σ-CrFe ($D8_b$) Structure: A4B4C4DE2_tP30_136_i_j_i_a_f-001

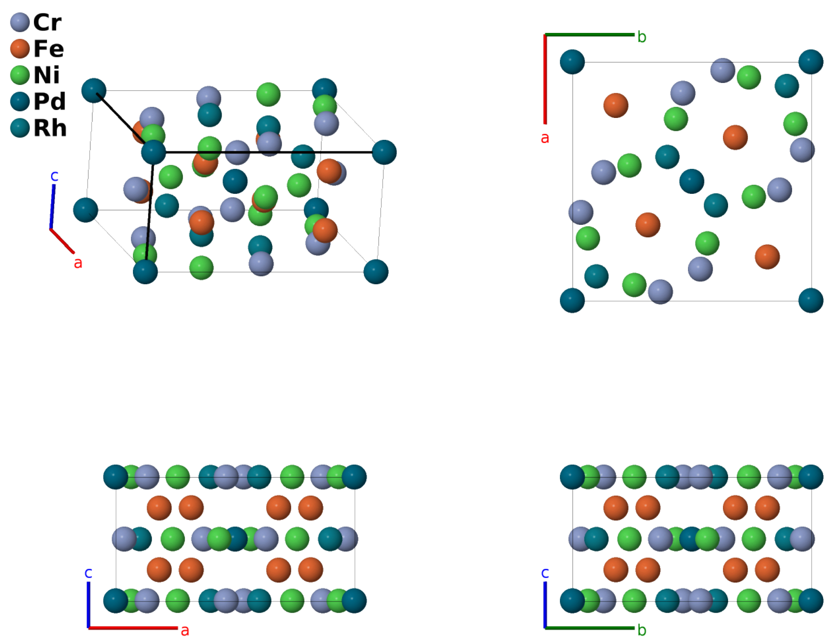
This structure originally had the label `sigma_tP30_136_bf2ij`. Calls to that address will be redirected here.

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/6EHC

https://aflow.org/p/A4B4C4DE2_tP30_136_i_j_i_a_f-001



Prototype	$Cr_4Fe_4Ni_4PdRh_2$
AFLOW prototype label	A4B4C4DE2_tP30_136_i_j_i_a_f-001
***Strukturbericht* designation**	$D8_b$
ICSD	none
Pearson symbol	tP30
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	`aflow --proto=A4B4C4DE2_tP30_136_i_j_i_a_f-001` `--params=`$a, c/a, x_2, x_3, y_3, x_4, y_4, x_5, z_5$

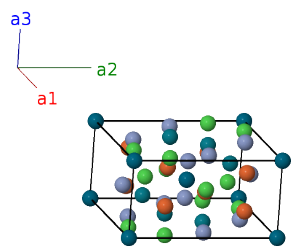
Other compounds with this structure

Al_3CoNb_6, $AlCrNb_3$, $AlNb_2$, $AuTa_2$, Co_2Mo_3, CoV, Cr_2Os, Cr_2Rus, Cr_8Ni_5W, CrFe, $CrMn_3$, Fe_3Re_2, $Fe_{21}Nb_{19}$, FeMo, FeV, $IrMo_2$, IrW_3, $IrZr_3$, Mn_2Os, Mn_3Re_2, $Mn_{45}Re_{55}$, MnTc, $Mo_{45}Ru_3$, $MoTc_3$, Nb_2Os_3, Nb_2Rh, Nb_3Pd_2, Ni_2V_3, $Ni_{34}Si_8V_{58}$, $PdTa_3$, Re_3Ta_2 (HT), Re_3V, $RhTa_2$, Ta_3V_7, TaV, Tc_3W

- The atoms in this lattice are completely disordered, that is, the Cr and Fe atoms are distributed randomly on the sites in the unit cell. This seems to be the case for all of the compounds listed below. We have chosen several of the atoms near Fe and Cr in the periodic table to color the above pictures. Except for a shift of the origin, this structure is crystallographically equivalent to β-U (A_b).
- We use the data for a sample of $Cr_{0.48}Fe_{0.52}$ annealed at 923K.
- Previously we had put the atom we labeled “Pd” on the (2b) site rather than the (2a) site, making the Pd-Rh distance too short. This is the corrected version. We thank Brandon Bocklund for pointing this out.
- Due to an origin shift, literature may list different Wyckoff designations. For instance, the structure in (Berne, 2001) lists a different Wyckoff sequence, af2ij, however it is structurally equivalent to this prototype and can be verified with AFLOW-XtalFinder.

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
$\mathbf{B_1}$	=	0	=	0	(2a)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Pd I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4f)	Rh I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4f)	Rh I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Rh I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Rh I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8i)	Cr I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8i)	Cr I
$\mathbf{B_9}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Cr I
$\mathbf{B_{10}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Cr I
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Cr I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Cr I
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8i)	Cr I
$\mathbf{B_{14}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8i)	Cr I
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8i)	Ni I
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8i)	Ni I
$\mathbf{B_{17}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Ni I

$\mathbf{B_{18}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Ni I
$\mathbf{B_{19}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Ni I
$\mathbf{B_{20}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Ni I
$\mathbf{B_{21}}$	=	$y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}$	(8i)	Ni I
$\mathbf{B_{22}}$	=	$-y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}$	(8i)	Ni I
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{24}}$	=	$-x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{25}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{26}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{27}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{28}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{29}}$	=	$x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(8j)	Fe I
$\mathbf{B_{30}}$	=	$-x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(8j)	Fe I

References

[1] H. L. Yakel, *Atom distributions in sigma phases. I. Fe and Cr atom distributions in a binary sigma phase equilibrated at 1063, 1013 and 923 K*, Acta Crystallogr. Sect. B **39**, 20–28 (1983), doi:10.1107/S0108768183001974.

Found in

[1] P. Villars and L. Calvert, eds., *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, Ohio, 1991), vol. 2, chap. , p. 2639, 2nd edn.