_6$, $HfMn_6Ge_6$, $HfMn_6Sn_6$, $HoCo_6Ge_6$, $HoCr_6Ge_6$, $HoFe_6Ge_6$, $HoMn_6Ge_6$, $HoMn_6Sn_6$, HoV_6Sn_6, $LiCo_6Ge_6$, $LuCo_6Ge_6$, $LuFe_6Ge_6$, $LuFe_6Sn_6$, $LuMn_6Ge_6$, LuV_6Sn_6, $MgCo_6Ge_6$, $MgNi_6Ge_6$, $MgNi_6Si_6$, $MgFe_6Ge_6$, $NbFe_6Ge_6$, $NdMn_6Ge_6$, $ScCo_6Ge_6$, $ScCr_6Ge_6$, $ScFe_6Ge_6$, $ScMn_6Ge_6$, $ScMn_6Sn_6$, $SmMn_6Ge_6$, $TbCo_6Ge_6$, $TbCr_6Ge_6$, $TbFe_6Ge_6$, $TbMn_6Ge_6$, $TbMn_6Sn_6$, $TbNb_6Sn_6$, $TiCo_6Ge_6$, $TiFe_6Ge_6$, $TmCo_6Ge_6$, $TmFe_6Ge_6$, $TmFe_6Sn_6$, $TmMn_6Ge_6$, $TmMn_6Sn_6$, TmV_6Sn_6, UCo_6Ge_6, YCr_6Ge_6, YFe_6Ge_6, YMn_6Ge_6, YMn_6Sn_6, YV_6Sn_6, $YbCo_6Ge_6$, $YbFe_6Ge_6$, $YbFe_6Sn_6$, $YbMn_6Ge_6$, $YbMn_6Sn_6$, YbV_6Sn_6, $ZrCo_6Ge_6$, $ZrFe_6Ge_6$, $ZrMn_6Sn_6$, $DyFe_6Sn_4Ge_2$, $ErFe_6Sn_4Ge_2$, $GdFe_6Sn_4Ge_2$, $HoFe_6Sn_4Ge_2$, $TbFe_6Sn_4Ge_2$, $YFe_6Sn_4Ge_2$

- (Zyubrik, 1982) originally determined the structure of $HfFe_6Ge_6$. While we do not have a copy of this paper, we were able to extract the data from the ICSD entry.
- This structure is related to the $D2_a$ $TiBe_{12}$ structure. That structure, however, is probably not the actual $TiBe_{12}$ structure, so we designate $HfFe_6Ge_6$ as the prototype for the ternary form.

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)	Hf 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)	Ge 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)	Ge I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Ge II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Ge II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2e)	Ge III
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(2e)	Ge III
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I

References

[1] A. A. Zyubrik, R. R. Olenych, I. A. Mizak, and Y. P. Yarmolyuk, *The (titanium, hafnium)-iron-germanium systems*, Dopov. Akad. Nauk Ukr. RSR A **44**, 78–81 (1982).

Found in

[1] T. Mazet, O. Isnard, and B. Malaman, *Neutron diffraction and ^{57}Fe Mössbauer study of the $HfFe_6Ge_6$-type RFe_6Ge_6 compounds (R=Sc, Ti, Zr, Hf, Nb)*, Solid State Commun. **114**, 91–96 (2000), doi:10.1016/S0038-1098(00)00003-X.

First cited in

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