

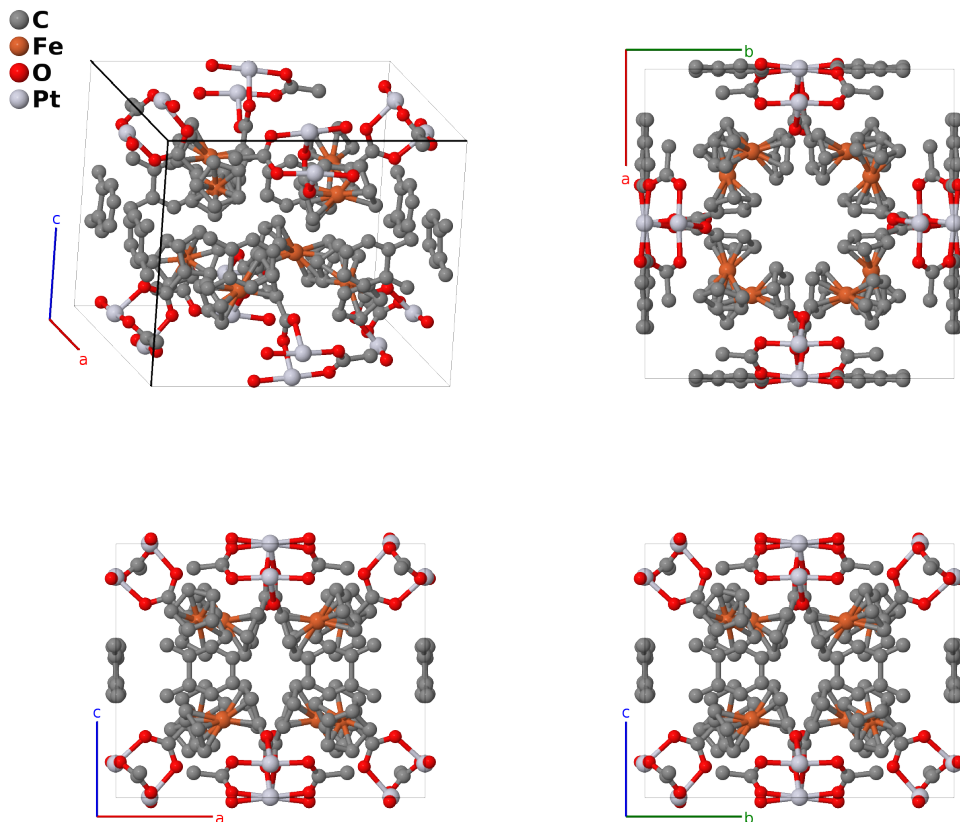
(CH)₁₇FeO₄Pt Structure (Original Page): A17BC4D_tP184_89_17p_p_4p_il-001

This structure originally had the label A17BC4D_tP184_89_17p_p_4p_io. Calls to that address will be redirected here.

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<https://aflow.org/p/EK6P>

https://aflow.org/p/A17BC4D_tP184_89_17p_p_4p_il-001

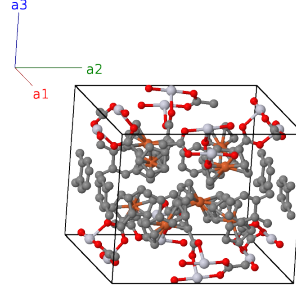


Prototype	C ₁₇ FeH ₁₇ O ₄ Pt
AFLOW prototype label	A17BC4D_tP184_89_17p_p_4p_il-001
CCDC	863010
Pearson symbol	tP184
Space group number	89
Space group symbol	P422
AFLOW prototype command	<pre>aflow --proto=A17BC4D_tP184_89_17p_p_4p_il-001 --params=a, c/a, z1, x2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24</pre>

- Structures exhibiting space group $P422$ #89 are quite rare. According to (Hoffmann, 2014) there are only two entries in the Inorganic Crystal Structure Database with space group #89; however the ones they list are incorrectly classified.
- This structure was not explicitly referenced in (Tanaka, 2011), but the authors did deposit it in the Cambridge Structure Database (ID=863010).
- This page (Hicks, 2019) does not include the hydrogen atom locations. Those are included on the A17BC17D4E.tP320_89_17p_p_17p_4p_il page.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4i)	Pt I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(4i)	Pt I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4i)	Pt I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_1 \hat{\mathbf{z}}$	(4i)	Pt I
\mathbf{B}_5	$= x_2 \mathbf{a}_1$	$=$	$ax_2 \hat{\mathbf{x}}$	(4l)	Pt II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1$	$=$	$-ax_2 \hat{\mathbf{x}}$	(4l)	Pt II
\mathbf{B}_7	$= x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{y}}$	(4l)	Pt II
\mathbf{B}_8	$= -x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{y}}$	(4l)	Pt II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{11}	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{12}	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{13}	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{14}	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{15}	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{16}	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8p)	C I
\mathbf{B}_{17}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8p)	C II
\mathbf{B}_{18}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8p)	C II
\mathbf{B}_{19}	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8p)	C II
\mathbf{B}_{20}	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8p)	C II
\mathbf{B}_{21}	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8p)	C II

References

- [1] S. Tanaka and K. Mashima, *Interaction of Ferrocene Moieties Across a Square Pt_4 Unit: Synthesis, Characterization, and Electrochemical Properties of Carboxylate-Bridged Bimetallic Pt_4Fe_n ($n = 2, 3,$ and 4) Complexes*, *Inorg. Chem.* **50**, 11384–11393 (2011), doi:10.1021/ic201012m.
- [2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, *Comput. Mater. Sci.* **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.