

Eisen(III)-Oximat 2a der Struktur [Fe₃^{III}O(H₂O)₃L₆][FeCl₄]

Empirical formula	C117 H216 Cl16 Fe16 N24 O100
Color	red
Formula weight	5019.94 g · mol ⁻¹
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	HEXAGONAL
Space group	P 63, (no. 173)
Unit cell dimensions	a = 17.107(2) Å α= 90°. b = 17.107(2) Å β= 90°. c = 24.704(3) Å β = 120°.
Volume	6260.9(13) Å ³
Z	1
Density (calculated)	1.331 Mg · m ⁻³
Absorption coefficient	1.148 mm ⁻¹
F(000)	2574 e
Crystal size	0.360 x 0.345 x 0.096 mm3
θ range for data collection	1.37 to 36.43°.
Index ranges -	28 ≤ h ≤ 28, -28 ≤ k ≤ 28, -41 ≤ l ≤ 41
Reflections collected	243304
Independent reflections	20334 [R _{int} = 0.0275]
Reflections with I>2σ (I)	18050
Completeness to θ = 27.50°	100.0 %
Absorption correction	Gaussian
Max. and min. transmission	0.83 and 0.50
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	20334 / 1 / 460
Goodness-of-fit on F ²	1.165
Final R indices [I>2σ (I)]	R ₁ = 0.0509 wR ² = 0.1500
R indices (all data)	R ₁ = 0.0606 wR ² = 0.1621
Absolute structure parameter	0.00(6)
Largest diff. peak and hole	2.255 and -1.250 e · Å ⁻³

Atom	Wyck	Site	S.O.F.	Atomic parameters			U [Å ²]
				x/a	y/b	z/c	
Fe1	6c	1		0.55898(2)	0.21870(2)	0.36573(2)	
Fe1A	6c	1		0.12828(1)	0.06288(1)	0.37759(1)	
Fe2	2a	3..		0	0	0.62768(2)	
Fe2A	2b	3..		1/3	2/3	0.12690(5)	
Cl1	6c	1		-0.08977(6)	0.04674(6)	0.65703(5)	
Cl1A	6c	1		0.34765(9)	0.55383(9)	0.15700(7)	
Cl2	2a	3..		0	0	0.53908(5)	
Cl2A	2b	3..		1/3	2/3	0.03718(7)	
O1	6c	1		0.35666(16)	0.24566(17)	0.17587(10)	
O1A	6c	1		0.13194(16)	0.36799(16)	0.2193(1)	
O2	6c	1		0.49754(12)	0.25161(12)	0.30748(9)	
O2A	6c	1		0.14295(10)	0.15007(11)	0.31827(7)	
O3	6c	1		0.59802(13)	0.16695(13)	0.30489(11)	
O3A	6c	1		0.14151(11)	-0.01647(11)	0.32214(8)	
O4	6c	1		0.59943(13)	0.16483(13)	0.42369(11)	
O4A	2a	3..		0	0	0.37773(13)	
O5	6c	1		0.49793(12)	0.24954(12)	0.42414(9)	
O5A	6c	1		0.14024(11)	0.15137(11)	0.43510(7)	
O6	6c	1		0.38794(17)	0.2473(2)	0.56736(11)	
O6A	6c	1		0.12642(19)	0.35650(19)	0.54528(11)	
O7	2b	3..		2/3	1/3	0.36585(13)	
O7A	6c	1		0.14281(11)	-0.00922(12)	0.43740(8)	
O8	6c	1		0.44531(10)	0.09299(10)	0.36616(9)	
H8A	6c	1		0.41180	0.08410	0.39620	0.0470
H8B	6c	1		0.40960	0.08530	0.33730	0.0470
O8A	6c	1		0.26764(8)	0.13419(9)	0.37736(8)	
H8AA	6c	1		0.28820	0.12030	0.34840	0.0330
H8AB	6c	1		0.28720	0.19250	0.37720	0.0330
O9	6c	1		-0.08819(14)	0.24511(18)	0.29163(8)	
H9A	6c	1		-0.06160	0.21900	0.27600	0.0550
H9B	6c	1		-0.13100	0.24130	0.27080	0.0550
O9A	6c	1		-0.07963(13)	0.26512(15)	0.45333(7)	
H9AA	6c	1		-0.05510	0.32240	0.46060	0.0450
H9AB	6c	1		-0.13650	0.23770	0.46220	0.0450
N1	6c	1		0.42195(15)	0.24438(18)	0.51742(10)	
N1A	6c	1		0.08408(16)	0.28931(16)	0.50622(9)	
N2	6c	1		0.40245(15)	0.24443(16)	0.22167(10)	
N2A	6c	1		0.08700(14)	0.29492(14)	0.25381(9)	
C1	6c	1		0.3394(3)	0.1574(3)	0.58928(18)	
H1A	6c	1		0.28810	0.11930	0.56570	0.0950
H1B	6c	1		0.31730	0.15940	0.62560	0.0950
H1C	6c	1		0.37970	0.13220	0.59140	0.0950
C1A	6c	1		0.0812(4)	0.4073(3)	0.54888(18)	
H1AA	6c	1		0.08110	0.43260	0.51330	0.0860
H1AB	6c	1		0.11250	0.45650	0.57500	0.0860
H1AC	6c	1		0.01880	0.36780	0.56080	0.0860
C2	6c	1		0.4942(3)	0.4092(3)	0.5244(2)	
H2A	6c	1		0.52590	0.41540	0.55860	0.0840
H2B	6c	1		0.43810	0.40970	0.53170	0.0840
H2C	6c	1		0.53270	0.45960	0.50040	0.0840
C2A	6c	1		0.2108(2)	0.2623(3)	0.52615(13)	
H2AA	6c	1		0.19470	0.21940	0.55610	0.0630
H2AB	6c	1		0.24320	0.32410	0.54030	0.0630
H2AC	6c	1		0.24970	0.25370	0.50060	0.0630
C3	6c	1		0.47283(18)	0.32298(18)	0.49812(12)	
C3A	6c	1		0.12674(16)	0.24669(17)	0.49774(10)	
C4	6c	1		0.51501(15)	0.32386(16)	0.44444(12)	
C4A	6c	1		0.08820(14)	0.17718(14)	0.45341(9)	
C5	6c	1		0.2823(2)	0.1553(3)	0.16646(17)	

H5A	6c	1		0.24220	0.15700	0.13880	0.0780
H5B	6c	1		0.24850	0.13100	0.20020	0.0780
H5C	6c	1		0.30590	0.11660	0.15410	0.0780
C5A	6c	1		0.0756(3)	0.4037(3)	0.20548(19)	
H5AA	6c	1		0.10910	0.45710	0.18250	0.0810
H5AB	6c	1		0.05600	0.42070	0.23850	0.0810
H5AC	6c	1		0.02260	0.35800	0.18580	0.0810
C6	6c	1		0.4815(3)	0.4099(2)	0.20978(18)	
H6A	6c	1		0.45720	0.44070	0.23170	0.0760
H6B	6c	1		0.45310	0.39620	0.17400	0.0760
H6C	6c	1		0.54690	0.44910	0.20580	0.0760
C6A	6c	1		0.23230(17)	0.2999(2)	0.24875(13)	
H6AA	6c	1		0.26350	0.27880	0.27280	0.0560
H6AB	6c	1		0.26350	0.36600	0.24930	0.0560
H6AC	6c	1		0.23230	0.27910	0.21180	0.0560
C7	6c	1		0.46212(18)	0.32379(18)	0.23721(12)	
C7A	6c	1		0.13801(14)	0.26318(15)	0.26743(10)	
C8	6c	1		0.51350(14)	0.32535(15)	0.28714(11)	
C8A	6c	1		0.09483(13)	0.18285(13)	0.30524(8)	
C11	6c	1	0.5	0.2685(4)	0.3766(3)	0.3847(2)	
H11	6c	1	0.5	0.22800	0.32050	0.40120	0.0390
C12	6c	1	0.5	0.3574(5)	0.3992(5)	0.3785(5)	
H12	6c	1	0.5	0.38130	0.36620	0.39590	0.0670
C13	6c	1	0.5	0.4134(4)	0.4774(6)	0.3434(5)	
H13	6c	1	0.5	0.47460	0.49440	0.33670	0.0740
C14	6c	1	0.5	0.3785(5)	0.5250(6)	0.3207(6)	
H14	6c	1	0.5	0.41470	0.57310	0.29670	0.0840
C15	6c	1	0.5	0.2909(6)	0.5053(5)	0.3317(5)	
H15	6c	1	0.5	0.26740	0.53960	0.31560	0.0760
C16	6c	1	0.5	0.2358(3)	0.4312(4)	0.3682(5)	
C17	6c	1	0.5	0.1388(3)	0.4043(4)	0.3798(3)	
H17A	6c	1	0.5	0.13580	0.43310	0.41340	0.0580
H17B	6c	1	0.5	0.10280	0.33860	0.38370	0.0580
H17C	6c	1	0.5	0.11500	0.42380	0.34980	0.0580

Anisotropic displacement parameters, in Å²

Atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Fe1	0.01371(9)	0.01440(9)	0.04695(18)	0.00625(8)	0.00292(10)	-0.00151(10)
Fe1A	0.01220(8)	0.01290(8)	0.02855(11)	0.00628(7)	-0.00024(9)	0.00012(9)
Fe2	0.02370(12)	0.02370(12)	0.02232(18)	0.01185(6)	0.00000	0.00000
Fe2A	0.0387(2)	0.0387(2)	0.0661(5)	0.01933(12)	0.00000	0.00000
Cl1	0.0427(4)	0.0454(4)	0.0699(5)	0.0272(3)	0.0110(4)	-0.0070(4)
Cl1A	0.0684(7)	0.0556(6)	0.0931(9)	0.0328(5)	-0.0178(6)	0.0081(6)
Cl2	0.0642(5)	0.0642(5)	0.0259(4)	0.0321(3)	0.00000	0.00000
Cl2A	0.0332(3)	0.0332(3)	0.0660(8)	0.01660(15)	0.00000	0.00000
O1	0.0318(9)	0.0415(11)	0.0405(10)	0.0082(8)	-0.0075(8)	-0.0078(8)
O1A	0.0375(10)	0.0388(10)	0.0461(11)	0.0228(8)	0.0127(8)	0.0222(9)
O2	0.0198(7)	0.0199(6)	0.0479(10)	0.0051(5)	-0.0037(6)	-0.0029(6)
O2A	0.0164(6)	0.0214(6)	0.0307(7)	0.0105(5)	0.0023(5)	0.0058(5)
O3	0.0211(7)	0.0224(7)	0.0668(14)	0.0071(6)	0.0117(8)	-0.0090(8)
O3A	0.0166(6)	0.0177(6)	0.0478(10)	0.0068(5)	0.0007(6)	-0.0097(6)
O4	0.0219(7)	0.0211(7)	0.0676(14)	0.0088(6)	-0.0001(8)	0.0099(8)
O4A	0.0133(4)	0.0133(4)	0.0296(9)	0.0066(2)	0.00000	0.00000
O5	0.0224(7)	0.0205(7)	0.0467(10)	0.0079(6)	0.0072(6)	-0.0021(6)
O5A	0.0180(6)	0.0229(6)	0.0305(7)	0.0090(5)	-0.0026(5)	-0.0051(5)
O6	0.0374(11)	0.0582(15)	0.0449(12)	0.0187(11)	0.0046(9)	-0.0123(10)
O6A	0.0531(13)	0.0526(13)	0.0493(12)	0.0375(12)	-0.0231(10)	-0.0300(11)
O7	0.0145(5)	0.0145(5)	0.0432(15)	0.0072(2)	0.00000	0.00000

O7A	0.0155(6)	0.0235(7)	0.0410(9)	0.0085(5)	0.0020(5)	0.0114(6)
O8	0.0161(5)	0.0177(5)	0.0563(11)	0.0059(4)	0.0050(6)	-0.0022(6)
O8A	0.0142(4)	0.0186(5)	0.0315(6)	0.0071(4)	0.0006(5)	0.0015(5)
O9	0.0324(9)	0.0638(13)	0.0290(7)	0.0359(10)	0.0078(6)	0.0116(8)
O9A	0.0309(8)	0.0415(9)	0.0275(7)	0.0258(7)	-0.0044(6)	-0.0056(6)
N1	0.0252(9)	0.0421(11)	0.0363(10)	0.0154(8)	-0.0002(7)	-0.0046(9)
N1A	0.0358(10)	0.0328(10)	0.0307(9)	0.0220(8)	-0.0107(7)	-0.0112(7)
N2	0.0235(8)	0.032(1)	0.0369(10)	0.0075(7)	-0.0015(7)	-0.0061(8)
N2A	0.0267(8)	0.0245(8)	0.0309(8)	0.0146(7)	0.0048(6)	0.0086(6)
C1	0.057(2)	0.068(3)	0.0436(17)	0.0142(19)	0.0094(16)	0.0000(16)
C1A	0.077(3)	0.059(2)	0.060(2)	0.052(2)	-0.0269(19)	-0.0340(18)
C2	0.0509(18)	0.0429(16)	0.076(3)	0.0247(15)	0.0100(17)	-0.0181(16)
C2A	0.0375(13)	0.0560(17)	0.0440(14)	0.0313(13)	-0.0200(11)	-0.0224(13)
C3	0.0257(10)	0.0301(10)	0.0489(14)	0.0144(8)	0.0018(9)	-0.0084(9)
C3A	0.0262(9)	0.0294(9)	0.032(1)	0.0161(8)	-0.0085(7)	-0.0085(8)
C4	0.0184(8)	0.0243(9)	0.0499(13)	0.0125(7)	0.0011(8)	-0.0034(8)
C4A	0.0211(8)	0.0189(7)	0.0264(8)	0.0108(6)	-0.0049(6)	-0.0023(6)
C5	0.0337(13)	0.0457(17)	0.0560(19)	0.0049(12)	-0.0111(13)	-0.0134(14)
C5A	0.054(2)	0.053(2)	0.070(2)	0.0378(18)	0.0139(17)	0.0315(18)
C6	0.0485(18)	0.0321(13)	0.061(2)	0.0125(12)	-0.0157(15)	0.0022(13)
C6A	0.0231(9)	0.0419(13)	0.0464(14)	0.0154(9)	0.0102(9)	0.0185(11)
C7	0.0240(9)	0.029(1)	0.0427(12)	0.0093(8)	-0.0032(8)	-0.0045(9)
C7A	0.0183(7)	0.0244(8)	0.0325(10)	0.0097(6)	0.0047(7)	0.0078(7)
C8	0.0168(7)	0.0211(8)	0.0452(12)	0.0079(6)	-0.0028(7)	-0.0065(8)
C8A	0.0167(7)	0.0164(7)	0.0268(8)	0.0076(6)	0.0026(6)	0.0028(6)
C11	0.034(2)	0.0308(19)	0.028(2)	0.0129(16)	-0.0034(15)	0.0038(15)
C12	0.037(3)	0.051(3)	0.089(5)	0.029(3)	-0.016(4)	-0.006(4)
C13	0.019(2)	0.054(4)	0.108(7)	0.014(2)	-0.002(3)	-0.005(4)
C14	0.034(3)	0.041(4)	0.121(9)	0.009(3)	0.022(4)	0.018(4)
C15	0.041(3)	0.037(3)	0.116(8)	0.021(3)	0.010(4)	0.017(4)
C16	0.0172(16)	0.032(2)	0.117(7)	0.0097(15)	-0.005(3)	-0.003(3)
C17	0.0244(17)	0.050(3)	0.042(2)	0.0191(18)	0.0012(19)	-0.003(2)

Bond length [Å] und angles [°]

Fe(1)-O(4)	2.0639(6)	Fe(1)-O(4)#1	2.0639(6)	Fe(1)-O(1)#1	2.1145(6)
Fe(1)-O(2)	2.021(2)	Fe(1)-O(3)	2.020(2)	Fe(1)-O(4)	2.004(2)
Fe(1)-O(5)	2.0005(19)	Fe(1)-O(7)	1.9043(4)	Fe(1)-O(8)	2.0553(15)
Fe(1A)-O(2A)	2.0152(16)	Fe(1A)-O(3A)	2.0192(17)	Fe(1A)-O(4A)	1.9006(3)
Fe(1A)-O(5A)	2.0105(17)	Fe(1A)-O(7A)	2.0182(17)	Fe(1A)-O(8A)	2.0649(13)
Fe(2)-Cl(1)*	2.1798(8)	Fe(2)-Cl(1)* ²	2.1798(8)	Fe(2)-Cl(1)	2.1798(8)
Fe(2)-Cl(2)	2.1887(14)	Fe(2A)-Cl(1A)	2.1935(13)	Fe(2A)-Cl(1A)* ³	2.1935(13)
Fe(2A)-Cl(1A)* ⁴	2.1935(13)	Fe(2A)-Cl(2A)	2.216(2)	O(1)-N(2)	1.382(3)
O(1)-C(5)	1.448(4)	O(1A)-N(2A)	1.385(3)	O(1A)-C(5A)	1.418(4)
O(2)-C(8)	1.255(3)	O(2A)-C(8A)	1.248(2)	O(3A)-C(8A)* ²	1.258(2)
O(4A)-Fe(1A)* ²	1.9006(3)	O(4A)-Fe(1A)*	1.9006(3)	O(5)-C(4)	1.258(3)
O(5A)-C(4A)	1.259(3)	O(6)-N(1)	1.376(3)	O(6)-C(1)	1.440(6)
O(6A)-N(1A)	1.394(3)	O(6A)-C(1A)	1.427(4)	O(7A)-C(4A)* ²	1.259(3)
N(1)-C(3)	1.274(4)	N(1A)-C(3A)	1.281(3)	N(2)-C(7)	1.283(3)

N(2A)-C(7A)	1.282(3)	C(2)-C(3)	1.481(4)	C(2A)-C(3A)	1.500(3)
C(3)-C(4)	1.506(4)	C(3A)-C(4A)	1.505(3)	C(4A)-O(7A)*	1.259(3)
C(6)-C(7)	1.500(5)	C(6A)-C(7A)	1.482(3)	C(7)-C(8)	1.507(4)
C(7A)-C(8A)	1.514(3)	C(8A)-O(3A)*	1.258(2)	C(11)-C(12)	1.377(9)
C(11)-C(16)	1.369(8)	C(12)-C(13)	1.476(14)	C(13)-C(14)	1.349(14)
C(14)-C(15)	1.388(12)	C(15)-C(16)	1.454(13)	C(16)-C(17)	1.510(7)

O(2)-Fe(1)-O(8)	86.76(8)	O(3)-Fe(1)-O(2)	85.66(10)
O(3)-Fe(1)-O(8)	83.82(8)	O(4)-Fe(1)-O(2)	169.78(8)
O(4)-Fe(1)-O(3)	93.68(10)	O(4)-Fe(1)-O(8)	83.03(8)
O(5)-Fe(1)-O(2)	91.57(8)	O(5)-Fe(1)-O(3)	169.38(8)
O(5)-Fe(1)-O(4)	87.23(10)	O(5)-Fe(1)-O(8)	85.79(7)
O(7)-Fe(1)-O(2)	94.84(9)	O(7)-Fe(1)-O(3)	95.21(9)
O(7)-Fe(1)-O(4)	95.38(9)	O(7)-Fe(1)-O(5)	95.23(9)
O(7)-Fe(1)-O(8)	178.07(6)	O(2A)-Fe(1A)-O(3A)	89.42(8)
O(2A)-Fe(1A)-O(7A)	167.68(6)	O(2A)-Fe(1A)-O(8A)	83.17(6)
O(3A)-Fe(1A)-O(8A)	84.89(7)	O(4A)-Fe(1A)-O(2A)	95.83(8)
O(4A)-Fe(1A)-O(3A)	96.12(8)	O(4A)-Fe(1A)-O(5A)	94.52(8)
O(4A)-Fe(1A)-O(7A)	96.49(8)	O(4A)-Fe(1A)-O(8A)	178.57(4)
O(5A)-Fe(1A)-O(2A)	91.63(6)	O(5A)-Fe(1A)-O(3A)	169.14(7)
O(5A)-Fe(1A)-O(7A)	86.88(8)	O(5A)-Fe(1A)-O(8A)	84.51(7)
O(7A)-Fe(1A)-O(3A)	89.79(8)	O(7A)-Fe(1A)-O(8A)	84.51(7)
Cl(1)* ² -Fe(2)-Cl(1)*	109.51(3)	Cl(1)-Fe(2)-Cl(1)*	109.51(3)
Cl(1)-Fe(2)-Cl(1)* ²	109.52(3)	Cl(1)*-Fe(2)-Cl(2)	109.43(3)
Cl(1)* ² -Fe(2)-Cl(2)	109.43(3)	Cl(1)-Fe(2)-Cl(2)	109.43(3)
Cl(1A)* ³ -Fe(2A)-Cl(1A)	109.12(6)	Cl(1A)* ⁴ -Fe(2A)-Cl(1A)	109.12(6)
Cl(1A)* ⁴ -Fe(2A)-Cl(1A)* ³	109.12(6)	Cl(1A)-Fe(2A)-Cl(2A)	109.82(6)
Cl(1A)* ³ -Fe(2A)-Cl(2A)	109.82(6)	Cl(1A)* ⁴ -Fe(2A)-Cl(2A)	109.82(6)
N(2)-O(1)-C(5)	108.5(3)	N(2A)-O(1A)-C(5A)	110.3(2)
C(8)-O(2)-Fe(1)	133.10(16)	C(8A)-O(2A)-Fe(1A)	130.86(14)
C(8A)* ² -O(3A)-Fe(1A)	132.48(15)	Fe(1A)* ² -O(4A)-Fe(1A)*	120.000(1)
Fe(1A)-O(4A)-Fe(1A)*	120.000(1)	Fe(1A)-O(4A)-Fe(1A)* ²	119.999(1)
C(4)-O(5)-Fe(1)	131.76(17)	C(4A)-O(5A)-Fe(1A)	133.98(14)
N(1)-O(6)-C(1)	109.0(3)	N(1A)-O(6A)-C(1A)	109.2(2)
C(4A)* ² -O(7A)-Fe(1A)	129.65(15)	C(3)-N(1)-O(6)	112.0(3)
C(3A)-N(1A)-O(6A)	111.9(2)	C(7)-N(2)-O(1)	112.7(3)
C(7A)-N(2A)-O(1A)	110.8(2)	N(1)-C(3)-C(2)	125.8(3)
N(1)-C(3)-C(4)	114.3(2)	C(2)-C(3)-C(4)	119.9(3)

N(1A)-C(3A)-C(2A)	126.2(2)	N(1A)-C(3A)-C(4A)	114.8(2)
C(2A)-C(3A)-C(4A)	118.9(2)	O(5)-C(4)-C(3)	118.2(2)
O(5A)-C(4A)-O(7A) [*]	126.4(2)	O(5A)-C(4A)-C(3A)	115.57(18)
O(7A) ⁺ -C(4A)-C(3A)	118.01(19)	N(2)-C(7)-C(6)	124.9(3)
N(2)-C(7)-C(8)	114.3(3)	C(6)-C(7)-C(8)	120.8(2)
N(2A)-C(7A)-C(6A)	124.5(2)	N(2A)-C(7A)-C(8A)	114.83(18)
C(6A)-C(7A)-C(8A)	120.68(19)	O(2)-C(8)-C(7)	118.6(2)
O(2A)-C(8A)-O(3A) [*]	126.39(19)	O(2A)-C(8A)-C(7A)	115.79(17)
O(3A) ⁺ -C(8A)-C(7A)	117.75(18)	C(16)-C(11)-C(12)	123.1(6)
C(11)-C(12)-C(13)	116.4(6)	C(14)-C(13)-C(12)	120.6(6)
C(13)-C(14)-C(15)	121.4(9)	C(14)-C(15)-C(16)	119.0(8)
C(11)-C(16)-C(15)	118.0(6)	C(11)-C(16)-C(17)	119.8(6)
C(15)-C(16)-C(17)	121.2(6)		

Symmetry transformations used to generate equivalent atoms:

^{*} 1-x+y, 1-x, z ² 1-y, x-y, z ³ -x+y, -x, z ⁴ -y, x-y, z