Eisen(II)-oximat 1:

Empirical formula	C8 H16 Fe N2 O8
Color	yellow
Formula weight	324.08 g · mol^{-1}
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	p 21/c, (no. 14)
Unit cell dimensions	a = 10.0654(12) Å α= 90°.
	b = 8.9084(10) Å β= 98.313(2)°.
	c = 7.2243(9) Å γ = 90°.
Volume	640.97(13) $Å^3$
Z	2
Density (calculated)	1.679 Mg · m^{-3}
Absorption coefficient	1.214 mm^{-1}
F(000)	336 e
Crystal size	0.30 x 0.23 x 0.05 mm3
θ range for data collection	3.07 to 33.46°.
Index ranges	$-15 \leq h \leq 15$, $-13 \leq k \leq 13$, $-11 \leq l \leq 11$
Reflections collected	20811
Independent reflections	2508 [Rint = 0.0126]
Reflections with I>2σ (I)	2400
Completeness to θ = 27.50°	99.9 %
Absorption correction	Gaussian
Max. and min. transmission	0.94204 and 0.71359
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2508 / 1 / 96
Goodness-of-fit on F^2	1.093
Final R indices [I>2σ (I)]	R_1 = 0.0187 w R^2 = 0.0526
R indices (all data)	R_1 = 0.0195 w R^2 = 0.0532
Largest diff. peak and hole	0.500 and -0.457 e · $Å^{-3}$

Atomic parameters						
Atom	**Wyck**	**Site**	**x/a**	**y/b**	**z/c**	**U [Å^2]**
Fe1	2a	-1	1.00000	1/2	1/2	
O1	4e	1	0.93076(5)	0.27654(6)	0.51110(8)	
O4	4e	1	1.01608(6)	0.47267(7)	0.22041(8)	
H4A	4e	1	1.0759(14)	0.5145(14)	0.179(2)	0.0210
H4B	4e	1	0.9922(13)	0.4018(15)	0.1594(19)	0.0210
O2	4e	1	0.76883(6)	0.12314(7)	0.37764(9)	
O3	4e	1	0.68203(6)	0.62721(7)	0.39604(11)	
C2	4e	1	0.71882(7)	0.38216(8)	0.38483(11)	
C1	4e	1	0.81241(7)	0.24938(8)	0.42635(10)	
N1	4e	1	0.77375(7)	0.51027(7)	0.42796(10)	
C4	4e	1	0.74201(9)	0.76967(9)	0.44763(13)	
H4C	4e	1	0.82400	0.75460	0.53680	0.0270
H4D	4e	1	0.67880	0.83140	0.50560	0.0270
H4E	4e	1	0.76430	0.82050	0.33580	0.0270
C3	4e	1	0.57590(9)	0.35984(10)	0.30189(16)	
H3A	4e	1	0.56030	0.25350	0.27150	0.0360
H3B	4e	1	0.55600	0.42000	0.18770	0.0360
H3C	4e	1	0.51730	0.39130	0.39190	0.0360

Anisotropic displacement parameters, in Å^2

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.00925(7)	0.00737(7)	0.00949(7)	-0.00014(4)	0.00051(5)	-0.00034(4)
O1	0.0112(2)	0.0089(2)	0.0147(2)	-0.00022(17)	-0.00059(17)	0.00059(17)
O4	0.0172(3)	0.0131(2)	0.0121(2)	-0.0052(2)	0.00362(19)	-0.00281(19)
O2	0.0139(2)	0.0097(2)	0.0244(3)	-0.00165(19)	0.0020(2)	-0.0036(2)
O3	0.0108(2)	0.0087(2)	0.0444(4)	0.00213(19)	-0.0009(2)	0.0010(2)
C2	0.0102(3)	0.0106(3)	0.0160(3)	0.0000(2)	0.0012(2)	0.0001(2)
C1	0.0113(3)	0.0095(3)	0.0123(3)	0.0001(2)	0.0026(2)	0.0000(2)
N1	0.0106(3)	0.0089(2)	0.0148(3)	0.00199(19)	0.0014(2)	0.00101(19)
C4	0.0197(3)	0.0096(3)	0.0251(4)	0.0002(3)	0.0012(3)	-0.0006(3)
C3	0.0114(3)	0.0156(4)	0.0427(5)	-0.0013(3)	-0.0050(3)	-0.0008(3)

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(1)	2.1145(6)	Fe(1)-N(1)	2.2633(7)	Fe(1)-N(1)#1	2.2633(7)
O(1)-C(1)	1.2813(9)	O(4)-H(4A)	0.800(13)	O(4)-H(4B)	0.788(12)
O(2)-C(1)	1.2395(9)	O(3)-N(1)	1.3889(9)	O(3)-C(4)	1.4314(10)
C(2)-N(1)	1.2867(10)	C(2)-C(3)	1.4895(11)	C(2)-C(1)	1.5149(10)

C(4)-H(4C)	0.9800	C(4)-H(4D)	0.9800	C(4)-H(4E)	0.9800
C(3)-H(3A)	0.9800	C(3)-H(3B)	0.9800	C(3)-H(3C)	0.9800

O(4)-Fe(1)-O(4)#1	180.0	O(4)-Fe(1)-O(1)#1	90.06(2)
O(4)#1-Fe(1)-O(1)#1	89.94(2)	O(4)-Fe(1)-O(1)	89.94(2)
O(4)#1-Fe(1)-O(1)	90.06(2)	O(1)#1-Fe(1)-O(1)	180.0
O(4)-Fe(1)-N(1)	89.91(3)	O(4)#1-Fe(1)-N(1)	90.09(3)
O(1)#1-Fe(1)-N(1)	106.22(2)	O(1)-Fe(1)-N(1)	73.78(2)
O(4)-Fe(1)-N(1)#1	90.09(3)	O(4)#1-Fe(1)-N(1)#1	89.91(3)
O(1)#1-Fe(1)-N(1)#1	73.78(2)	O(1)-Fe(1)-N(1)#1	106.22(2)
N(1)-Fe(1)-N(1)#1	180.0	C(1)-O(1)-Fe(1)	116.64(5)
Fe(1)-O(4)-H(4A)	118.4(11)	Fe(1)-O(4)-H(4B)	125.6(10)
H(4A)-O(4)-H(4B)	110.6(14)	N(1)-O(3)-C(4)	112.12(6)
N(1)-C(2)-C(3)	124.89(7)	N(1)-C(2)-C(1)	114.30(6)
C(3)-C(2)-C(1)	120.81(7)	O(2)-C(1)-O(1)	124.99(7)
O(2)-C(1)-C(2)	117.90(7)	O(1)-C(1)-C(2)	117.11(6)
C(2)-N(1)-O(3)	111.90(6)	C(2)-N(1)-Fe(1)	113.75(5)
O(3)-N(1)-Fe(1)	133.72(5)	O(3)-C(4)-H(4C)	109.5
O(3)-C(4)-H(4D)	109.5	H(4C)-C(4)-H(4D)	109.5
O(3)-C(4)-H(4E)	109.5	H(4C)-C(4)-H(4E)	109.5
H(4D)-C(4)-H(4E)	109.5	C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5	H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5	H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1