Fe_7W_6 ($D8_5$) μ-phase Structure: A7B6_hR13_166_ah_3c-001

This structure originally had the label `A7B6_hR13_166_ah_3c`. Calls to that address will be redirected here.

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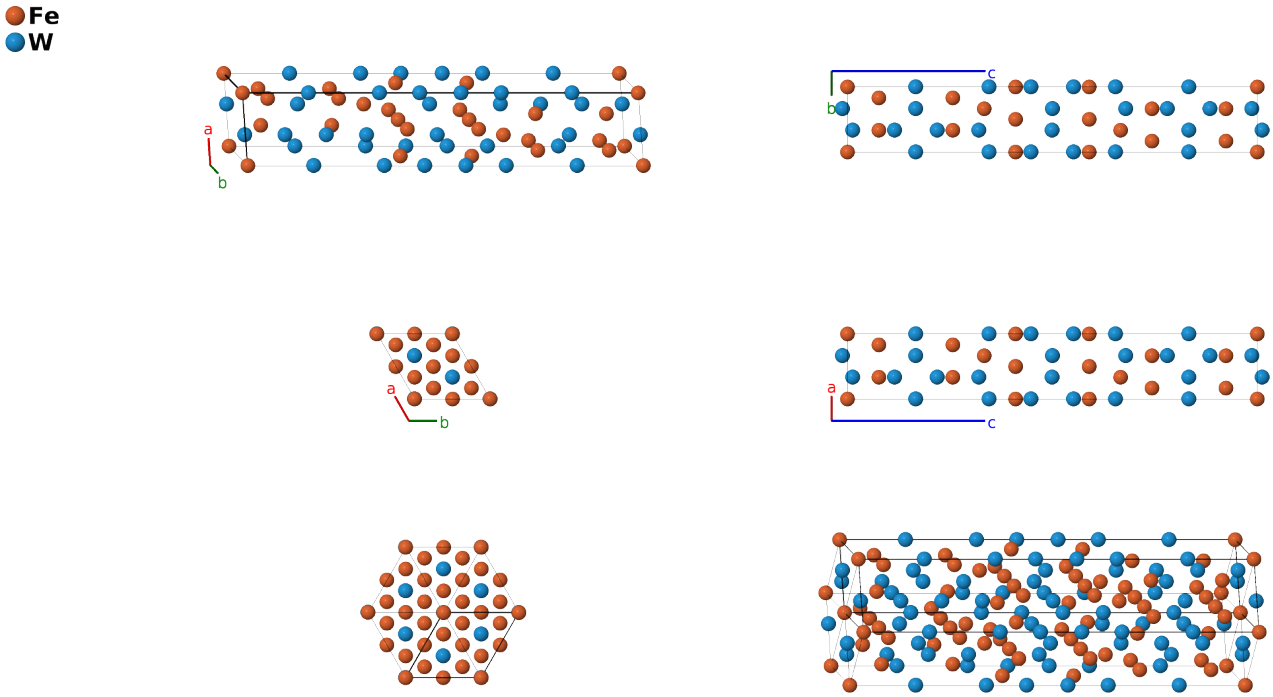
https://aflow.org/p/MXB3

https://aflow.org/p/A7B6_hR13_166_ah_3c-001



Prototype	Fe_7W_6
AFLOW prototype label	A7B6_hR13_166_ah_3c-001
***Strukturbericht* designation**	$D8_5$
ICSD	632620
Pearson symbol	hR13
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A7B6_hR13_166_ah_3c-001 --params=`$a, c/a, x_2, x_3, x_4, x_5, z_5$

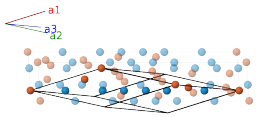
Other compounds with this structure

Co_7Mo_6, Co_7W_6, Fe_7Mo_6, Fe_7Nb_6, Fe_7Ta_6, Mo_7Co_6, Si_7Mn_6, Ta_7Fe_6, Zn_7Ta_6, Co_6Re_6Si

- For more information on the μ-phase, see (Pearson, 1972, p. 664). There it is referred to as a tetrahedrally close-packed Frank-Kasper structure. We have been unable to obtain a copy of the original reference for this structure (Arnfeldt, 1935), so we use the structure from (Villars, 1991, p.3415), which itself is taken from a secondary reference.
- See the $Ba_3Cr_2O_8$ page for ternary compounds with this structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Fe I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	W I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	W I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	W II
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	W II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	W III
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	W III
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Fe II
$\mathbf{B_9}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Fe II
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Fe II
$\mathbf{B_{11}}$	=	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Fe II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Fe II
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Fe II

References

[1] H. Arnfelt, *Crystal Structure of Fe_7W_6*, Jernkontorets Annaler **119**, 185–187 (1935).

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

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.