

Exploring Second Coordination Sphere Effects in Flavodiiron Nitric Oxide Reductase Model Complexes

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Table of Contents

¹H-NMR spectra:

H[BPMP(NHCO ^t Bu) ₂]	S3
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Solid state IR spectra:

IR (KBr) of 0 , 1 , and 2	S4
IR (KBr) of 1 and 1 with CH ₃ ¹³ COO	S5
IR (KBr) of 0 and 0(NO)₂ with CoCp ₂	S6

Solution IR spectra:

0 , 1 , 2 , 0(NO)₂ , 1(NO)₂ , and 2(NO)₂	S7
0 and 0(NO)₂	S8
1 and 1(NO)₂	S9
2 and 2(NO)₂	S10
0 , 1 , and 2	S11
0(NO)₂ , 1(NO)₂ , and 2(NO)₂	S12
0(¹⁵NO)₂ SEC-IR	S13
Comparison of 0(NO)₂ and 0(¹⁵NO)₂ after reduction	S14

UV-Vis spectra:

0 and 0(NO)₂	S15
1 and 1(NO)₂	S16
2 and 2(NO)₂	S17
0 , 1 , and 2	S18
0(NO)₂ , 1(NO)₂ , and 2(NO)₂	S19
0(NO)₂ with CoCp ₂	S20

Comparative IR Spectra:

IR (KBr) of 0 , 1 , 2 , 0(NO)₂ , 1(NO)₂ , and 2(NO)₂ , stacked	S21
Difference spectra of IR (KBr) of 0/0(NO)₂ , 1/1(NO)₂ , and 2/2(NO)₂	S22
Solution IR of 0 , 1 , 2 , 0(NO)₂ , 1(NO)₂ , and 2(NO)₂ , stacked	S23
Difference spectra of Solution IR of 0/0(NO)₂ , 1/1(NO)₂ , and 2/2(NO)₂	S24

Crystal Structures:

Crystal structure of 0 and essential structural parameters	S25-70
Crystal structure of 1 and essential structural parameters	S71-92

DFT Optimized Structures:

DFT optimized structure of 0(NO)₂ with BP86/TZVP and Cartesian coordinates	S93-92
DFT optimized structure of 1(NO)₂ with BP86/TZVP and Cartesian coordinates	S96-99
DFT optimized structure of 2(NO)₂ with BP86/TZVP and Cartesian coordinates	S99-102

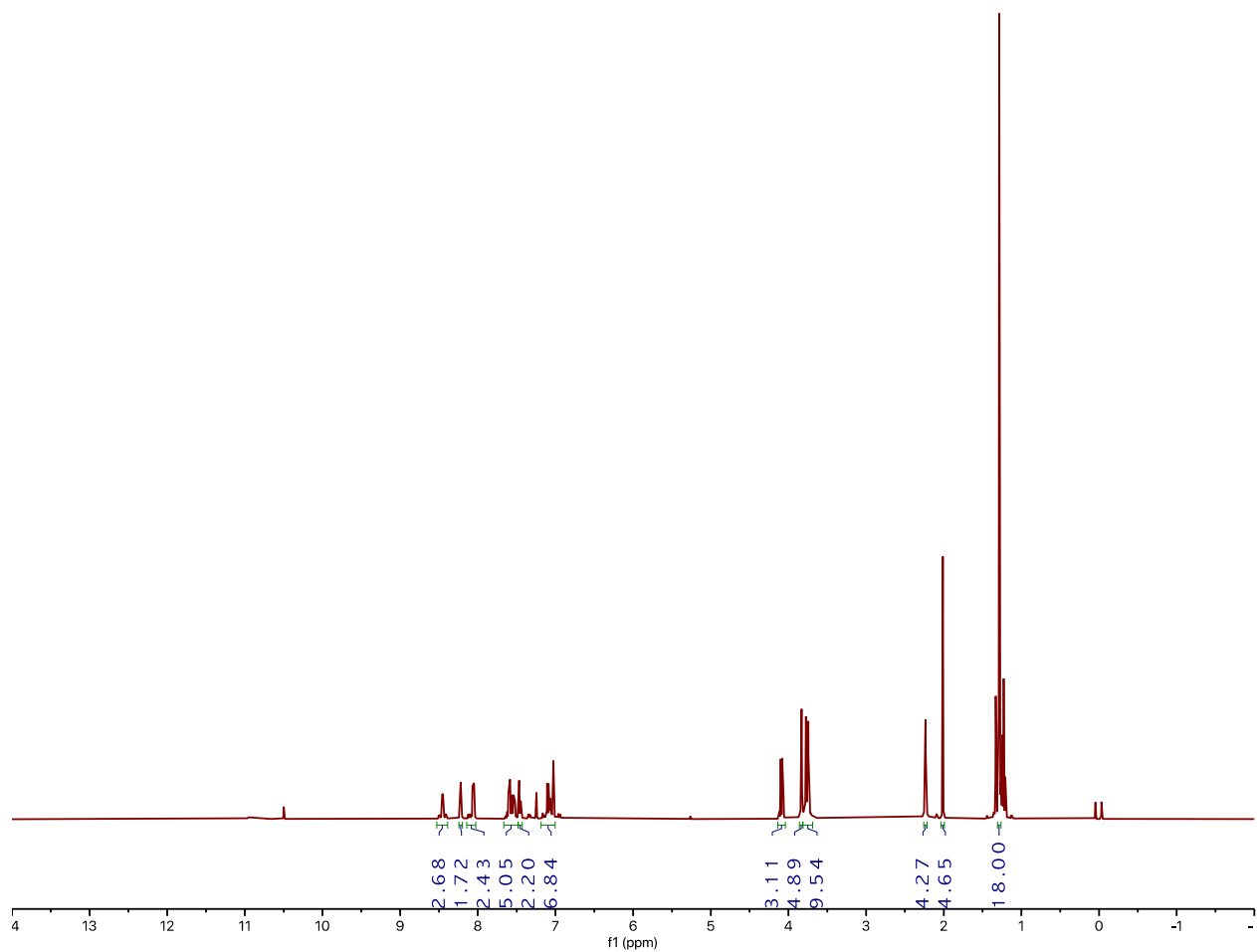


Figure S1. ¹H-NMR spectrum of H[BPMP(NHCO^tBu)₂] in CDCl₃ at room temperature.

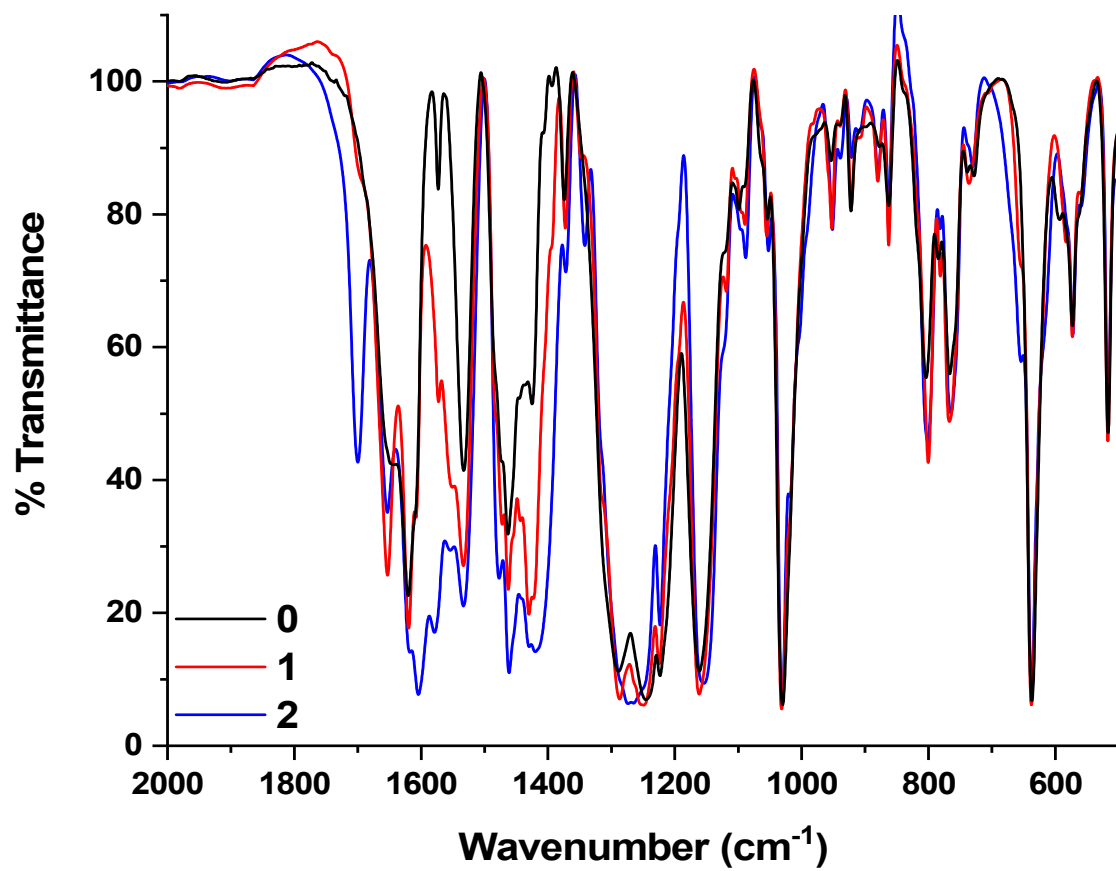


Figure S2. IR (KBr) spectra of solid precursor complexes **0**, **1**, and **2**.

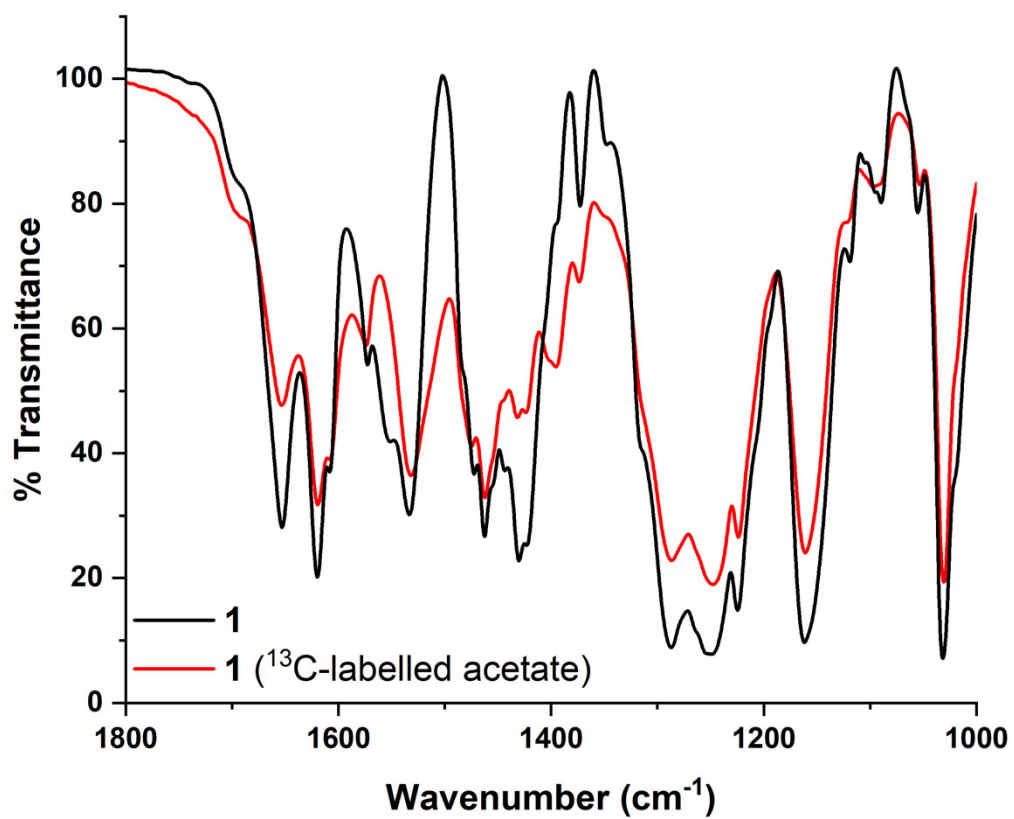


Figure S3. IR (KBr) spectra of solid precursor complexes **1** and **1** with CH₃¹³COO.

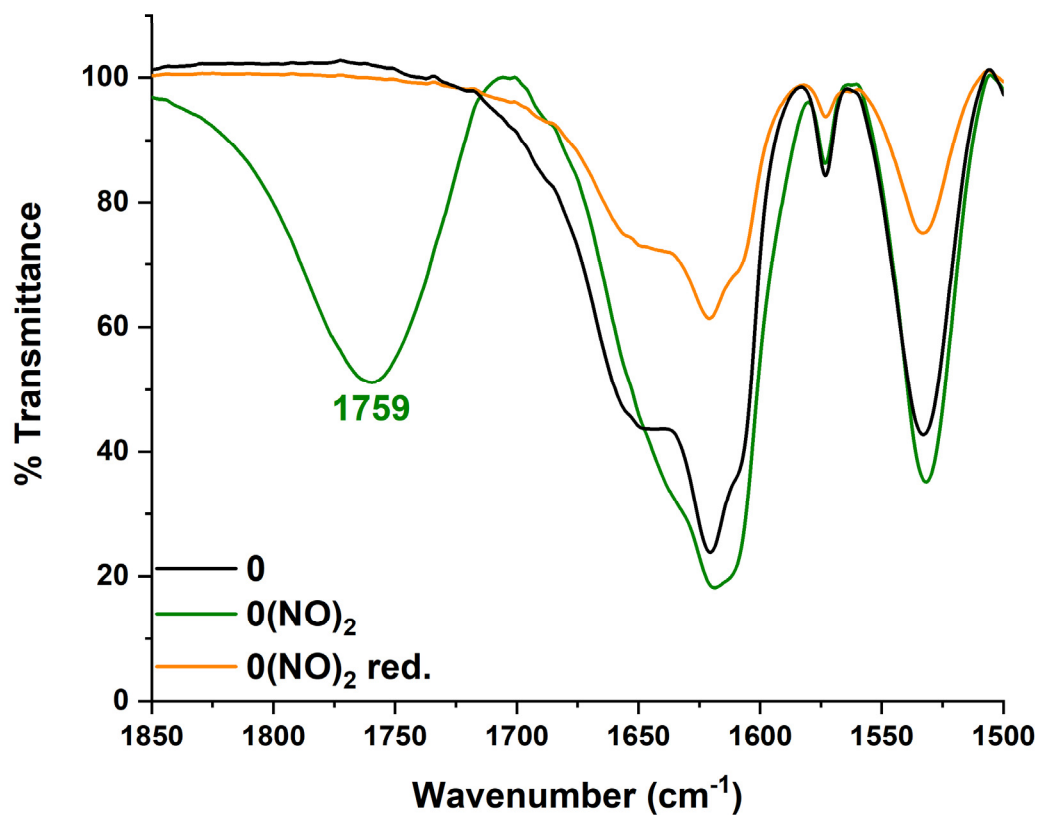


Figure S4. IR (KBr) spectra of **0**, and **0(NO)₂** before and after reduction with 1 equivalent of CoCp₂. The product after reduction was precipitated with diethyl ether from a CH₂Cl₂ solution, and does not show any DNIC signals.

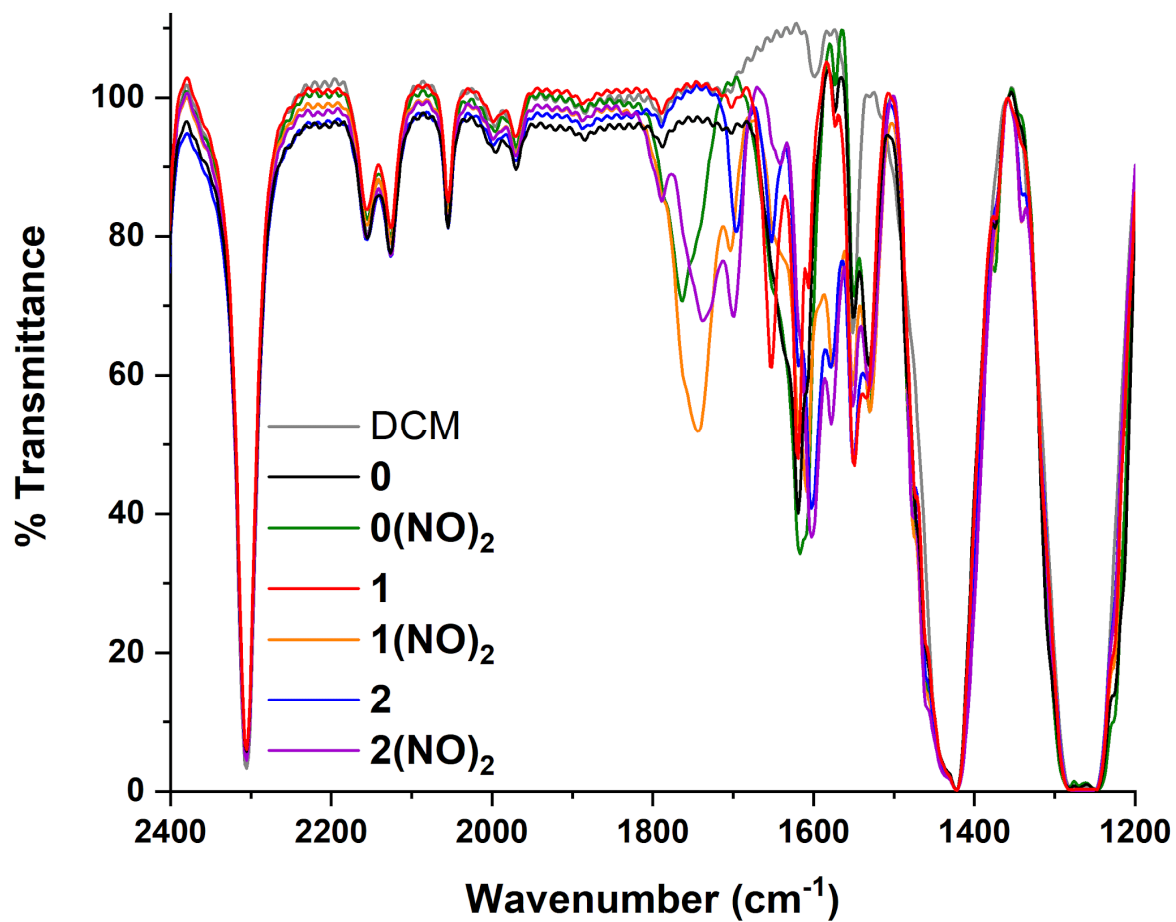


Figure S5. Solution IR spectra of precursor complexes **0**, **1**, and **2** and nitrosylated complexes **0(NO)₂**, **1(NO)₂**, and **2(NO)₂**, respectively. Conditions were 10 mM of precursor in CH₂Cl₂.

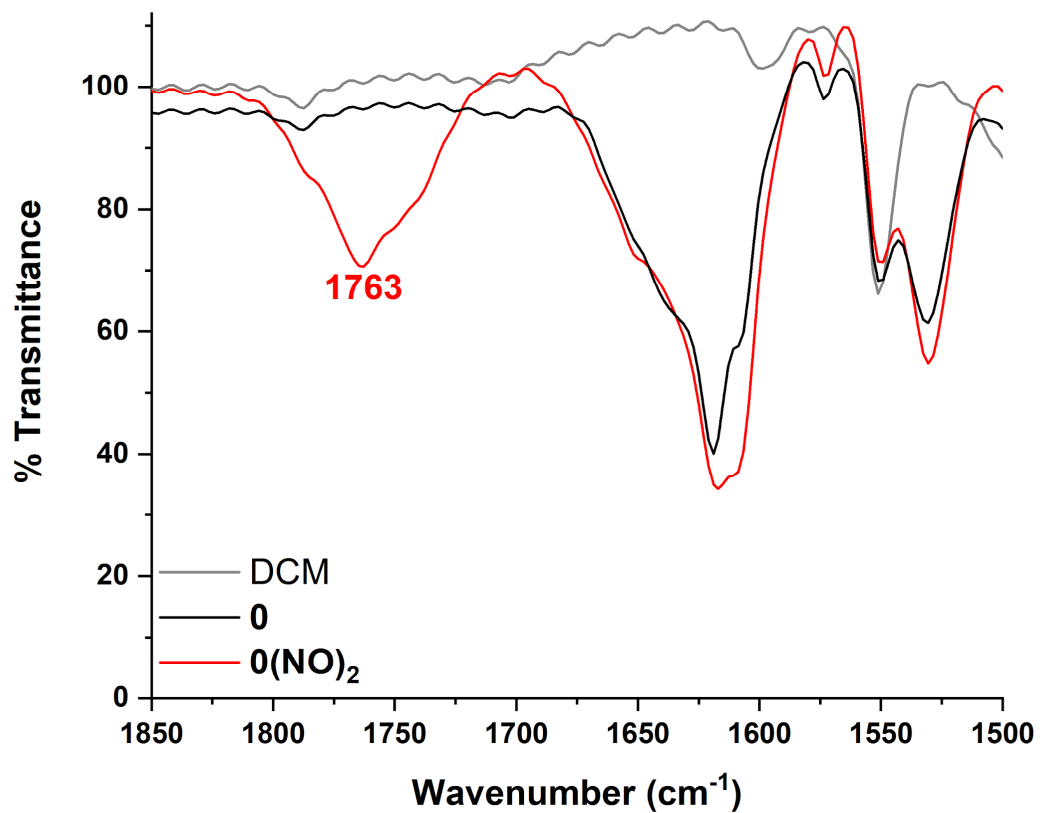


Figure S6. Solution IR spectra of precursor complex **0** and nitrosylated complex **0(NO)₂**. Conditions were 10 mM of precursor in CH₂Cl₂.

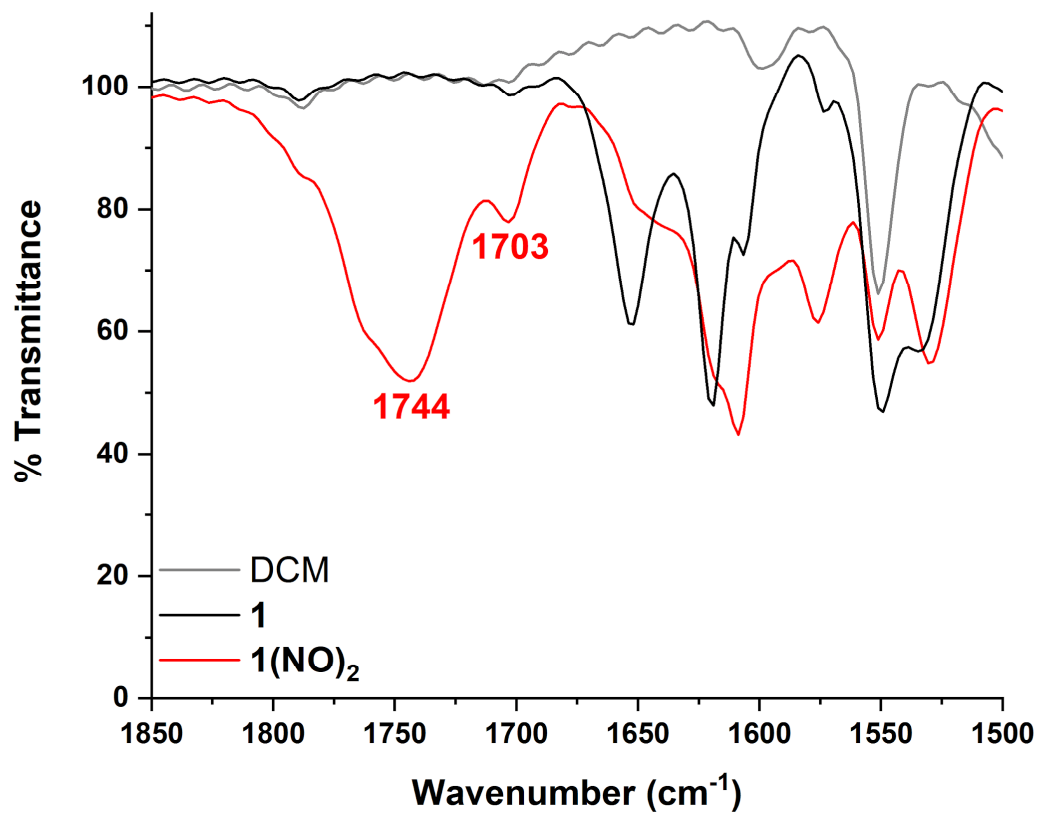


Figure S7. Solution IR spectra of precursor complex **1** and nitrosylated complex **1(NO)₂**. Conditions were 10 mM of precursor in CH₂Cl₂.

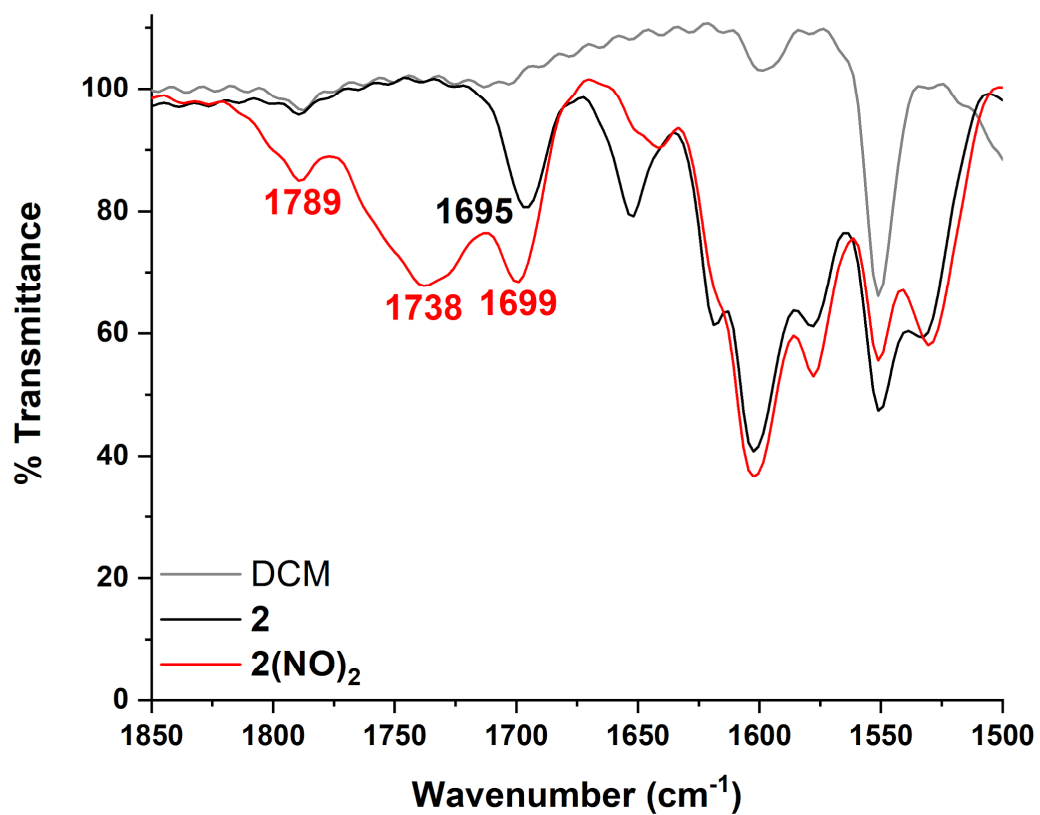


Figure S8. Solution IR spectra of precursor complex **2** and nitrosylated complex **2(NO)₂**. Conditions were 10 mM of precursor in CH₂Cl₂.

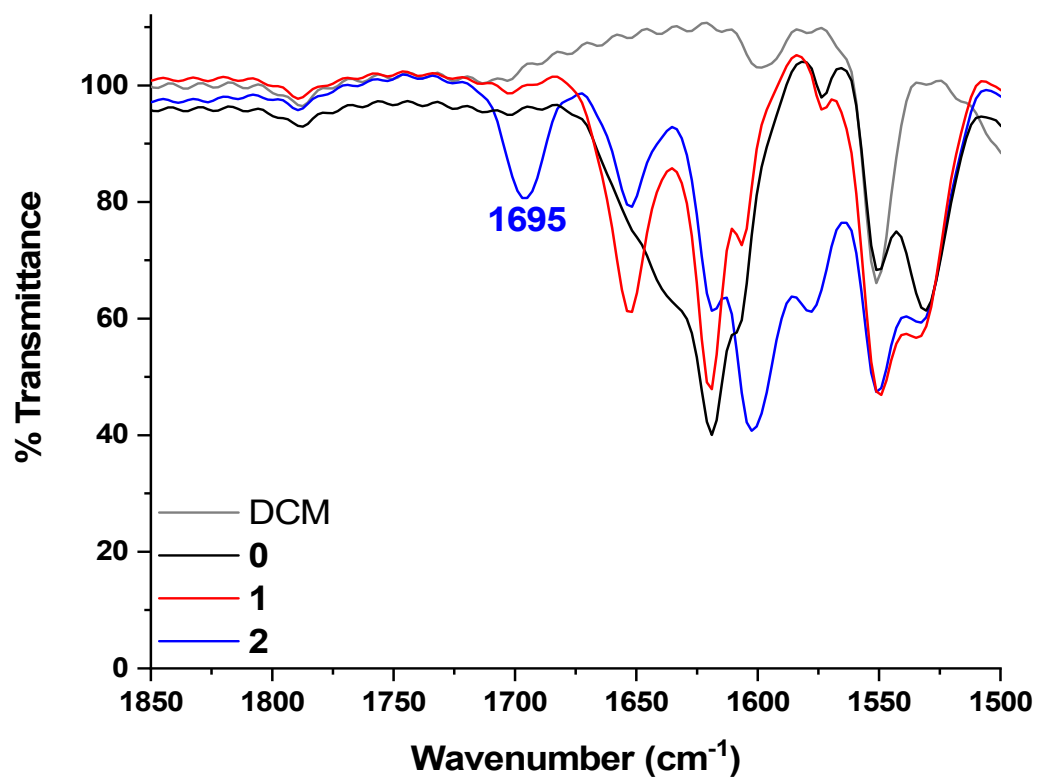


Figure S9. Solution IR spectra of precursor complexes **0**, **1**, and **2**. Conditions were 10 mM in CH₂Cl₂.

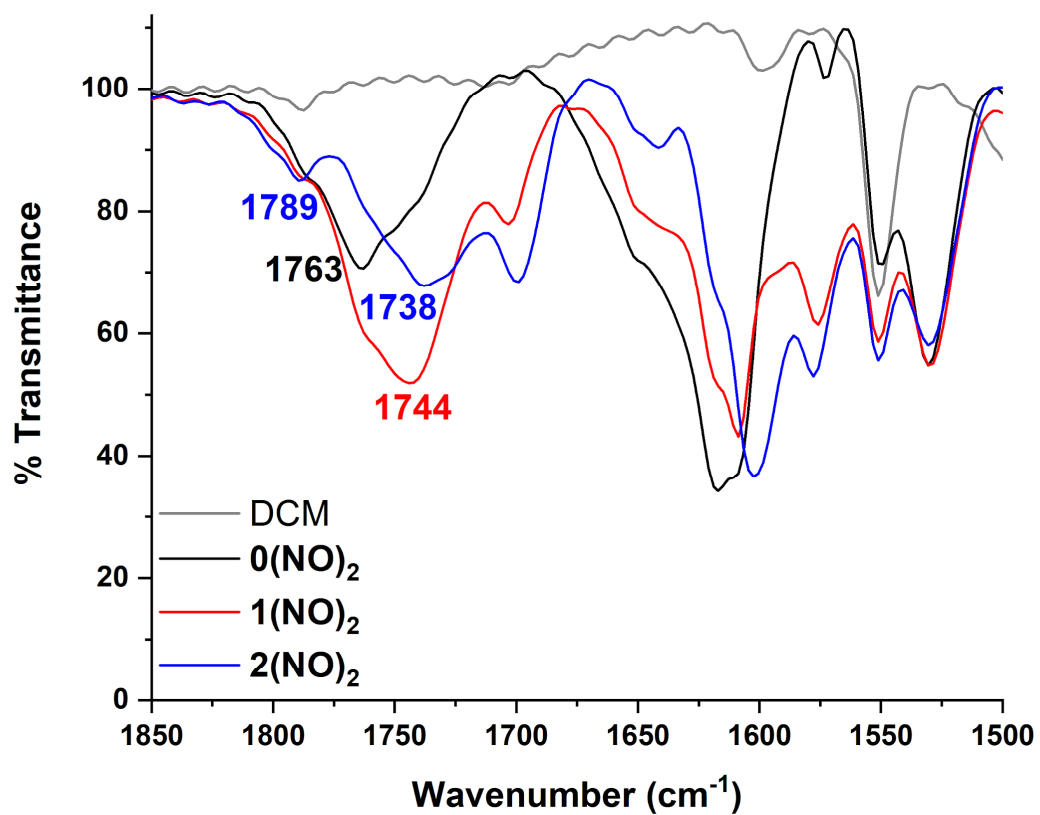


Figure S10. Solution IR spectra of nitrosylated complexes **0(NO)₂**, **1(NO)₂**, and **2(NO)₂**. Conditions were 10 mM of precursor in CH₂Cl₂.

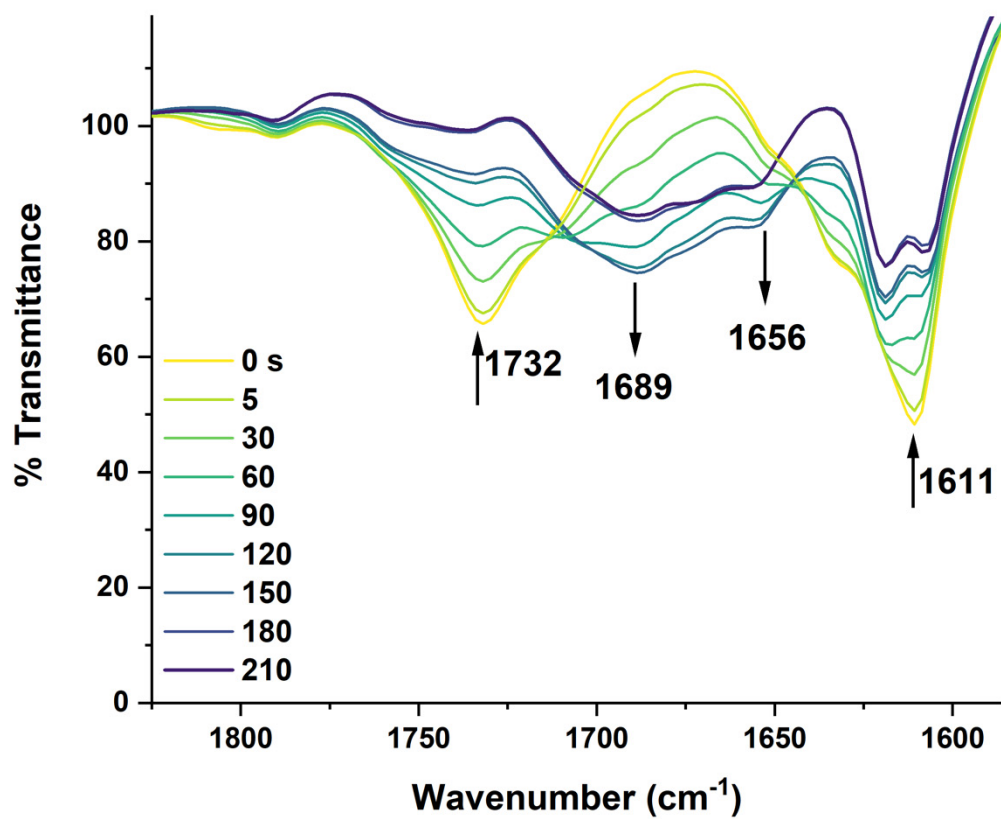


Figure S11. IR-spectroelectrochemical data of $0(^{15}\text{NO})_2$ with the potential held at -1.4 V vs. Ag wire. Conditions were 10 mM in CH_2Cl_2 with 0.1 M [TBA](OTf) as the supporting electrolyte.

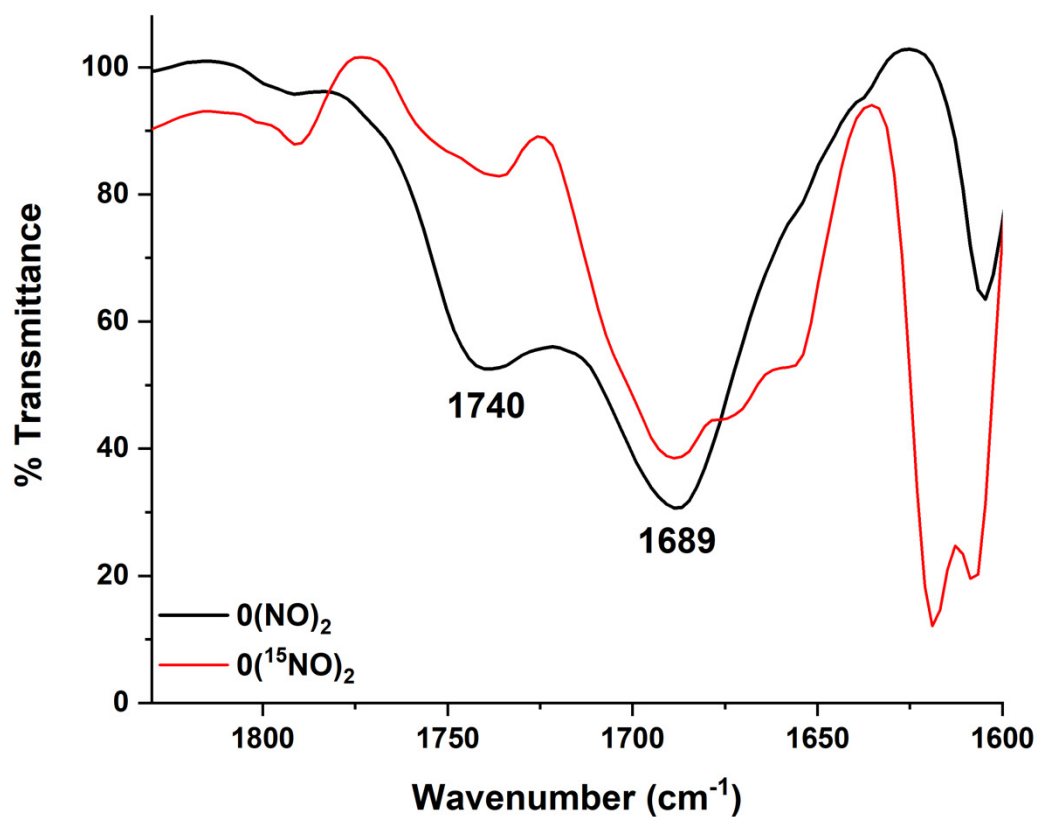


Figure S12. Solution IR data of $0(\text{NO})_2$ and $0(^{15}\text{NO})_2$ after holding the potential for 210 seconds at -1.4 V. Conditions were 10 mM in CH_2Cl_2 with 0.1 M $[\text{TBA}](\text{OTf})$ as the supporting electrolyte.

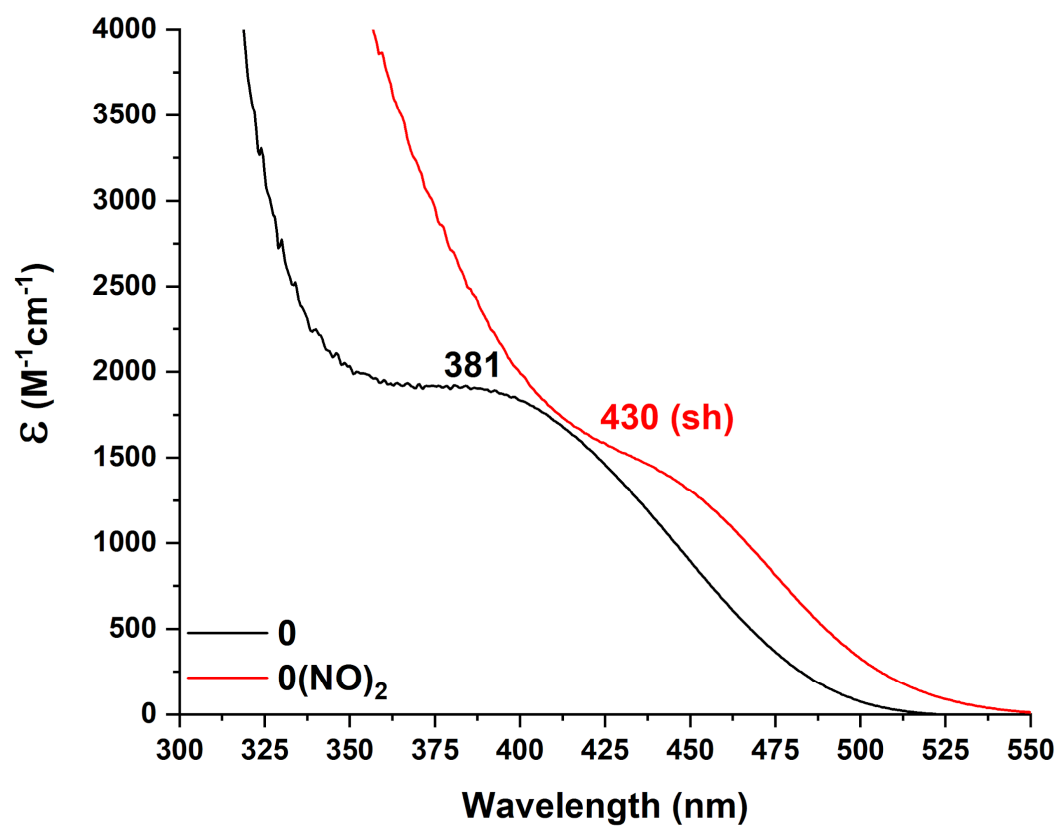


Figure S13. UV-Vis spectra of precursor complex **0** and nitrosylated complex **0(NO)₂**. Conditions were 0.2 mM of precursor in CH₂Cl₂.

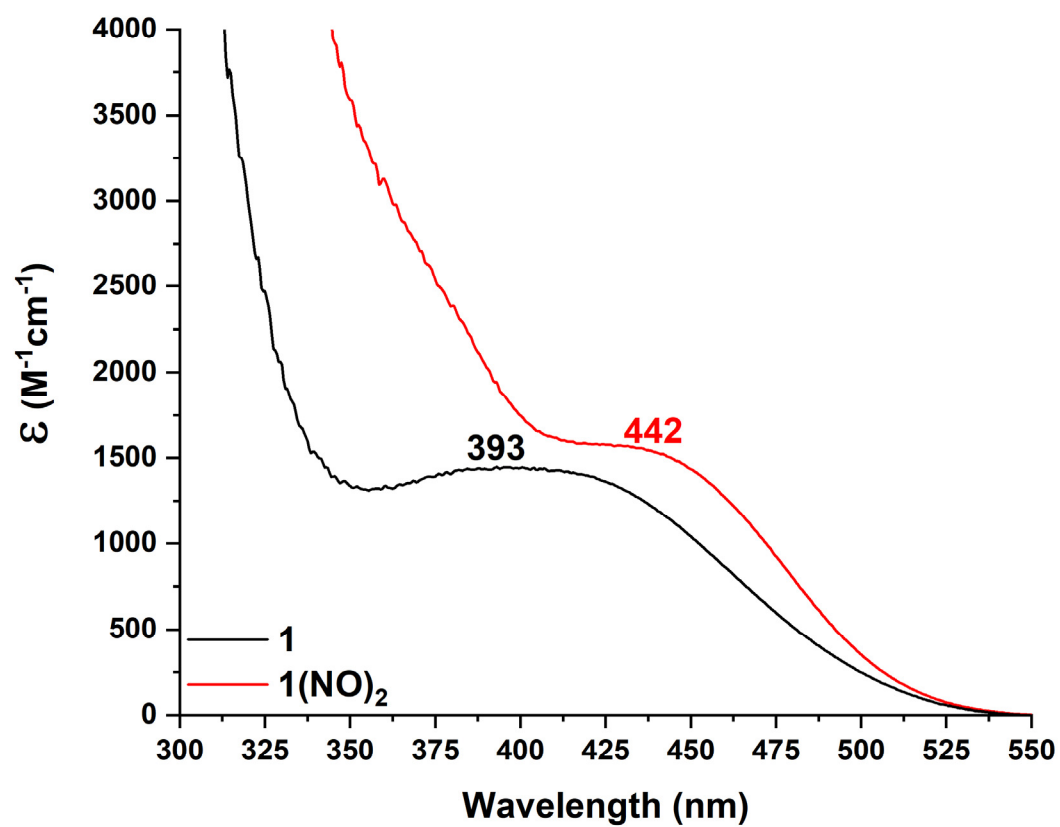


Figure S14. UV-Vis spectra of precursor complex **1** and nitrosylated complex **1(NO)₂**. Conditions were 0.2 mM of precursor in CH₂Cl₂.

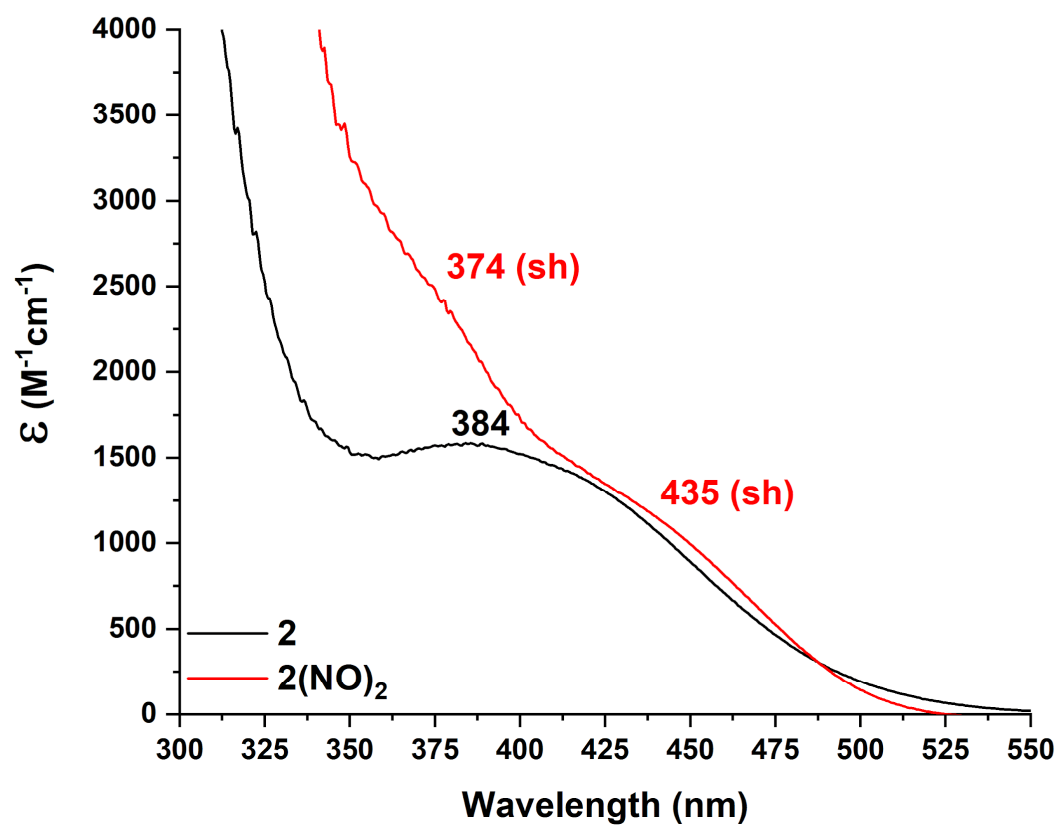


Figure S15. UV-Vis spectra of precursor complex **2** and nitrosylated complex **2(NO)₂**. Conditions were 0.2 mM of precursor in CH₂Cl₂.

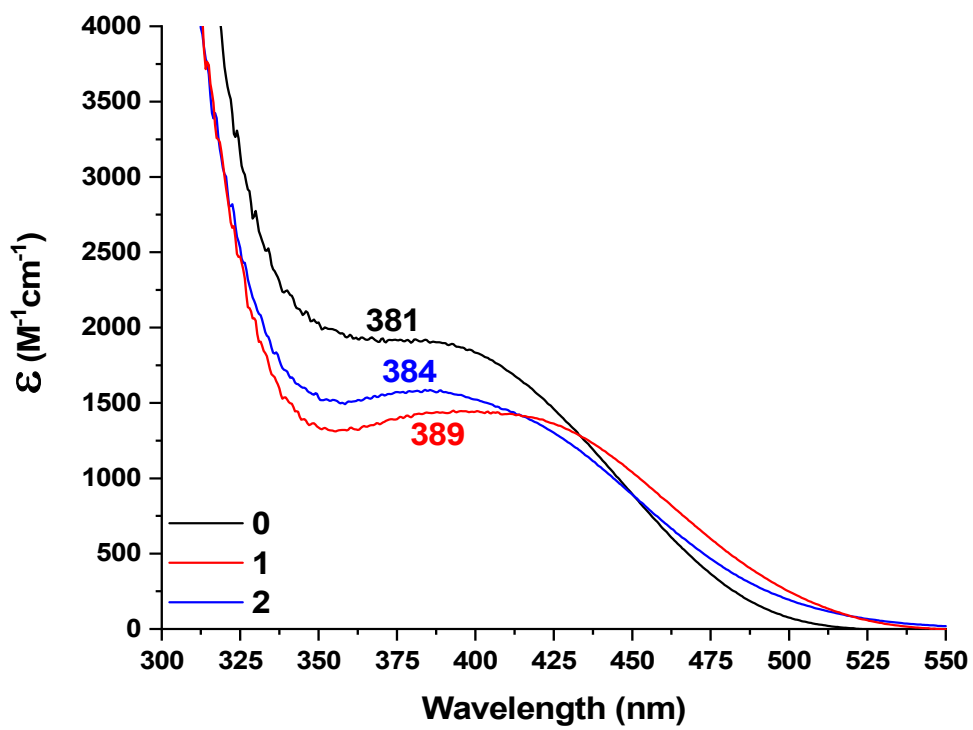


Figure S16. UV-Vis spectra of precursor complexes **0**, **1**, and **2**. Conditions were 0.2 mM in CH_2Cl_2 .

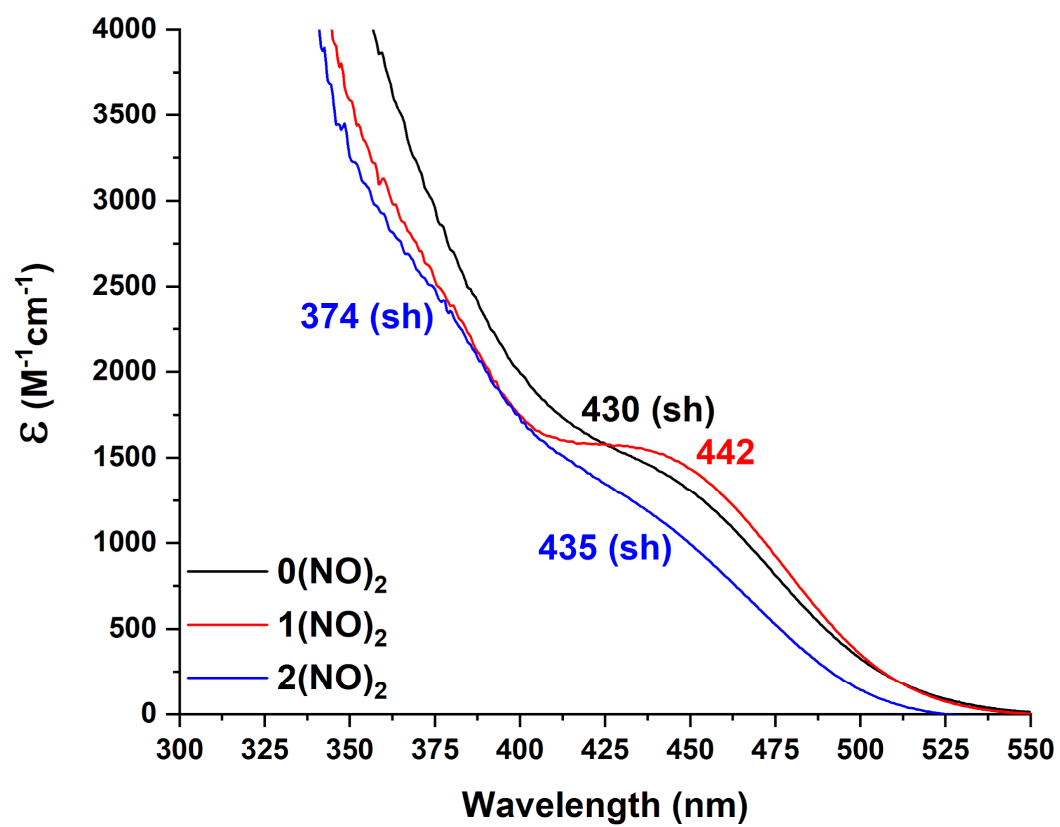


Figure S17. UV-vis spectra of nitrosylated complexes $0(\text{NO})_2$, $1(\text{NO})_2$, and $2(\text{NO})_2$. Conditions were 0.2 mM of precursor in CH_2Cl_2 .

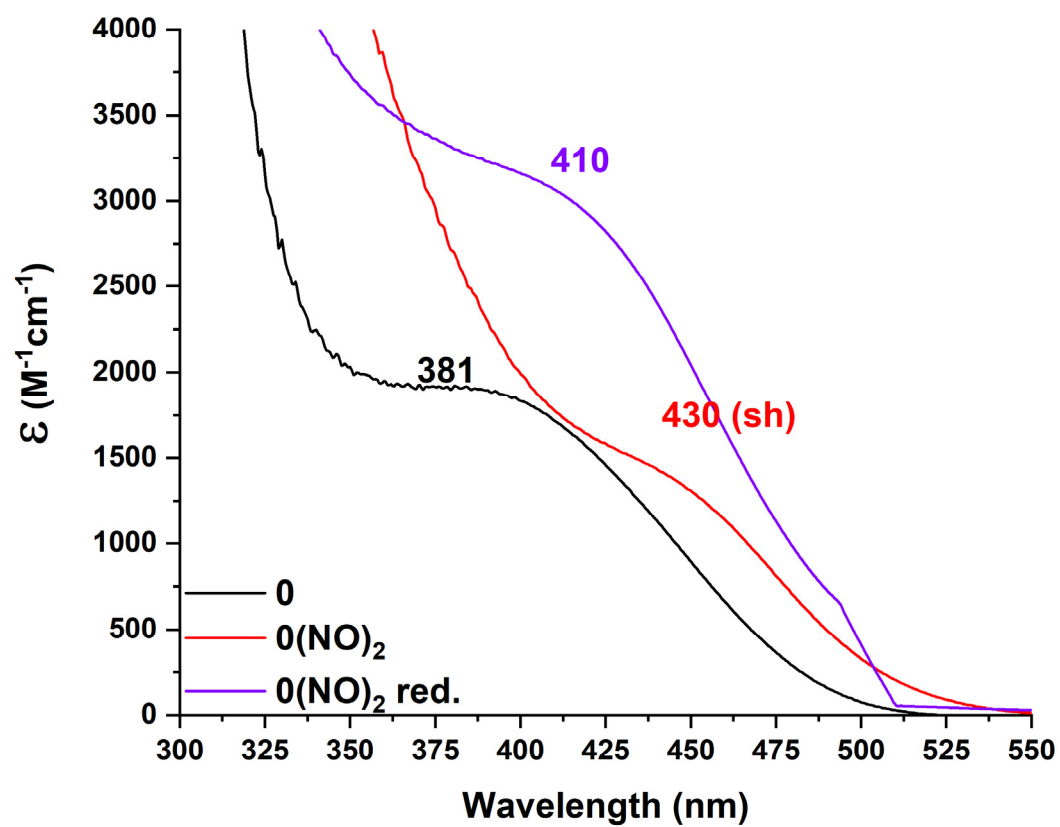


Figure S18. UV-vis spectra of **0** and **0(NO)₂** before and after reduction with 1 equivalent of CoCp₂. Conditions were 0.2 mM of precursor in CH₂Cl₂.

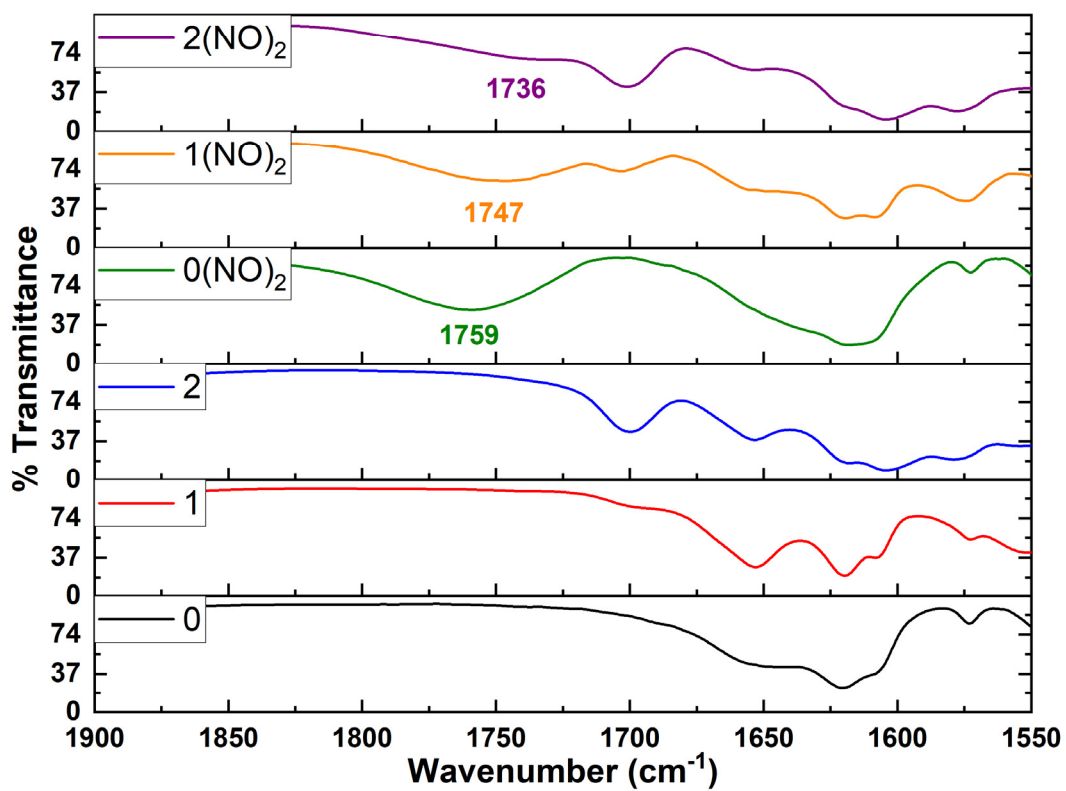


Figure S19. Stacked IR (KBr) spectra of the diferrous precursors **0**, **1**, and **2** and of the nitrosylated complexes **0(NO)₂**, **1(NO)₂**, and **2(NO)₂**.

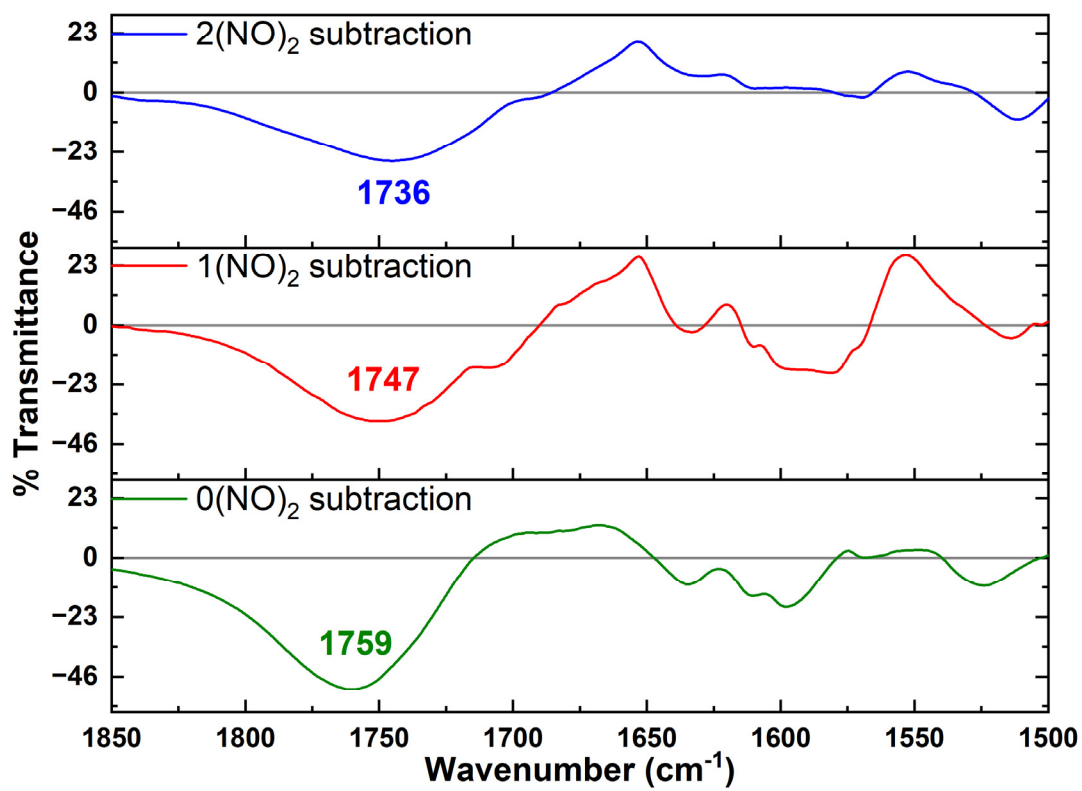


Figure S20. Difference spectra obtained from subtracting the IR (KBr) spectrum of **0**(NO)₂ from **0** (bottom), **1**(NO)₂ from **1** (middle), and **2**(NO)₂ from **2** (top). The NO vibrational bands are labelled.

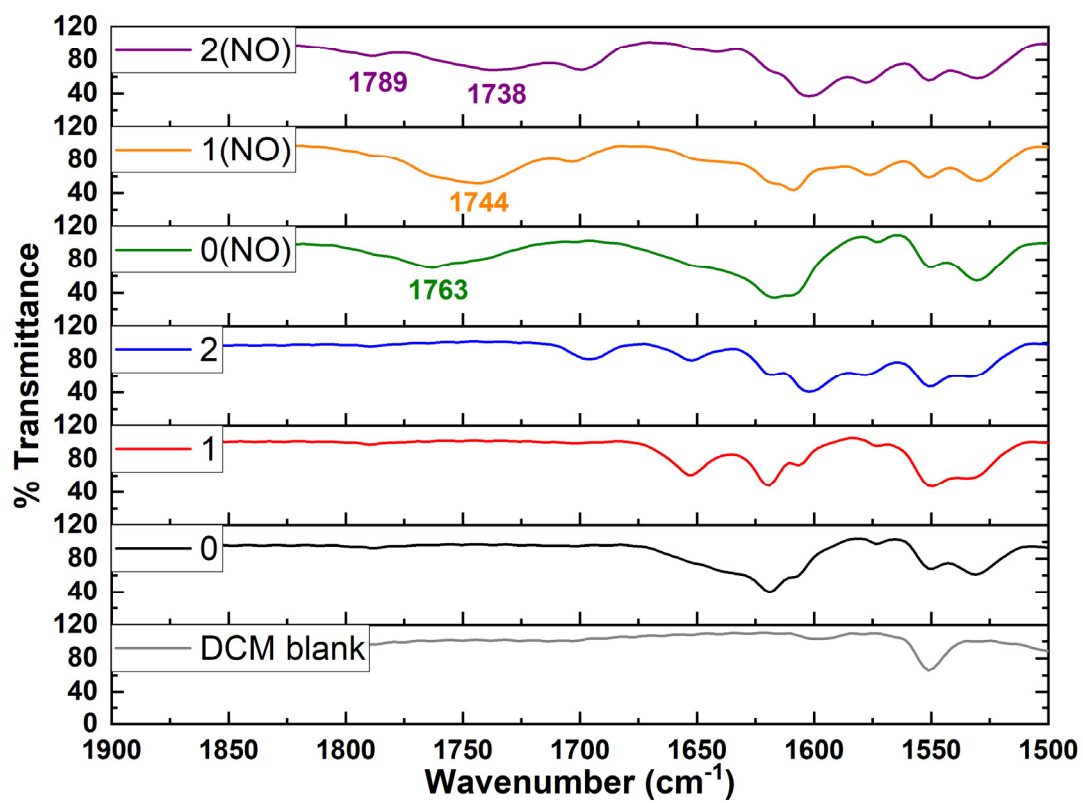


Figure S21. Stacked solution IR spectra of the diferrous precursors **0**, **1**, and **2** and of the nitrosylated complexes **0(NO)₂**, **1(NO)₂**, and **2(NO)₂**, at a concentration of 10 mM in CH₂Cl₂.

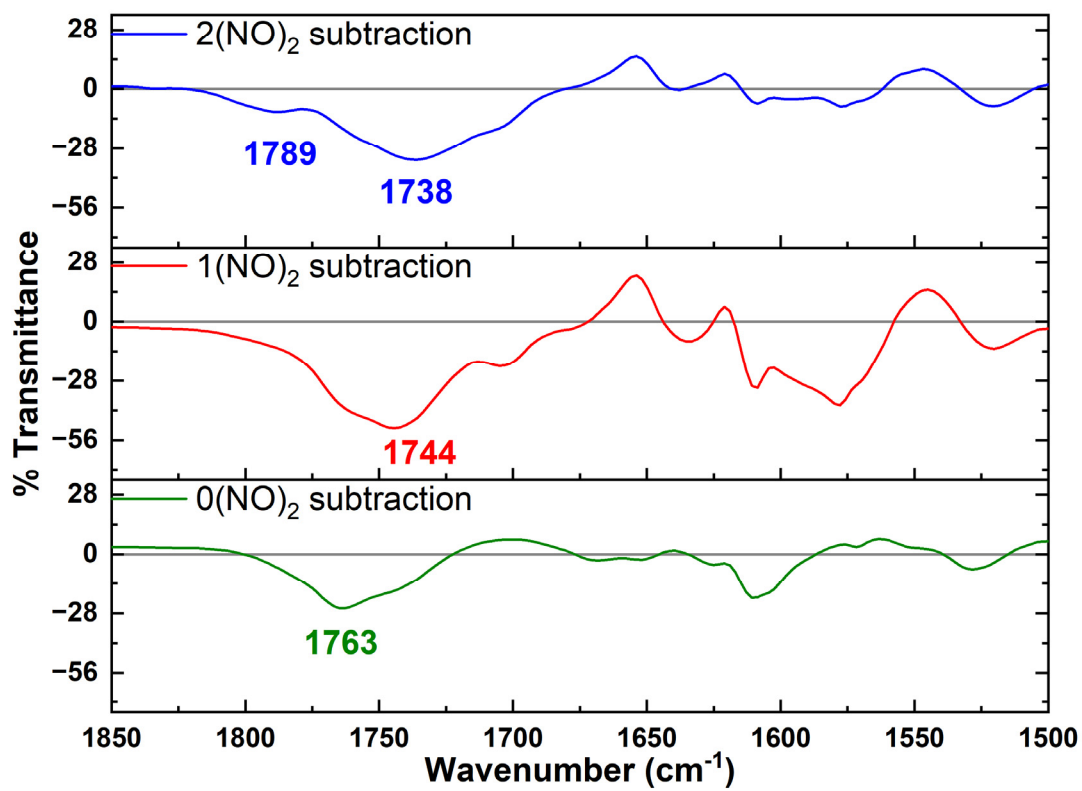


Figure S22. Difference spectra obtained from subtracting the solution IR spectrum of **0(NO)₂** from **0** (bottom), **1(NO)₂** from **1** (middle), and **2(NO)₂** from **2** (top). The NO vibrational bands are labelled.

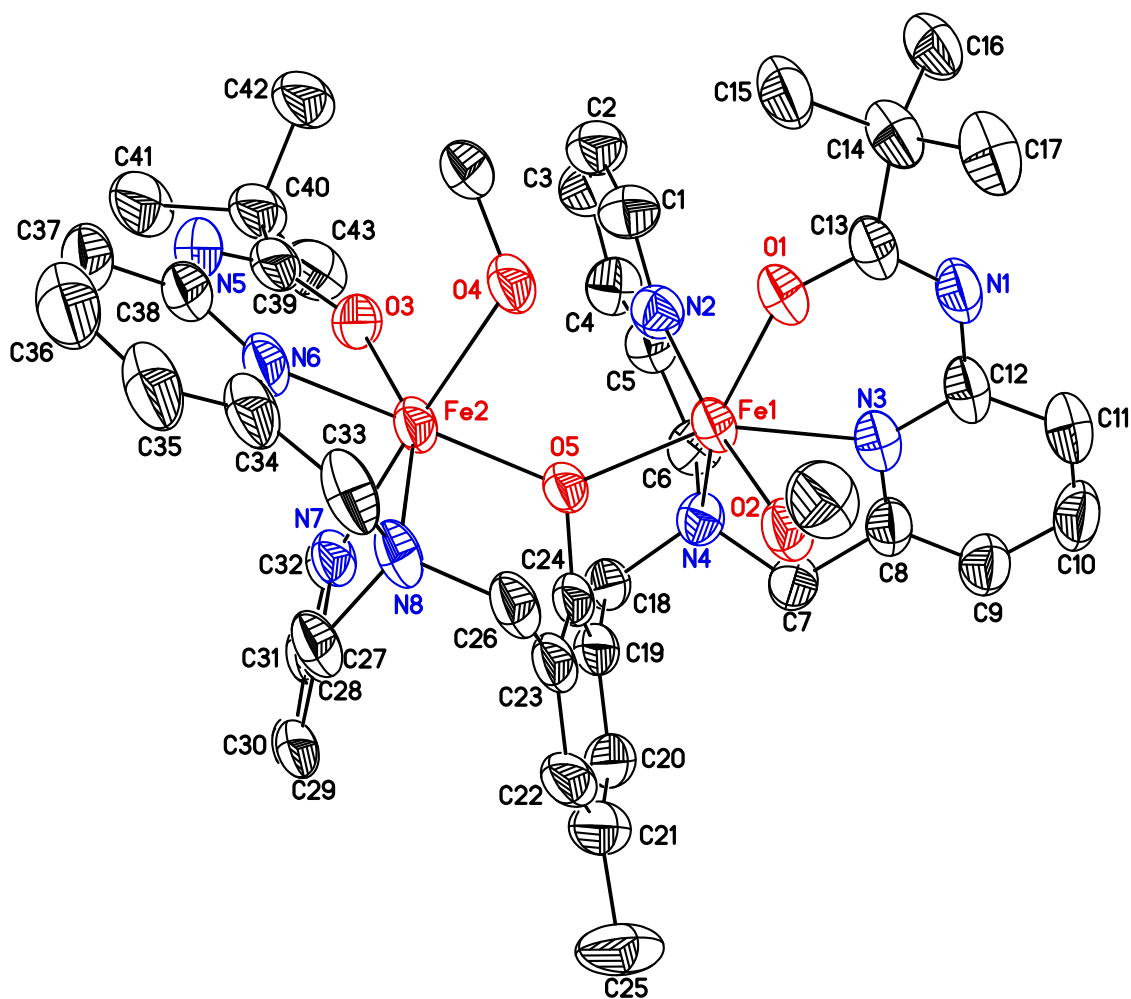


Figure S23. Crystal structure of complex **0** with ellipsoids drawn at 50% probability and atomic labeling scheme as indicated. Solvent molecules and hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for **0** (CCDC #2084746).

Identification Code	hd2128	
Empirical formula	C _{98.50} H ₁₂₈ F ₁₈ Fe ₄ N ₁₆ O _{30.50} S ₆	
Formula weight	2781.92	
Temperature	85(2) K	
Wavelength	1.54184 Å	
Crystal system, space group	Monoclinic, P2/n	
Unit cell dimensions	a = 25.1428(5) Å b = 11.31840(10) Å c = 42.5686(5) Å	alpha = 90 deg. beta = 99.770(2) deg. gamma = 90 deg.
Volume	11938.3(3) Å ³	
Z, Calculated density	4, 1.548 Mg/m ³	
Absorption coefficient	5.755 mm ⁻¹	
F(000)	5748	
Crystal size	0.120 x 0.120 x 0.040 mm	
Theta range for data collection	2.219 to 69.860 deg.	
Limiting indices	-30 ≤ h ≤ 29, -13 ≤ k ≤ 13, -49 ≤ l ≤ 51	
Reflections collected / unique	181810 / 22253 [R(int) = 0.1014]	
Completeness to theta = 67.684	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.51462	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	22253 / 217 / 1678	
Goodness-of-fit on F ²	1.049	
Final R indices [I > 2σ(I)]	R1 = 0.0859, wR2 = 0.2388	
R indices (all data)	R1 = 0.0973, wR2 = 0.2589	
Extinction coefficient	0.00032(4)	
Largest diff. peak and hole	1.348 and -0.850 e x Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **0**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	6646(1)	6460(1)	3623(1)	42(1)
Fe(2)	7294(1)	8303(1)	4332(1)	42(1)
Fe(3)	3500(1)	3616(1)	1217(1)	40(1)
Fe(4)	3802(1)	1841(1)	1974(1)	52(1)
O(1)	6366(1)	7743(3)	3288(1)	48(1)
O(2)	7341(1)	6383(3)	3369(1)	51(1)
O(3)	6647(1)	8542(3)	4563(1)	48(1)
O(4)	6877(1)	9351(3)	3930(1)	46(1)
O(5)	7200(1)	6932(3)	4018(1)	40(1)
O(6)	2678(1)	3781(3)	1214(1)	49(1)
O(7)	3703(2)	4703(3)	1644(1)	59(1)
O(8)	3938(2)	3205(4)	2310(1)	74(1)
O(9)	2909(3)	2013(10)	1834(2)	56(2)
C(90)	2639(12)	2610(40)	2043(7)	182(18)
O(9A)	3025(3)	2693(11)	1940(3)	79(3)
C(90A)	2545(6)	2270(20)	2006(4)	91(7)
O(10)	3851(1)	2245(3)	1498(1)	44(1)
N(1)	5979(2)	6735(4)	2852(1)	57(1)
N(2)	5923(2)	6719(4)	3822(1)	49(1)
N(3)	6316(2)	5243(4)	3230(1)	49(1)
N(4)	6556(2)	4704(3)	3857(1)	44(1)
N(5)	6840(2)	10254(5)	4843(1)	68(1)
N(6)	7568(2)	9989(4)	4564(1)	53(1)
N(7)	7663(2)	7152(4)	4720(1)	44(1)
N(8)	8165(2)	8409(4)	4288(1)	49(1)
N(9)	2414(2)	5306(4)	875(1)	49(1)
N(10)	3370(2)	5288(3)	946(1)	42(1)
N(11)	3367(2)	2487(3)	797(1)	42(1)
N(12)	4256(1)	3894(3)	1026(1)	40(1)
N(13)	3973(2)	2302(5)	2789(1)	68(1)
N(14)	3631(2)	859(5)	2406(1)	61(1)
N(15)	4649(2)	1400(3)	2046(1)	48(1)
N(16)	3753(2)	-57(4)	1839(1)	52(1)
C(1)	5652(2)	7748(5)	3821(1)	54(1)
C(2)	5189(2)	7870(5)	3948(1)	60(1)
C(3)	5008(2)	6925(5)	4099(2)	63(1)
C(4)	5286(2)	5861(5)	4108(1)	59(1)
C(5)	5731(2)	5776(4)	3958(1)	49(1)

C(6)	5994(2)	4605(4)	3916(1)	52(1)
C(7)	6669(2)	3780(4)	3633(1)	50(1)
C(8)	6442(2)	4097(5)	3296(1)	50(1)
C(9)	6400(2)	3239(5)	3062(1)	61(1)
C(10)	6237(3)	3586(6)	2743(1)	69(2)
C(11)	6106(3)	4740(6)	2677(1)	68(2)
C(12)	6140(2)	5552(5)	2925(1)	56(1)
C(13)	6097(2)	7736(5)	3020(1)	51(1)
C(14)	5897(2)	8901(5)	2856(1)	58(1)
C(15)	6048(3)	9925(5)	3079(1)	66(1)
C(16)	5275(2)	8869(6)	2758(1)	64(1)
C(17)	6167(3)	9016(6)	2564(1)	72(2)
C(18)	6937(2)	4608(4)	4162(1)	46(1)
C(19)	7502(2)	4956(4)	4122(1)	44(1)
C(20)	7920(2)	4109(5)	4144(1)	54(1)
C(21)	8438(2)	4417(6)	4108(1)	63(1)
C(22)	8543(2)	5614(5)	4063(1)	56(1)
C(23)	8139(2)	6475(5)	4036(1)	48(1)
C(24)	7611(2)	6115(4)	4057(1)	42(1)
C(25)	8876(3)	3511(7)	4118(2)	88(2)
C(26)	8255(2)	7746(5)	4001(1)	50(1)
C(27)	8496(2)	7905(5)	4581(1)	52(1)
C(28)	8205(2)	6983(4)	4736(1)	46(1)
C(29)	8470(2)	6052(5)	4905(1)	50(1)
C(30)	8180(2)	5281(4)	5063(1)	53(1)
C(31)	7628(2)	5449(5)	5049(1)	53(1)
C(32)	7388(2)	6385(4)	4872(1)	47(1)
C(33)	8284(2)	9674(5)	4259(1)	64(1)
C(34)	8043(2)	10382(5)	4495(1)	59(1)
C(35)	8292(3)	11392(5)	4625(1)	73(2)
C(36)	8044(3)	12059(6)	4825(2)	80(2)
C(37)	7566(3)	11716(5)	4890(1)	75(2)
C(38)	7328(2)	10636(5)	4760(1)	59(1)
C(39)	6524(2)	9272(5)	4759(1)	56(1)
C(40)	6029(2)	9119(6)	4903(1)	67(2)
C(41)	6104(3)	9582(8)	5248(1)	91(2)
C(42)	5573(3)	9830(7)	4694(1)	79(2)
C(43)	5877(3)	7827(7)	4897(2)	74(2)
C(44)	7520(3)	7258(7)	3172(2)	76(2)
C(45)	6563(2)	10381(5)	3971(1)	56(1)
C(46)	2901(2)	5852(4)	847(1)	45(1)
C(47)	2881(2)	6979(4)	714(1)	53(1)
C(48)	3361(2)	7496(4)	670(1)	57(1)
C(49)	3846(2)	6911(4)	759(1)	53(1)
C(50)	3839(2)	5826(4)	901(1)	45(1)
C(51)	4350(2)	5172(4)	1028(1)	45(1)

C(52)	4186(2)	3432(4)	694(1)	44(1)
C(53)	3785(2)	2434(4)	639(1)	41(1)
C(54)	3835(2)	1533(4)	424(1)	47(1)
C(55)	3431(2)	688(4)	364(1)	50(1)
C(56)	2999(2)	749(4)	523(1)	48(1)
C(57)	2981(2)	1653(4)	742(1)	44(1)
C(58)	2314(2)	4353(5)	1048(1)	49(1)
C(59)	1723(2)	3995(5)	1021(1)	56(1)
C(60)	1673(2)	3057(6)	1273(2)	68(2)
C(61)	1545(2)	3482(6)	688(1)	62(1)
C(62)	1369(2)	5059(6)	1071(2)	70(2)
C(63)	4708(2)	3270(4)	1234(1)	44(1)
C(64)	4603(2)	1969(4)	1228(1)	42(1)
C(65)	4935(2)	1193(5)	1092(1)	47(1)
C(66)	4838(2)	-20(5)	1075(1)	53(1)
C(67)	4398(2)	-434(4)	1190(1)	49(1)
C(68)	4061(2)	296(4)	1331(1)	45(1)
C(69)	4168(2)	1504(4)	1352(1)	41(1)
C(70)	5227(2)	-822(6)	941(2)	69(2)
C(71)	3618(2)	-210(5)	1486(1)	51(1)
C(72)	4293(2)	-594(5)	1966(1)	57(1)
C(73)	4743(2)	293(4)	1961(1)	50(1)
C(74)	5227(2)	-41(5)	1879(1)	54(1)
C(75)	5625(2)	810(5)	1873(1)	58(1)
C(76)	5529(2)	1952(5)	1965(1)	57(1)
C(77)	5031(2)	2209(5)	2050(1)	51(1)
C(78)	3336(2)	-597(6)	1997(1)	66(2)
C(79)	3403(2)	-211(6)	2340(1)	69(2)
C(80)	3245(3)	-910(7)	2571(2)	81(2)
C(81)	3332(3)	-532(8)	2882(2)	92(2)
C(82)	3574(3)	555(7)	2958(2)	78(2)
C(83)	3716(2)	1221(6)	2707(1)	65(1)
C(84)	4044(3)	3241(5)	2604(1)	65(1)
C(85)	4270(3)	4354(6)	2777(2)	75(2)
C(86)	4872(4)	4225(9)	2843(2)	107(3)
C(87)	4045(4)	4544(8)	3085(2)	101(3)
C(88)	4113(6)	5396(7)	2555(2)	123(4)
C(89)	3461(4)	5769(7)	1697(2)	107(3)
S(3)	5113(1)	6210(1)	1900(1)	60(1)
S(4)	5029(1)	1595(1)	3585(1)	58(1)
S(5)	7806(1)	1000(1)	3404(1)	58(1)
O(17)	4860(2)	5072(4)	1898(1)	81(1)
O(18)	4793(2)	7012(4)	1674(1)	81(1)
O(19)	5317(2)	6733(4)	2199(1)	83(1)
O(20)	5450(2)	2300(4)	3492(1)	71(1)
O(21)	5134(2)	365(4)	3607(1)	83(1)

O(22)	4490(2)	1897(4)	3434(1)	67(1)
O(23)	8357(2)	795(6)	3533(1)	98(2)
O(24)	7453(2)	96(5)	3480(1)	90(2)
O(25)	7638(3)	2160(5)	3435(1)	108(2)
O(29)	7825(3)	4418(6)	3221(2)	104(2)
C(93)	5687(3)	5964(9)	1709(2)	89(2)
C(94)	5036(2)	2046(5)	3998(1)	59(1)
C(95)	7766(3)	829(7)	2972(1)	71(2)
C(97)	7782(5)	4329(11)	2888(3)	120(3)
O(30)	2500	5142(10)	2500	161(5)
C(98)	2956(6)	4450(17)	2454(7)	131(9)
O(31)	2472(3)	7197(9)	3010(2)	159(4)
C(99)	2865(12)	6348(15)	2990(5)	318(18)
F(1)	5571(2)	2569(5)	5237(1)	68(1)
F(2)	5302(3)	3623(14)	4818(2)	72(2)
F(3)	5545(2)	4466(5)	5269(1)	74(2)
C(91)	5652(3)	3586(7)	5087(2)	56(2)
S(1)	6344(1)	3640(2)	5018(1)	49(1)
O(11)	6661(6)	3644(17)	5329(4)	64(4)
O(12)	6385(2)	2592(6)	4837(2)	68(2)
O(13)	6352(3)	4744(5)	4850(2)	65(2)
F(1A)	5753(11)	5145(14)	4999(6)	219(11)
F(2A)	5417(7)	3680(30)	4733(4)	87(6)
F(3A)	6228(7)	4130(30)	4705(4)	219(11)
C(91A)	5871(6)	4100(14)	4896(4)	103(5)
S(1A)	6152(1)	3151(3)	5227(1)	55(1)
O(11A)	6654(9)	3650(30)	5369(8)	63(7)
O(12A)	6188(9)	2044(14)	5085(5)	143(9)
O(13A)	5743(7)	3300(30)	5416(4)	154(10)
F(4)	3772(2)	8521(7)	3610(1)	144(3)
F(5)	3749(2)	8171(6)	4094(1)	119(2)
F(6)	3852(2)	9913(6)	3950(2)	129(2)
C(92)	3600(3)	8925(7)	3862(2)	80(2)
S(2)	2872(1)	9140(2)	3784(1)	83(1)
O(14)	2672(3)	8004(6)	3677(2)	126(2)
O(15)	2795(2)	10074(6)	3543(1)	102(2)
O(16)	2765(3)	9441(6)	4083(1)	103(2)
F(7)	5559(2)	5525(4)	1420(1)	82(1)
F(8)	6020(2)	5182(8)	1887(1)	156(3)
F(9)	5976(2)	6913(6)	1699(1)	126(2)
F(10)	4708(2)	1385(4)	4138(1)	81(1)
F(11)	5534(1)	1960(4)	4166(1)	80(1)
F(12)	4878(2)	3157(3)	4014(1)	71(1)
F(13)	8101(2)	1507(4)	2857(1)	80(1)
F(14)	7895(3)	-262(5)	2904(1)	130(2)
F(15)	7271(2)	1084(6)	2826(1)	108(2)

F(16)	581(2)	8825(5)	4799(1)	101(2)
F(17)	370(2)	8519(6)	5288(1)	114(2)
F(18)	-279(2)	8784(5)	4875(1)	98(1)
C(96)	249(2)	8407(5)	4987(1)	114(2)
S(6)	172(1)	6693(3)	4876(1)	91(1)
O(26)	-146(3)	6325(6)	5087(2)	121(2)
O(27)	715(2)	6348(6)	4968(2)	119(2)
O(28)	-27(3)	6606(6)	4568(2)	130(2)
F(16A)	-146(3)	6325(6)	5087(2)	121(2)
F(17A)	715(2)	6348(6)	4968(2)	119(2)
F(18A)	-27(3)	6606(6)	4568(2)	130(2)
C(96A)	172(1)	6693(3)	4876(1)	91(1)
S(6A)	249(2)	8407(5)	4987(1)	114(2)
O(26A)	581(2)	8825(5)	4799(1)	101(2)
O(27A)	370(2)	8519(6)	5288(1)	114(2)
O(28A)	-279(2)	8784(5)	4875(1)	98(1)

Table S3. Bond lengths [Å] and angles [deg] for **0**.

Fe(1)-O(5)	2.065(3)
Fe(1)-O(1)	2.072(3)
Fe(1)-N(2)	2.154(4)
Fe(1)-O(2)	2.204(3)
Fe(1)-N(3)	2.216(4)
Fe(1)-N(4)	2.252(4)
Fe(2)-O(5)	2.036(3)
Fe(2)-O(3)	2.056(3)
Fe(2)-N(7)	2.182(4)
Fe(2)-O(4)	2.199(3)
Fe(2)-N(6)	2.204(4)
Fe(2)-N(8)	2.231(4)
Fe(3)-O(10)	2.063(3)
Fe(3)-O(6)	2.074(3)
Fe(3)-N(11)	2.178(4)
Fe(3)-O(7)	2.182(3)
Fe(3)-N(10)	2.211(4)
Fe(3)-N(12)	2.214(4)
Fe(4)-O(8)	2.094(4)
Fe(4)-O(10)	2.103(3)
Fe(4)-N(15)	2.158(4)
Fe(4)-O(9A)	2.160(9)
Fe(4)-N(16)	2.222(5)
Fe(4)-O(9)	2.231(7)
Fe(4)-N(14)	2.253(4)
O(1)-C(13)	1.224(5)
O(2)-C(44)	1.419(8)
O(2)-H(2O)	0.9500
O(3)-C(39)	1.250(6)
O(4)-C(45)	1.436(6)
O(4)-H(4O)	0.9500
O(5)-C(24)	1.376(5)
O(6)-C(58)	1.238(6)
O(7)-C(89)	1.387(8)
O(7)-H(7)	0.9500
O(8)-C(84)	1.234(7)
O(9)-C(90)	1.387(17)
O(9)-H(9O1)	0.9500
C(90)-H(90A)	0.9800
C(90)-H(90B)	0.9800
C(90)-H(90C)	0.9800
O(9A)-C(90A)	1.371(15)
O(9A)-H(9O2)	0.9500

C(90A)-H(90D)	0.9800
C(90A)-H(90E)	0.9800
C(90A)-H(90F)	0.9800
O(10)-C(69)	1.375(6)
N(1)-C(13)	1.345(7)
N(1)-C(12)	1.418(7)
N(1)-H(1A)	0.8800
N(2)-C(5)	1.344(6)
N(2)-C(1)	1.348(6)
N(3)-C(12)	1.344(6)
N(3)-C(8)	1.353(7)
N(4)-C(7)	1.473(6)
N(4)-C(6)	1.480(6)
N(4)-C(18)	1.483(6)
N(5)-C(39)	1.377(8)
N(5)-C(38)	1.400(8)
N(5)-H(5A)	0.8800
N(6)-C(38)	1.331(7)
N(6)-C(34)	1.351(8)
N(7)-C(32)	1.344(6)
N(7)-C(28)	1.366(6)
N(8)-C(33)	1.473(7)
N(8)-C(26)	1.486(6)
N(8)-C(27)	1.492(6)
N(9)-C(58)	1.354(7)
N(9)-C(46)	1.395(6)
N(9)-H(9A)	0.8800
N(10)-C(46)	1.344(6)
N(10)-C(50)	1.371(6)
N(11)-C(53)	1.341(6)
N(11)-C(57)	1.345(6)
N(12)-C(51)	1.466(6)
N(12)-C(52)	1.488(5)
N(12)-C(63)	1.495(5)
N(13)-C(84)	1.352(8)
N(13)-C(83)	1.400(9)
N(13)-H(13A)	0.8800
N(14)-C(83)	1.327(7)
N(14)-C(79)	1.349(8)
N(15)-C(77)	1.325(7)
N(15)-C(73)	1.336(7)
N(16)-C(78)	1.469(7)
N(16)-C(71)	1.494(6)
N(16)-C(72)	1.503(7)
C(1)-C(2)	1.372(8)
C(1)-H(1)	0.9500

C(2)-C(3)	1.365(9)
C(2)-H(2)	0.9500
C(3)-C(4)	1.390(8)
C(3)-H(3)	0.9500
C(4)-C(5)	1.380(8)
C(4)-H(4)	0.9500
C(5)-C(6)	1.506(7)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.497(7)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.382(7)
C(9)-C(10)	1.407(9)
C(9)-H(9)	0.9500
C(10)-C(11)	1.364(9)
C(10)-H(10)	0.9500
C(11)-C(12)	1.391(8)
C(11)-H(11)	0.9500
C(13)-C(14)	1.535(7)
C(14)-C(15)	1.505(8)
C(14)-C(17)	1.524(9)
C(14)-C(16)	1.550(8)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.511(7)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(24)	1.377(7)
C(19)-C(20)	1.415(7)
C(20)-C(21)	1.380(8)
C(20)-H(20)	0.9500
C(21)-C(22)	1.400(9)
C(21)-C(25)	1.501(8)
C(22)-C(23)	1.398(7)
C(22)-H(22)	0.9500
C(23)-C(24)	1.406(7)
C(23)-C(26)	1.480(8)
C(25)-H(25A)	0.9800

C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.491(7)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.380(7)
C(29)-C(30)	1.382(8)
C(29)-H(29)	0.9500
C(30)-C(31)	1.393(8)
C(30)-H(30)	0.9500
C(31)-C(32)	1.377(7)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(34)	1.492(9)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.374(8)
C(35)-C(36)	1.366(11)
C(35)-H(35)	0.9500
C(36)-C(37)	1.336(11)
C(36)-H(36)	0.9500
C(37)-C(38)	1.431(8)
C(37)-H(37)	0.9500
C(39)-C(40)	1.489(9)
C(40)-C(43)	1.511(10)
C(40)-C(41)	1.541(8)
C(40)-C(42)	1.552(8)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.394(7)
C(47)-C(48)	1.381(8)

C(47)-H(47)	0.9500
C(48)-C(49)	1.383(8)
C(48)-H(48)	0.9500
C(49)-C(50)	1.371(7)
C(49)-H(49)	0.9500
C(50)-C(51)	1.503(7)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(52)-C(53)	1.506(6)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(54)	1.391(6)
C(54)-C(55)	1.386(7)
C(54)-H(54)	0.9500
C(55)-C(56)	1.376(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.391(7)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(59)	1.525(7)
C(59)-C(61)	1.527(8)
C(59)-C(60)	1.530(8)
C(59)-C(62)	1.534(8)
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-C(64)	1.495(7)
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(64)-C(69)	1.396(7)
C(64)-C(65)	1.403(7)
C(65)-C(66)	1.395(7)
C(65)-H(65)	0.9500
C(66)-C(67)	1.365(8)
C(66)-C(70)	1.516(8)
C(67)-C(68)	1.391(7)
C(67)-H(67)	0.9500
C(68)-C(69)	1.394(7)
C(68)-C(71)	1.501(7)
C(70)-H(70A)	0.9800

C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-H(71A)	0.9900
C(71)-H(71B)	0.9900
C(72)-C(73)	1.515(7)
C(72)-H(72A)	0.9900
C(72)-H(72B)	0.9900
C(73)-C(74)	1.375(8)
C(74)-C(75)	1.392(8)
C(74)-H(74)	0.9500
C(75)-C(76)	1.384(8)
C(75)-H(75)	0.9500
C(76)-C(77)	1.392(8)
C(76)-H(76)	0.9500
C(77)-H(77)	0.9500
C(78)-C(79)	1.507(8)
C(78)-H(78A)	0.9900
C(78)-H(78B)	0.9900
C(79)-C(80)	1.372(9)
C(80)-C(81)	1.375(10)
C(80)-H(80)	0.9500
C(81)-C(82)	1.386(11)
C(81)-H(81)	0.9500
C(82)-C(83)	1.399(8)
C(82)-H(82)	0.9500
C(84)-C(85)	1.521(10)
C(85)-C(86)	1.500(12)
C(85)-C(88)	1.520(10)
C(85)-C(87)	1.529(9)
C(86)-H(86A)	0.9800
C(86)-H(86B)	0.9800
C(86)-H(86C)	0.9800
C(87)-H(87A)	0.9800
C(87)-H(87B)	0.9800
C(87)-H(87C)	0.9800
C(88)-H(88A)	0.9800
C(88)-H(88B)	0.9800
C(88)-H(88C)	0.9800
C(89)-H(89A)	0.9800
C(89)-H(89B)	0.9800
C(89)-H(89C)	0.9800
S(3)-O(19)	1.419(4)
S(3)-O(17)	1.436(5)
S(3)-O(18)	1.459(5)
S(3)-C(93)	1.796(8)
S(4)-O(21)	1.418(4)

S(4)-O(20)	1.435(4)
S(4)-O(22)	1.439(4)
S(4)-C(94)	1.826(6)
S(5)-O(25)	1.393(6)
S(5)-O(23)	1.419(5)
S(5)-O(24)	1.430(5)
S(5)-C(95)	1.836(6)
O(29)-C(97)	1.406(12)
O(29)-H(29O)	0.92(2)
C(93)-F(9)	1.302(10)
C(93)-F(7)	1.315(8)
C(93)-F(8)	1.359(10)
C(94)-F(12)	1.324(7)
C(94)-F(10)	1.328(6)
C(94)-F(11)	1.337(6)
C(95)-F(13)	1.295(7)
C(95)-F(14)	1.320(9)
C(95)-F(15)	1.327(8)
C(97)-H(97A)	0.9800
C(97)-H(97B)	0.9800
C(97)-H(97C)	0.9800
O(30)-C(98)	1.429(17)
O(30)-H(30A)	0.8400
O(30)-H(30A)#1	0.8401
C(98)-H(98A)	0.9800
C(98)-H(98B)	0.9800
C(98)-H(98C)	0.9800
O(31)-C(99)	1.39(2)
O(31)-H(31A)	0.8400
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
F(1)-C(91)	1.350(9)
F(2)-C(91)	1.318(10)
F(3)-C(91)	1.319(9)
C(91)-S(1)	1.815(8)
S(1)-O(11)	1.422(12)
S(1)-O(12)	1.427(6)
S(1)-O(13)	1.443(6)
F(1A)-C(91A)	1.314(16)
F(2A)-C(91A)	1.322(14)
F(3A)-C(91A)	1.309(16)
C(91A)-S(1A)	1.814(12)
S(1A)-O(12A)	1.401(12)
S(1A)-O(13A)	1.420(12)
S(1A)-O(11A)	1.420(15)

F(4)-C(92)	1.305(8)
F(5)-C(92)	1.311(8)
F(6)-C(92)	1.308(9)
C(92)-S(2)	1.821(7)
S(2)-O(16)	1.386(6)
S(2)-O(14)	1.427(6)
S(2)-O(15)	1.464(6)
F(16)-C(96)	1.335(6)
F(17)-C(96)	1.272(7)
F(18)-C(96)	1.399(6)
C(96)-S(6)	1.998(7)
S(6)-O(28)	1.327(8)
S(6)-O(26)	1.363(6)
S(6)-O(27)	1.411(6)
F(16A)-C(96A)	1.363(6)
F(17A)-C(96A)	1.411(6)
F(18A)-C(96A)	1.327(8)
C(96A)-S(6A)	1.998(7)
S(6A)-O(27A)	1.272(7)
S(6A)-O(26A)	1.335(6)
S(6A)-O(28A)	1.399(6)
O(5)-Fe(1)-O(1)	118.89(13)
O(5)-Fe(1)-N(2)	98.13(14)
O(1)-Fe(1)-N(2)	87.91(15)
O(5)-Fe(1)-O(2)	85.93(12)
O(1)-Fe(1)-O(2)	84.05(13)
N(2)-Fe(1)-O(2)	171.96(14)
O(5)-Fe(1)-N(3)	152.97(14)
O(1)-Fe(1)-N(3)	82.90(14)
N(2)-Fe(1)-N(3)	98.50(15)
O(2)-Fe(1)-N(3)	80.40(14)
O(5)-Fe(1)-N(4)	88.40(13)
O(1)-Fe(1)-N(4)	150.98(14)
N(2)-Fe(1)-N(4)	77.89(15)
O(2)-Fe(1)-N(4)	109.28(14)
N(3)-Fe(1)-N(4)	74.49(14)
O(5)-Fe(2)-O(3)	113.60(13)
O(5)-Fe(2)-N(7)	91.62(13)
O(3)-Fe(2)-N(7)	89.29(13)
O(5)-Fe(2)-O(4)	84.97(12)
O(3)-Fe(2)-O(4)	89.43(12)
N(7)-Fe(2)-O(4)	175.53(14)
O(5)-Fe(2)-N(6)	161.16(16)
O(3)-Fe(2)-N(6)	83.42(16)
N(7)-Fe(2)-N(6)	96.81(14)

O(4)-Fe(2)-N(6)	87.29(13)
O(5)-Fe(2)-N(8)	89.52(14)
O(3)-Fe(2)-N(8)	154.24(14)
N(7)-Fe(2)-N(8)	78.37(14)
O(4)-Fe(2)-N(8)	104.45(13)
N(6)-Fe(2)-N(8)	75.82(17)
O(10)-Fe(3)-O(6)	113.54(13)
O(10)-Fe(3)-N(11)	91.41(13)
O(6)-Fe(3)-N(11)	91.88(14)
O(10)-Fe(3)-O(7)	85.77(13)
O(6)-Fe(3)-O(7)	92.68(14)
N(11)-Fe(3)-O(7)	175.31(15)
O(10)-Fe(3)-N(10)	163.10(14)
O(6)-Fe(3)-N(10)	81.97(14)
N(11)-Fe(3)-N(10)	94.86(13)
O(7)-Fe(3)-N(10)	86.85(13)
O(10)-Fe(3)-N(12)	90.62(13)
O(6)-Fe(3)-N(12)	154.39(13)
N(11)-Fe(3)-N(12)	78.59(13)
O(7)-Fe(3)-N(12)	97.66(14)
N(10)-Fe(3)-N(12)	75.32(14)
O(8)-Fe(4)-O(10)	117.99(14)
O(8)-Fe(4)-N(15)	91.74(17)
O(10)-Fe(4)-N(15)	88.20(13)
O(8)-Fe(4)-O(9A)	76.0(4)
O(10)-Fe(4)-O(9A)	92.2(3)
N(15)-Fe(4)-O(9A)	166.3(4)
O(8)-Fe(4)-N(16)	152.29(15)
O(10)-Fe(4)-N(16)	88.32(14)
N(15)-Fe(4)-N(16)	79.82(15)
O(9A)-Fe(4)-N(16)	113.9(4)
O(8)-Fe(4)-O(9)	99.2(3)
O(10)-Fe(4)-O(9)	86.8(2)
N(15)-Fe(4)-O(9)	169.1(3)
N(16)-Fe(4)-O(9)	90.3(3)
O(8)-Fe(4)-N(14)	80.62(17)
O(10)-Fe(4)-N(14)	161.03(17)
N(15)-Fe(4)-N(14)	95.23(16)
O(9A)-Fe(4)-N(14)	88.9(3)
N(16)-Fe(4)-N(14)	74.01(17)
O(9)-Fe(4)-N(14)	86.5(2)
C(13)-O(1)-Fe(1)	135.0(3)
C(44)-O(2)-Fe(1)	128.2(4)
C(44)-O(2)-H(2O)	115.9
Fe(1)-O(2)-H(2O)	115.9
C(39)-O(3)-Fe(2)	135.2(4)

C(45)-O(4)-Fe(2)	122.8(3)
C(45)-O(4)-H(4O)	118.6
Fe(2)-O(4)-H(4O)	118.6
C(24)-O(5)-Fe(2)	115.6(2)
C(24)-O(5)-Fe(1)	108.2(2)
Fe(2)-O(5)-Fe(1)	136.05(15)
C(58)-O(6)-Fe(3)	133.5(3)
C(89)-O(7)-Fe(3)	125.3(4)
C(89)-O(7)-H(7)	117.4
Fe(3)-O(7)-H(7)	117.4
C(84)-O(8)-Fe(4)	134.3(4)
C(90)-O(9)-Fe(4)	116.8(15)
C(90)-O(9)-H(9O1)	121.6
Fe(4)-O(9)-H(9O1)	121.6
O(9)-C(90)-H(90A)	109.5
O(9)-C(90)-H(90B)	109.5
H(90A)-C(90)-H(90B)	109.5
O(9)-C(90)-H(90C)	109.5
H(90A)-C(90)-H(90C)	109.5
H(90B)-C(90)-H(90C)	109.5
C(90A)-O(9A)-Fe(4)	130.5(12)
C(90A)-O(9A)-H(9O2)	114.8
Fe(4)-O(9A)-H(9O2)	114.8
O(9A)-C(90A)-H(90D)	109.5
O(9A)-C(90A)-H(90E)	109.5
H(90D)-C(90A)-H(90E)	109.5
O(9A)-C(90A)-H(90F)	109.5
H(90D)-C(90A)-H(90F)	109.5
H(90E)-C(90A)-H(90F)	109.5
C(69)-O(10)-Fe(3)	114.9(2)
C(69)-O(10)-Fe(4)	115.9(2)
Fe(3)-O(10)-Fe(4)	129.21(16)
C(13)-N(1)-C(12)	130.5(4)
C(13)-N(1)-H(1A)	114.7
C(12)-N(1)-H(1A)	114.7
C(5)-N(2)-C(1)	118.0(4)
C(5)-N(2)-Fe(1)	116.8(3)
C(1)-N(2)-Fe(1)	125.2(3)
C(12)-N(3)-C(8)	118.5(4)
C(12)-N(3)-Fe(1)	125.9(3)
C(8)-N(3)-Fe(1)	113.2(3)
C(7)-N(4)-C(6)	110.4(4)
C(7)-N(4)-C(18)	110.3(4)
C(6)-N(4)-C(18)	109.9(4)
C(7)-N(4)-Fe(1)	107.2(3)
C(6)-N(4)-Fe(1)	108.2(3)

C(18)-N(4)-Fe(1)	110.7(3)
C(39)-N(5)-C(38)	132.4(5)
C(39)-N(5)-H(5A)	113.8
C(38)-N(5)-H(5A)	113.8
C(38)-N(6)-C(34)	117.9(5)
C(38)-N(6)-Fe(2)	128.1(4)
C(34)-N(6)-Fe(2)	114.1(4)
C(32)-N(7)-C(28)	118.4(4)
C(32)-N(7)-Fe(2)	124.2(3)
C(28)-N(7)-Fe(2)	114.5(3)
C(33)-N(8)-C(26)	111.2(4)
C(33)-N(8)-C(27)	110.3(4)
C(26)-N(8)-C(27)	110.7(4)
C(33)-N(8)-Fe(2)	106.1(3)
C(26)-N(8)-Fe(2)	109.4(3)
C(27)-N(8)-Fe(2)	109.0(3)
C(58)-N(9)-C(46)	130.2(4)
C(58)-N(9)-H(9A)	114.9
C(46)-N(9)-H(9A)	114.9
C(46)-N(10)-C(50)	118.3(4)
C(46)-N(10)-Fe(3)	128.0(3)
C(50)-N(10)-Fe(3)	113.5(3)
C(53)-N(11)-C(57)	119.0(4)
C(53)-N(11)-Fe(3)	114.4(3)
C(57)-N(11)-Fe(3)	124.1(3)
C(51)-N(12)-C(52)	110.3(3)
C(51)-N(12)-C(63)	110.8(3)
C(52)-N(12)-C(63)	110.6(3)
C(51)-N(12)-Fe(3)	106.6(3)
C(52)-N(12)-Fe(3)	109.3(3)
C(63)-N(12)-Fe(3)	109.2(3)
C(84)-N(13)-C(83)	130.1(5)
C(84)-N(13)-H(13A)	115.0
C(83)-N(13)-H(13A)	115.0
C(83)-N(14)-C(79)	118.2(5)
C(83)-N(14)-Fe(4)	127.9(4)
C(79)-N(14)-Fe(4)	113.8(4)
C(77)-N(15)-C(73)	119.4(5)
C(77)-N(15)-Fe(4)	122.5(3)
C(73)-N(15)-Fe(4)	113.3(3)
C(78)-N(16)-C(71)	110.7(4)
C(78)-N(16)-C(72)	109.8(4)
C(71)-N(16)-C(72)	110.7(4)
C(78)-N(16)-Fe(4)	107.3(4)
C(71)-N(16)-Fe(4)	111.4(3)
C(72)-N(16)-Fe(4)	106.9(3)

N(2)-C(1)-C(2)	123.1(5)
N(2)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(3)-C(2)-C(1)	118.8(5)
C(3)-C(2)-H(2)	120.6
C(1)-C(2)-H(2)	120.6
C(2)-C(3)-C(4)	118.9(5)
C(2)-C(3)-H(3)	120.5
C(4)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	119.4(5)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
N(2)-C(5)-C(4)	121.5(5)
N(2)-C(5)-C(6)	116.7(4)
C(4)-C(5)-C(6)	121.6(4)
N(4)-C(6)-C(5)	113.9(4)
N(4)-C(6)-H(6A)	108.8
C(5)-C(6)-H(6A)	108.8
N(4)-C(6)-H(6B)	108.8
C(5)-C(6)-H(6B)	108.8
H(6A)-C(6)-H(6B)	107.7
N(4)-C(7)-C(8)	111.5(4)
N(4)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
N(4)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	108.0
N(3)-C(8)-C(9)	122.5(5)
N(3)-C(8)-C(7)	117.8(4)
C(9)-C(8)-C(7)	119.5(5)
C(8)-C(9)-C(10)	118.2(6)
C(8)-C(9)-H(9)	120.9
C(10)-C(9)-H(9)	120.9
C(11)-C(10)-C(9)	119.2(5)
C(11)-C(10)-H(10)	120.4
C(9)-C(10)-H(10)	120.4
C(10)-C(11)-C(12)	119.6(5)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
N(3)-C(12)-C(11)	121.9(5)
N(3)-C(12)-N(1)	119.5(4)
C(11)-C(12)-N(1)	118.6(5)
O(1)-C(13)-N(1)	122.5(5)
O(1)-C(13)-C(14)	120.3(5)
N(1)-C(13)-C(14)	117.2(4)
C(15)-C(14)-C(17)	110.5(5)

C(15)-C(14)-C(13)	110.3(4)
C(17)-C(14)-C(13)	106.6(5)
C(15)-C(14)-C(16)	108.9(5)
C(17)-C(14)-C(16)	110.5(4)
C(13)-C(14)-C(16)	109.9(4)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(4)-C(18)-C(19)	111.1(4)
N(4)-C(18)-H(18A)	109.4
C(19)-C(18)-H(18A)	109.4
N(4)-C(18)-H(18B)	109.4
C(19)-C(18)-H(18B)	109.4
H(18A)-C(18)-H(18B)	108.0
C(24)-C(19)-C(20)	119.2(5)
C(24)-C(19)-C(18)	119.6(4)
C(20)-C(19)-C(18)	121.2(4)
C(21)-C(20)-C(19)	121.7(5)
C(21)-C(20)-H(20)	119.2
C(19)-C(20)-H(20)	119.2
C(20)-C(21)-C(22)	117.7(5)
C(20)-C(21)-C(25)	121.7(6)
C(22)-C(21)-C(25)	120.6(6)
C(23)-C(22)-C(21)	122.3(5)
C(23)-C(22)-H(22)	118.9
C(21)-C(22)-H(22)	118.9
C(22)-C(23)-C(24)	118.2(5)
C(22)-C(23)-C(26)	122.2(5)
C(24)-C(23)-C(26)	119.5(4)
O(5)-C(24)-C(19)	119.5(4)
O(5)-C(24)-C(23)	119.7(4)

C(19)-C(24)-C(23)	120.8(4)
C(21)-C(25)-H(25A)	109.5
C(21)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(21)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-N(8)	110.2(4)
C(23)-C(26)-H(26A)	109.6
N(8)-C(26)-H(26A)	109.6
C(23)-C(26)-H(26B)	109.6
N(8)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	108.1
C(28)-C(27)-N(8)	113.0(4)
C(28)-C(27)-H(27A)	109.0
N(8)-C(27)-H(27A)	109.0
C(28)-C(27)-H(27B)	109.0
N(8)-C(27)-H(27B)	109.0
H(27A)-C(27)-H(27B)	107.8
N(7)-C(28)-C(29)	121.5(5)
N(7)-C(28)-C(27)	116.1(4)
C(29)-C(28)-C(27)	122.3(5)
C(28)-C(29)-C(30)	119.2(5)
C(28)-C(29)-H(29)	120.4
C(30)-C(29)-H(29)	120.4
C(29)-C(30)-C(31)	119.8(5)
C(29)-C(30)-H(30)	120.1
C(31)-C(30)-H(30)	120.1
C(32)-C(31)-C(30)	118.0(5)
C(32)-C(31)-H(31)	121.0
C(30)-C(31)-H(31)	121.0
N(7)-C(32)-C(31)	123.1(5)
N(7)-C(32)-H(32)	118.5
C(31)-C(32)-H(32)	118.5
N(8)-C(33)-C(34)	110.7(4)
N(8)-C(33)-H(33A)	109.5
C(34)-C(33)-H(33A)	109.5
N(8)-C(33)-H(33B)	109.5
C(34)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	108.1
N(6)-C(34)-C(35)	123.1(6)
N(6)-C(34)-C(33)	116.4(5)
C(35)-C(34)-C(33)	120.4(6)
C(36)-C(35)-C(34)	119.0(7)
C(36)-C(35)-H(35)	120.5
C(34)-C(35)-H(35)	120.5

C(37)-C(36)-C(35)	119.4(6)
C(37)-C(36)-H(36)	120.3
C(35)-C(36)-H(36)	120.3
C(36)-C(37)-C(38)	120.0(6)
C(36)-C(37)-H(37)	120.0
C(38)-C(37)-H(37)	120.0
N(6)-C(38)-N(5)	119.9(5)
N(6)-C(38)-C(37)	120.5(6)
N(5)-C(38)-C(37)	119.6(6)
O(3)-C(39)-N(5)	120.8(5)
O(3)-C(39)-C(40)	121.1(5)
N(5)-C(39)-C(40)	118.2(5)
C(39)-C(40)-C(43)	109.4(5)
C(39)-C(40)-C(41)	112.2(6)
C(43)-C(40)-C(41)	109.6(6)
C(39)-C(40)-C(42)	106.9(5)
C(43)-C(40)-C(42)	109.4(6)
C(41)-C(40)-C(42)	109.3(5)
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(40)-C(43)-H(43A)	109.5
C(40)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(40)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
O(2)-C(44)-H(44A)	109.5
O(2)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
O(2)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
O(4)-C(45)-H(45A)	109.5
O(4)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
O(4)-C(45)-H(45C)	109.5

H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
N(10)-C(46)-C(47)	122.1(5)
N(10)-C(46)-N(9)	119.9(4)
C(47)-C(46)-N(9)	118.0(4)
C(48)-C(47)-C(46)	118.1(5)
C(48)-C(47)-H(47)	121.0
C(46)-C(47)-H(47)	121.0
C(47)-C(48)-C(49)	120.7(5)
C(47)-C(48)-H(48)	119.6
C(49)-C(48)-H(48)	119.6
C(50)-C(49)-C(48)	118.2(5)
C(50)-C(49)-H(49)	120.9
C(48)-C(49)-H(49)	120.9
N(10)-C(50)-C(49)	122.5(4)
N(10)-C(50)-C(51)	115.7(4)
C(49)-C(50)-C(51)	121.8(4)
N(12)-C(51)-C(50)	110.8(4)
N(12)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51A)	109.5
N(12)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	108.1
N(12)-C(52)-C(53)	112.1(4)
N(12)-C(52)-H(52A)	109.2
C(53)-C(52)-H(52A)	109.2
N(12)-C(52)-H(52B)	109.2
C(53)-C(52)-H(52B)	109.2
H(52A)-C(52)-H(52B)	107.9
N(11)-C(53)-C(54)	122.0(4)
N(11)-C(53)-C(52)	116.8(4)
C(54)-C(53)-C(52)	121.1(4)
C(55)-C(54)-C(53)	118.8(5)
C(55)-C(54)-H(54)	120.6
C(53)-C(54)-H(54)	120.6
C(56)-C(55)-C(54)	119.4(4)
C(56)-C(55)-H(55)	120.3
C(54)-C(55)-H(55)	120.3
C(55)-C(56)-C(57)	119.0(4)
C(55)-C(56)-H(56)	120.5
C(57)-C(56)-H(56)	120.5
N(11)-C(57)-C(56)	121.9(5)
N(11)-C(57)-H(57)	119.0
C(56)-C(57)-H(57)	119.0
O(6)-C(58)-N(9)	122.7(5)
O(6)-C(58)-C(59)	121.3(5)

N(9)-C(58)-C(59)	115.9(4)
C(58)-C(59)-C(61)	107.5(4)
C(58)-C(59)-C(60)	109.0(4)
C(61)-C(59)-C(60)	109.9(5)
C(58)-C(59)-C(62)	111.2(5)
C(61)-C(59)-C(62)	110.0(5)
C(60)-C(59)-C(62)	109.1(5)
C(59)-C(60)-H(60A)	109.5
C(59)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(59)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(59)-C(61)-H(61A)	109.5
C(59)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(59)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(59)-C(62)-H(62A)	109.5
C(59)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(59)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(64)-C(63)-N(12)	109.9(3)
C(64)-C(63)-H(63A)	109.7
N(12)-C(63)-H(63A)	109.7
C(64)-C(63)-H(63B)	109.7
N(12)-C(63)-H(63B)	109.7
H(63A)-C(63)-H(63B)	108.2
C(69)-C(64)-C(65)	118.7(4)
C(69)-C(64)-C(63)	120.8(4)
C(65)-C(64)-C(63)	120.5(4)
C(66)-C(65)-C(64)	121.7(5)
C(66)-C(65)-H(65)	119.1
C(64)-C(65)-H(65)	119.1
C(67)-C(66)-C(65)	117.7(5)
C(67)-C(66)-C(70)	122.9(5)
C(65)-C(66)-C(70)	119.3(5)
C(66)-C(67)-C(68)	122.8(5)
C(66)-C(67)-H(67)	118.6
C(68)-C(67)-H(67)	118.6
C(67)-C(68)-C(69)	119.0(5)
C(67)-C(68)-C(71)	121.1(5)
C(69)-C(68)-C(71)	119.7(4)

O(10)-C(69)-C(68)	120.4(4)
O(10)-C(69)-C(64)	119.5(4)
C(68)-C(69)-C(64)	120.1(4)
C(66)-C(70)-H(70A)	109.5
C(66)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(66)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
N(16)-C(71)-C(68)	109.8(4)
N(16)-C(71)-H(71A)	109.7
C(68)-C(71)-H(71A)	109.7
N(16)-C(71)-H(71B)	109.7
C(68)-C(71)-H(71B)	109.7
H(71A)-C(71)-H(71B)	108.2
N(16)-C(72)-C(73)	111.1(4)
N(16)-C(72)-H(72A)	109.4
C(73)-C(72)-H(72A)	109.4
N(16)-C(72)-H(72B)	109.4
C(73)-C(72)-H(72B)	109.4
H(72A)-C(72)-H(72B)	108.0
N(15)-C(73)-C(74)	122.1(5)
N(15)-C(73)-C(72)	116.7(5)
C(74)-C(73)-C(72)	121.1(5)
C(73)-C(74)-C(75)	119.0(5)
C(73)-C(74)-H(74)	120.5
C(75)-C(74)-H(74)	120.5
C(76)-C(75)-C(74)	118.7(5)
C(76)-C(75)-H(75)	120.7
C(74)-C(75)-H(75)	120.7
C(75)-C(76)-C(77)	118.5(5)
C(75)-C(76)-H(76)	120.7
C(77)-C(76)-H(76)	120.7
N(15)-C(77)-C(76)	122.3(5)
N(15)-C(77)-H(77)	118.9
C(76)-C(77)-H(77)	118.9
N(16)-C(78)-C(79)	110.6(5)
N(16)-C(78)-H(78A)	109.5
C(79)-C(78)-H(78A)	109.5
N(16)-C(78)-H(78B)	109.5
C(79)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	108.1
N(14)-C(79)-C(80)	122.1(6)
N(14)-C(79)-C(78)	116.0(5)
C(80)-C(79)-C(78)	121.9(6)
C(79)-C(80)-C(81)	119.5(7)

C(79)-C(80)-H(80)	120.2
C(81)-C(80)-H(80)	120.2
C(80)-C(81)-C(82)	119.4(6)
C(80)-C(81)-H(81)	120.3
C(82)-C(81)-H(81)	120.3
C(81)-C(82)-C(83)	117.4(6)
C(81)-C(82)-H(82)	121.3
C(83)-C(82)-H(82)	121.3
N(14)-C(83)-C(82)	123.2(6)
N(14)-C(83)-N(13)	120.0(5)
C(82)-C(83)-N(13)	116.7(5)
O(8)-C(84)-N(13)	122.5(6)
O(8)-C(84)-C(85)	121.1(5)
N(13)-C(84)-C(85)	116.4(5)
C(86)-C(85)-C(88)	109.8(8)
C(86)-C(85)-C(84)	107.0(6)
C(88)-C(85)-C(84)	107.8(6)
C(86)-C(85)-C(87)	111.3(7)
C(88)-C(85)-C(87)	109.2(6)
C(84)-C(85)-C(87)	111.7(6)
C(85)-C(86)-H(86A)	109.5
C(85)-C(86)-H(86B)	109.5
H(86A)-C(86)-H(86B)	109.5
C(85)-C(86)-H(86C)	109.5
H(86A)-C(86)-H(86C)	109.5
H(86B)-C(86)-H(86C)	109.5
C(85)-C(87)-H(87A)	109.5
C(85)-C(87)-H(87B)	109.5
H(87A)-C(87)-H(87B)	109.5
C(85)-C(87)-H(87C)	109.5
H(87A)-C(87)-H(87C)	109.5
H(87B)-C(87)-H(87C)	109.5
C(85)-C(88)-H(88A)	109.5
C(85)-C(88)-H(88B)	109.5
H(88A)-C(88)-H(88B)	109.5
C(85)-C(88)-H(88C)	109.5
H(88A)-C(88)-H(88C)	109.5
H(88B)-C(88)-H(88C)	109.5
O(7)-C(89)-H(89A)	109.5
O(7)-C(89)-H(89B)	109.5
H(89A)-C(89)-H(89B)	109.5
O(7)-C(89)-H(89C)	109.5
H(89A)-C(89)-H(89C)	109.5
H(89B)-C(89)-H(89C)	109.5
O(19)-S(3)-O(17)	118.0(3)
O(19)-S(3)-O(18)	114.0(3)

O(17)-S(3)-O(18)	111.2(3)
O(19)-S(3)-C(93)	105.9(3)
O(17)-S(3)-C(93)	104.4(4)
O(18)-S(3)-C(93)	101.2(4)
O(21)-S(4)-O(20)	115.2(3)
O(21)-S(4)-O(22)	114.5(3)
O(20)-S(4)-O(22)	115.3(3)
O(21)-S(4)-C(94)	103.9(3)
O(20)-S(4)-C(94)	102.9(2)
O(22)-S(4)-C(94)	102.6(3)
O(25)-S(5)-O(23)	114.2(4)
O(25)-S(5)-O(24)	116.3(4)
O(23)-S(5)-O(24)	113.5(3)
O(25)-S(5)-C(95)	103.2(3)
O(23)-S(5)-C(95)	104.7(3)
O(24)-S(5)-C(95)	102.8(3)
C(97)-O(29)-H(29O)	122(3)
F(9)-C(93)-F(7)	109.4(7)
F(9)-C(93)-F(8)	105.1(7)
F(7)-C(93)-F(8)	107.8(7)
F(9)-C(93)-S(3)	112.5(7)
F(7)-C(93)-S(3)	113.2(5)
F(8)-C(93)-S(3)	108.3(6)
F(12)-C(94)-F(10)	107.3(5)
F(12)-C(94)-F(11)	107.7(5)
F(10)-C(94)-F(11)	108.4(4)
F(12)-C(94)-S(4)	111.2(4)
F(10)-C(94)-S(4)	111.6(4)
F(11)-C(94)-S(4)	110.4(4)
F(13)-C(95)-F(14)	105.9(6)
F(13)-C(95)-F(15)	108.3(5)
F(14)-C(95)-F(15)	110.3(6)
F(13)-C(95)-S(5)	112.8(4)
F(14)-C(95)-S(5)	110.0(5)
F(15)-C(95)-S(5)	109.5(5)
O(29)-C(97)-H(97A)	109.5
O(29)-C(97)-H(97B)	109.5
H(97A)-C(97)-H(97B)	109.5
O(29)-C(97)-H(97C)	109.5
H(97A)-C(97)-H(97C)	109.5
H(97B)-C(97)-H(97C)	109.5
C(98)-O(30)-H(30A)	109.5
C(98)-O(30)-H(30A)#1	130.4(7)
H(30A)-O(30)-H(30A)#1	53.0
O(30)-C(98)-H(98A)	109.5
O(30)-C(98)-H(98B)	109.5

H(98A)-C(98)-H(98B)	109.5
O(30)-C(98)-H(98C)	109.5
H(98A)-C(98)-H(98C)	109.5
H(98B)-C(98)-H(98C)	109.5
C(99)-O(31)-H(31A)	109.5
O(31)-C(99)-H(99A)	109.5
O(31)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5
O(31)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5
H(99B)-C(99)-H(99C)	109.5
F(2)-C(91)-F(3)	108.4(9)
F(2)-C(91)-F(1)	107.9(9)
F(3)-C(91)-F(1)	107.6(7)
F(2)-C(91)-S(1)	112.1(7)
F(3)-C(91)-S(1)	111.4(6)
F(1)-C(91)-S(1)	109.3(5)
O(11)-S(1)-O(12)	115.2(8)
O(11)-S(1)-O(13)	114.0(8)
O(12)-S(1)-O(13)	116.3(4)
O(11)-S(1)-C(91)	104.6(9)
O(12)-S(1)-C(91)	102.5(4)
O(13)-S(1)-C(91)	101.7(4)
F(3A)-C(91A)-F(1A)	113.6(19)
F(3A)-C(91A)-F(2A)	107.7(16)
F(1A)-C(91A)-F(2A)	106.1(18)
F(3A)-C(91A)-S(1A)	106.3(12)
F(1A)-C(91A)-S(1A)	110.7(12)
F(2A)-C(91A)-S(1A)	112.5(14)
O(12A)-S(1A)-O(13A)	117.0(15)
O(12A)-S(1A)-O(11A)	114.7(14)
O(13A)-S(1A)-O(11A)	113.0(17)
O(12A)-S(1A)-C(91A)	103.9(10)
O(13A)-S(1A)-C(91A)	98.6(11)
O(11A)-S(1A)-C(91A)	107.3(14)
F(4)-C(92)-F(6)	108.8(7)
F(4)-C(92)-F(5)	107.4(7)
F(6)-C(92)-F(5)	106.2(6)
F(4)-C(92)-S(2)	111.0(5)
F(6)-C(92)-S(2)	111.1(5)
F(5)-C(92)-S(2)	112.0(5)
O(16)-S(2)-O(14)	113.8(4)
O(16)-S(2)-O(15)	116.4(4)
O(14)-S(2)-O(15)	115.3(4)
O(16)-S(2)-C(92)	102.1(4)
O(14)-S(2)-C(92)	103.1(4)

O(15)-S(2)-C(92)	103.5(3)
F(17)-C(96)-F(16)	120.1(5)
F(17)-C(96)-F(18)	111.3(5)
F(16)-C(96)-F(18)	110.0(4)
F(17)-C(96)-S(6)	109.3(4)
F(16)-C(96)-S(6)	104.5(4)
F(18)-C(96)-S(6)	99.6(4)
O(28)-S(6)-O(26)	117.7(5)
O(28)-S(6)-O(27)	115.9(5)
O(26)-S(6)-O(27)	112.4(4)
O(28)-S(6)-C(96)	108.0(4)
O(26)-S(6)-C(96)	100.8(4)
O(27)-S(6)-C(96)	98.8(4)
F(18A)-C(96A)-F(16A)	117.7(5)
F(18A)-C(96A)-F(17A)	115.9(5)
F(16A)-C(96A)-F(17A)	112.4(4)
F(18A)-C(96A)-S(6A)	108.0(4)
F(16A)-C(96A)-S(6A)	100.8(4)
F(17A)-C(96A)-S(6A)	98.8(4)
O(27A)-S(6A)-O(26A)	120.1(5)
O(27A)-S(6A)-O(28A)	111.3(5)
O(26A)-S(6A)-O(28A)	110.0(4)
O(27A)-S(6A)-C(96A)	109.3(4)
O(26A)-S(6A)-C(96A)	104.5(4)
O(28A)-S(6A)-C(96A)	99.6(4)

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **0**. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	40(1)	53(1)	29(1)	1(1)	1(1)	-3(1)
Fe(2)	46(1)	53(1)	24(1)	-1(1)	1(1)	1(1)
Fe(3)	41(1)	52(1)	25(1)	1(1)	0(1)	1(1)
Fe(4)	53(1)	70(1)	34(1)	14(1)	7(1)	7(1)
O(1)	49(2)	61(2)	32(2)	6(1)	-2(1)	-3(1)
O(2)	48(2)	71(2)	33(2)	3(1)	7(1)	-1(2)
O(3)	57(2)	57(2)	32(2)	1(1)	11(1)	9(1)
O(4)	52(2)	59(2)	26(1)	3(1)	1(1)	3(1)
O(5)	38(2)	53(2)	28(1)	0(1)	2(1)	4(1)
O(6)	50(2)	60(2)	39(2)	3(1)	8(1)	2(1)
O(7)	77(2)	64(2)	34(2)	-5(1)	2(2)	7(2)
O(8)	113(4)	77(2)	39(2)	10(2)	29(2)	23(2)
O(9)	41(4)	92(6)	36(4)	3(4)	12(3)	9(4)
C(90)	97(18)	350(40)	104(14)	-70(20)	21(13)	110(20)
O(9A)	50(4)	101(7)	89(7)	26(6)	15(4)	-2(5)
C(90A)	44(5)	162(16)	60(8)	50(10)	-9(5)	-14(7)
O(10)	43(2)	58(2)	32(1)	4(1)	5(1)	6(1)
N(1)	66(3)	65(2)	34(2)	-5(2)	-6(2)	-2(2)
N(2)	42(2)	55(2)	49(2)	-2(2)	4(2)	-1(2)
N(3)	49(2)	61(2)	35(2)	-2(2)	2(2)	-8(2)
N(4)	49(2)	48(2)	37(2)	0(2)	12(2)	-1(2)
N(5)	80(3)	76(3)	42(2)	-19(2)	-6(2)	21(3)
N(6)	69(2)	53(2)	31(2)	-1(2)	-13(2)	2(2)
N(7)	48(2)	60(2)	22(2)	1(2)	4(1)	2(2)
N(8)	53(2)	67(2)	24(2)	4(2)	-2(2)	-7(2)
N(9)	45(2)	62(2)	38(2)	4(2)	2(2)	7(2)
N(10)	48(2)	51(2)	23(2)	2(1)	-1(1)	2(2)
N(11)	44(2)	52(2)	26(2)	0(1)	-2(1)	1(2)
N(12)	42(2)	53(2)	22(2)	-1(1)	-3(1)	-1(2)
N(13)	74(3)	86(3)	45(2)	8(2)	11(2)	-5(3)
N(14)	54(2)	89(3)	40(2)	17(2)	8(2)	-7(2)
N(15)	52(2)	58(2)	29(2)	4(2)	-4(2)	-1(2)
N(16)	48(2)	68(2)	38(2)	9(2)	1(2)	-9(2)
C(1)	48(3)	52(3)	64(3)	2(2)	11(2)	3(2)
C(2)	54(3)	64(3)	63(3)	1(2)	11(2)	8(2)
C(3)	53(3)	77(4)	62(3)	-4(3)	16(2)	6(3)
C(4)	57(3)	62(3)	59(3)	0(2)	15(2)	-4(2)
C(5)	43(2)	58(3)	46(3)	0(2)	9(2)	-6(2)

C(6)	51(3)	53(3)	55(3)	2(2)	17(2)	-6(2)
C(7)	57(3)	49(2)	45(3)	-4(2)	10(2)	0(2)
C(8)	46(2)	63(3)	40(2)	-10(2)	6(2)	-6(2)
C(9)	61(3)	68(3)	52(3)	-13(2)	5(2)	-3(2)
C(10)	74(4)	84(4)	48(3)	-28(3)	5(3)	-5(3)
C(11)	77(4)	83(4)	40(3)	-12(3)	-6(2)	-3(3)
C(12)	58(3)	72(3)	35(2)	-6(2)	-1(2)	-9(2)
C(13)	50(3)	68(3)	33(2)	0(2)	-2(2)	-3(2)
C(14)	60(3)	62(3)	45(3)	7(2)	-8(2)	-10(2)
C(15)	77(4)	68(3)	43(3)	-1(2)	-12(3)	-6(3)
C(16)	58(3)	76(3)	50(3)	0(3)	-12(2)	-3(3)
C(17)	80(4)	84(4)	48(3)	3(3)	-2(3)	-17(3)
C(18)	55(3)	52(2)	31(2)	4(2)	10(2)	7(2)
C(19)	49(2)	57(2)	27(2)	2(2)	7(2)	7(2)
C(20)	64(3)	70(3)	31(2)	6(2)	14(2)	18(2)
C(21)	63(3)	92(4)	37(2)	16(2)	17(2)	29(3)
C(22)	42(2)	94(4)	32(2)	6(2)	6(2)	17(2)
C(23)	42(2)	77(3)	22(2)	-1(2)	2(2)	3(2)
C(24)	42(2)	60(2)	22(2)	-2(2)	3(2)	5(2)
C(25)	70(4)	116(6)	87(5)	37(4)	40(4)	46(4)
C(26)	40(2)	84(3)	26(2)	0(2)	3(2)	-4(2)
C(27)	48(2)	76(3)	28(2)	3(2)	-4(2)	-5(2)
C(28)	49(2)	64(3)	23(2)	-4(2)	-3(2)	2(2)
C(29)	52(3)	67(3)	27(2)	-5(2)	-4(2)	4(2)
C(30)	70(3)	57(3)	28(2)	-4(2)	-8(2)	5(2)
C(31)	72(3)	59(3)	26(2)	-1(2)	5(2)	-2(2)
C(32)	55(3)	61(3)	26(2)	1(2)	6(2)	5(2)
C(33)	70(3)	81(4)	34(2)	9(2)	-6(2)	-23(3)
C(34)	77(3)	62(3)	32(2)	9(2)	-9(2)	-9(2)
C(35)	97(4)	67(3)	46(3)	8(2)	-17(3)	-21(3)
C(36)	112(5)	59(3)	59(3)	4(3)	-16(3)	-15(3)
C(37)	108(4)	62(3)	44(3)	-12(2)	-18(3)	16(3)
C(38)	73(3)	55(3)	41(2)	-5(2)	-12(2)	11(2)
C(39)	64(3)	74(3)	28(2)	2(2)	0(2)	22(3)
C(40)	68(3)	96(4)	37(3)	4(3)	8(2)	28(3)
C(41)	91(5)	148(7)	34(3)	-2(3)	12(3)	46(5)
C(42)	73(4)	118(5)	45(3)	1(3)	8(3)	42(4)
C(43)	57(3)	116(5)	50(3)	13(3)	19(3)	17(3)
C(44)	65(4)	105(5)	63(4)	8(3)	20(3)	-1(3)
C(45)	71(3)	57(3)	36(2)	3(2)	-5(2)	11(2)
C(46)	52(3)	53(2)	29(2)	1(2)	2(2)	6(2)
C(47)	60(3)	55(3)	40(2)	0(2)	-1(2)	8(2)
C(48)	75(3)	49(2)	43(3)	3(2)	-2(2)	2(2)
C(49)	63(3)	55(3)	36(2)	-3(2)	-2(2)	-10(2)
C(50)	55(3)	53(2)	26(2)	-2(2)	-2(2)	-7(2)
C(51)	48(2)	56(2)	28(2)	1(2)	0(2)	-7(2)

C(52)	45(2)	58(2)	27(2)	0(2)	4(2)	-3(2)
C(53)	44(2)	52(2)	24(2)	0(2)	-2(2)	2(2)
C(54)	51(3)	60(3)	28(2)	1(2)	2(2)	-1(2)
C(55)	63(3)	52(2)	30(2)	1(2)	0(2)	3(2)
C(56)	54(3)	49(2)	37(2)	0(2)	-5(2)	-2(2)
C(57)	39(2)	54(2)	36(2)	-1(2)	0(2)	-4(2)
C(58)	47(2)	63(3)	35(2)	-2(2)	1(2)	7(2)
C(59)	42(2)	79(3)	47(3)	2(2)	6(2)	3(2)
C(60)	48(3)	98(4)	60(3)	13(3)	12(2)	-3(3)
C(61)	51(3)	83(4)	51(3)	-7(3)	2(2)	-4(3)
C(62)	53(3)	95(4)	61(3)	-7(3)	13(3)	14(3)
C(63)	39(2)	59(3)	31(2)	4(2)	-1(2)	2(2)
C(64)	40(2)	56(2)	28(2)	2(2)	-2(2)	3(2)
C(65)	40(2)	67(3)	34(2)	2(2)	3(2)	2(2)
C(66)	49(3)	66(3)	41(2)	-2(2)	-3(2)	13(2)
C(67)	50(3)	57(3)	34(2)	-3(2)	-8(2)	4(2)
C(68)	43(2)	60(3)	29(2)	1(2)	-5(2)	0(2)
C(69)	34(2)	59(2)	29(2)	3(2)	-2(2)	5(2)
C(70)	63(3)	78(4)	65(3)	-7(3)	8(3)	16(3)
C(71)	46(2)	62(3)	42(2)	2(2)	-2(2)	-8(2)
C(72)	60(3)	62(3)	43(3)	10(2)	-6(2)	-3(2)
C(73)	50(3)	61(3)	33(2)	4(2)	-7(2)	0(2)
C(74)	47(3)	68(3)	44(3)	-1(2)	-5(2)	3(2)
C(75)	47(3)	84(4)	41(3)	1(2)	0(2)	2(2)
C(76)	52(3)	75(3)	41(2)	-1(2)	-1(2)	-11(2)
C(77)	64(3)	57(3)	31(2)	1(2)	6(2)	-4(2)
C(78)	57(3)	91(4)	46(3)	17(3)	-1(2)	-16(3)
C(79)	63(3)	98(4)	42(3)	15(3)	-2(2)	-17(3)
C(80)	79(4)	112(5)	50(3)	16(3)	4(3)	-22(4)
C(81)	102(5)	125(6)	50(3)	21(4)	11(3)	-33(5)
C(82)	77(4)	110(5)	47(3)	14(3)	10(3)	-15(4)
C(83)	60(3)	98(4)	38(3)	12(3)	11(2)	-2(3)
C(84)	77(4)	75(3)	47(3)	7(2)	25(3)	10(3)
C(85)	105(5)	75(4)	54(3)	3(3)	39(3)	5(3)
C(86)	108(6)	111(6)	108(7)	-20(5)	40(5)	-28(5)
C(87)	157(8)	93(5)	66(4)	1(4)	53(5)	6(5)
C(88)	244(13)	75(4)	61(4)	5(3)	60(6)	15(6)
C(89)	147(8)	88(5)	77(5)	-24(4)	-5(5)	33(5)
S(3)	73(1)	68(1)	38(1)	-10(1)	1(1)	-1(1)
S(4)	55(1)	60(1)	59(1)	-4(1)	12(1)	-4(1)
S(5)	60(1)	78(1)	37(1)	3(1)	12(1)	6(1)
O(17)	122(4)	64(2)	58(2)	-1(2)	21(2)	-3(2)
O(18)	95(3)	77(3)	62(3)	1(2)	-10(2)	5(2)
O(19)	96(3)	105(3)	40(2)	-20(2)	-12(2)	0(3)
O(20)	68(2)	76(2)	75(3)	-17(2)	32(2)	-22(2)
O(21)	87(3)	53(2)	110(4)	-8(2)	22(3)	-2(2)

O(22)	55(2)	93(3)	52(2)	6(2)	5(2)	2(2)
O(23)	62(3)	183(6)	49(2)	32(3)	6(2)	15(3)
O(24)	87(3)	136(4)	48(2)	9(2)	15(2)	-34(3)
O(25)	154(6)	96(4)	79(3)	-5(3)	32(3)	38(4)
O(29)	119(4)	111(4)	92(4)	0(3)	49(3)	16(4)
C(93)	67(4)	137(7)	60(4)	-11(4)	-3(3)	-20(4)
C(94)	51(3)	67(3)	57(3)	9(2)	6(2)	-5(2)
C(95)	66(4)	101(5)	46(3)	2(3)	5(3)	-12(3)
C(97)	123(8)	136(8)	106(7)	-20(6)	33(6)	-12(6)
O(30)	61(5)	127(8)	309(18)	0	68(7)	0
C(98)	48(7)	106(12)	240(30)	-62(15)	10(11)	-7(8)
O(31)	105(5)	199(8)	184(8)	77(7)	55(5)	59(5)
C(99)	600(50)	147(13)	175(16)	39(12)	-20(20)	200(20)
F(1)	66(3)	79(3)	63(3)	12(2)	20(2)	-9(2)
F(2)	46(3)	106(5)	59(5)	9(4)	-2(3)	3(3)
F(3)	65(3)	91(4)	67(3)	-6(3)	17(3)	20(3)
C(91)	49(4)	70(4)	48(4)	6(3)	5(3)	5(3)
S(1)	42(1)	60(1)	42(1)	-2(1)	4(1)	2(1)
O(11)	54(6)	92(10)	40(5)	-6(5)	-4(4)	-16(6)
O(12)	57(3)	66(3)	78(4)	-26(3)	2(3)	6(3)
O(13)	81(5)	59(3)	57(4)	5(3)	17(3)	-8(3)
F(1A)	270(20)	96(9)	220(20)	-1(11)	-161(16)	18(12)
F(2A)	69(9)	122(11)	59(10)	3(9)	-20(8)	-9(9)
F(3A)	118(12)	430(30)	95(13)	103(16)	-27(8)	-103(16)
C(91A)	89(11)	106(9)	94(11)	38(10)	-45(7)	-41(9)
S(1A)	50(2)	69(2)	45(2)	1(2)	6(1)	-1(2)
O(11A)	62(11)	71(13)	50(12)	14(9)	-7(8)	4(10)
O(12A)	146(16)	99(10)	152(17)	-51(11)	-64(14)	44(11)
O(13A)	82(10)	330(30)	63(9)	-26(14)	41(8)	-26(14)
F(4)	82(3)	291(9)	63(3)	-7(4)	22(2)	30(4)
F(5)	105(4)	167(5)	87(3)	26(3)	20(3)	42(3)
F(6)	79(3)	155(5)	142(5)	14(4)	-11(3)	-29(3)
C(92)	66(4)	118(6)	56(4)	0(4)	9(3)	-7(4)
S(2)	61(1)	120(1)	70(1)	-15(1)	16(1)	-8(1)
O(14)	99(4)	131(5)	148(6)	-49(5)	20(4)	-30(4)
O(15)	74(3)	164(5)	63(3)	7(3)	-2(2)	-2(3)
O(16)	113(4)	123(4)	78(3)	-5(3)	27(3)	-11(3)
F(7)	68(2)	123(3)	57(2)	-21(2)	16(2)	-16(2)
F(8)	104(4)	272(9)	86(3)	12(4)	-1(3)	83(5)
F(9)	93(3)	168(5)	121(4)	-41(4)	27(3)	-67(3)
F(10)	75(2)	106(3)	60(2)	15(2)	10(2)	-26(2)
F(11)	62(2)	102(3)	69(2)	14(2)	-11(2)	-10(2)
F(12)	74(2)	79(2)	61(2)	-14(2)	17(2)	-5(2)
F(13)	70(2)	127(3)	45(2)	11(2)	11(2)	-8(2)
F(14)	229(7)	99(3)	82(3)	-16(2)	79(4)	-6(4)
F(15)	63(2)	213(5)	45(2)	13(3)	1(2)	-13(3)

F(16)	90(3)	136(4)	78(3)	4(3)	18(2)	-13(3)
F(17)	110(4)	159(5)	71(3)	-1(3)	6(3)	3(3)
F(18)	74(3)	148(4)	68(3)	-9(3)	2(2)	3(3)
C(96)	84(2)	184(5)	73(2)	15(2)	14(2)	7(2)
S(6)	76(2)	135(3)	66(2)	19(2)	23(1)	18(2)
O(26)	124(5)	159(5)	91(4)	1(3)	46(3)	-9(4)
O(27)	87(4)	155(5)	120(5)	30(4)	31(3)	25(3)
O(28)	131(5)	159(6)	110(5)	-20(4)	51(4)	-7(4)
F(16A)	124(5)	159(5)	91(4)	1(3)	46(3)	-9(4)
F(17A)	87(4)	155(5)	120(5)	30(4)	31(3)	25(3)
F(18A)	131(5)	159(6)	110(5)	-20(4)	51(4)	-7(4)
C(96A)	76(2)	135(3)	66(2)	19(2)	23(1)	18(2)
S(6A)	84(2)	184(5)	73(2)	15(2)	14(2)	7(2)
O(26A)	90(3)	136(4)	78(3)	4(3)	18(2)	-13(3)
O(27A)	110(4)	159(5)	71(3)	-1(3)	6(3)	3(3)
O(28A)	74(3)	148(4)	68(3)	-9(3)	2(2)	3(3)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **0**.

	x	y	z	U(eq)
H(2O)	7547	5675	3395	61
H(4O)	6907	9112	3719	55
H(7)	3980	4424	1807	71
H(9O1)	2723	1692	1639	67
H(90A)	2252	2632	1957	274
H(90B)	2697	2206	2250	274
H(90C)	2777	3421	2072	274
H(9O2)	3015	3488	1867	95
H(90D)	2270	2894	1964	136
H(90E)	2431	1589	1870	136
H(90F)	2590	2037	2230	136
H(1A)	5767	6830	2667	68
H(5A)	6710	10735	4974	81
H(9A)	2126	5632	762	59
H(13A)	4111	2382	2992	82
H(1)	5789	8421	3727	65
H(2)	4999	8598	3932	72
H(3)	4696	6993	4196	76
H(4)	5172	5198	4216	70
H(6A)	5992	4121	4109	62
H(6B)	5776	4184	3734	62
H(7A)	6509	3024	3688	60
H(7B)	7064	3669	3655	60
H(9)	6480	2436	3116	73
H(10)	6217	3024	2576	83
H(11)	5993	4988	2463	82
H(15A)	5927	10664	2970	98
H(15B)	6441	9944	3146	98
H(15C)	5874	9832	3267	98
H(16A)	5106	8852	2949	96
H(16B)	5170	8160	2630	96
H(16C)	5154	9573	2632	96
H(17A)	6110	9815	2476	108
H(17B)	6011	8439	2402	108
H(17C)	6555	8868	2624	108
H(18A)	6940	3785	4241	55
H(18B)	6815	5128	4323	55
H(20)	7843	3307	4185	65
H(22)	8901	5849	4050	67

H(25A)	9106	3519	4328	131
H(25B)	9095	3696	3954	131
H(25C)	8714	2726	4077	131
H(26A)	8017	8063	3810	61
H(26B)	8634	7846	3970	61
H(27A)	8829	7555	4525	62
H(27B)	8606	8551	4735	62
H(29)	8846	5942	4912	60
H(30)	8357	4639	5181	64
H(31)	7423	4933	5158	64
H(32)	7010	6495	4858	57
H(33A)	8138	9949	4041	76
H(33B)	8680	9793	4296	76
H(35)	8632	11623	4576	88
H(36)	8209	12761	4917	97
H(37)	7384	12189	5023	90
H(41A)	6456	9328	5364	137
H(41B)	5818	9265	5354	137
H(41C)	6086	10447	5246	137
H(42A)	5653	10676	4715	119
H(42B)	5229	9668	4764	119
H(42C)	5550	9594	4470	119
H(43A)	5802	7550	4676	110
H(43B)	5555	7723	4995	110
H(43C)	6176	7369	5016	110
H(44A)	7364	7104	2949	115
H(44B)	7914	7236	3198	115
H(44C)	7405	8039	3234	115
H(45A)	6296	10185	4106	84
H(45B)	6377	10654	3762	84
H(45C)	6801	11008	4072	84
H(47)	2547	7380	654	63
H(48)	3358	8262	579	69
H(49)	4176	7252	722	63
H(51A)	4628	5357	897	54
H(51B)	4487	5434	1249	54
H(52A)	4539	3150	649	52
H(52B)	4063	4080	543	52
H(54)	4140	1496	320	56
H(55)	3453	73	215	59
H(56)	2716	183	483	58
H(57)	2688	1683	857	52
H(60A)	1900	2377	1243	103
H(60B)	1296	2803	1251	103
H(60C)	1790	3391	1486	103
H(61A)	1595	4074	527	94

H(61B)	1163	3260	661	94
H(61C)	1762	2781	661	94
H(62A)	1493	5397	1283	104
H(62B)	993	4802	1054	104
H(62C)	1395	5658	908	104
H(63A)	5051	3430	1157	52
H(63B)	4741	3566	1455	52
H(65)	5235	1502	1009	57
H(67)	4319	-1254	1173	59
H(70A)	5107	-1644	948	103
H(70B)	5589	-741	1068	103
H(70C)	5237	-600	720	103
H(71A)	3274	198	1404	62
H(71B)	3572	-1060	1434	62
H(72A)	4353	-1288	1835	68
H(72B)	4298	-867	2188	68
H(74)	5289	-840	1827	65
H(75)	5956	610	1807	69
H(76)	5796	2547	1970	68
H(77)	4962	2992	2113	61
H(78A)	3364	-1469	1987	79
H(78B)	2975	-364	1884	79
H(80)	3077	-1651	2516	97
H(81)	3226	-1010	3044	111
H(82)	3642	836	3171	94
H(86A)	5032	4903	2968	160
H(86B)	5009	4193	2641	160
H(86C)	4969	3495	2963	160
H(87A)	4266	4111	3259	152
H(87B)	3672	4255	3057	152
H(87C)	4051	5389	3137	152
H(88A)	4291	6112	2650	184
H(88B)	3721	5504	2523	184
H(88C)	4226	5242	2350	184
H(89A)	3616	6402	1584	160
H(89B)	3522	5941	1926	160
H(89C)	3072	5718	1618	160
H(29O)	7800(50)	3770(40)	3347(8)	156
H(97A)	7659	5085	2789	180
H(97B)	7521	3709	2808	180
H(97C)	8135	4130	2834	180
H(30A)	2515	5806	2414	242
H(98A)	2832	3734	2334	197
H(98B)	3164	4230	2662	197
H(98C)	3184	4912	2335	197
H(31A)	2347	7098	3179	239

H(99A)	3118	6317	3193	477
H(99B)	3061	6555	2818	477
H(99C)	2693	5575	2947	477

Table S6. Torsion angles [deg] for **0**.

C(5)-N(2)-C(1)-C(2)	-0.9(8)
Fe(1)-N(2)-C(1)-C(2)	179.4(4)
N(2)-C(1)-C(2)-C(3)	3.7(9)
C(1)-C(2)-C(3)-C(4)	-2.4(9)
C(2)-C(3)-C(4)-C(5)	-1.4(9)
C(1)-N(2)-C(5)-C(4)	-3.1(7)
Fe(1)-N(2)-C(5)-C(4)	176.6(4)
C(1)-N(2)-C(5)-C(6)	171.7(5)
Fe(1)-N(2)-C(5)-C(6)	-8.7(5)
C(3)-C(4)-C(5)-N(2)	4.3(8)
C(3)-C(4)-C(5)-C(6)	-170.2(5)
C(7)-N(4)-C(6)-C(5)	-144.6(4)
C(18)-N(4)-C(6)-C(5)	93.5(5)
Fe(1)-N(4)-C(6)-C(5)	-27.5(5)
N(2)-C(5)-C(6)-N(4)	25.3(6)
C(4)-C(5)-C(6)-N(4)	-159.9(5)
C(6)-N(4)-C(7)-C(8)	79.0(5)
C(18)-N(4)-C(7)-C(8)	-159.3(4)
Fe(1)-N(4)-C(7)-C(8)	-38.7(5)
C(12)-N(3)-C(8)-C(9)	0.4(8)
Fe(1)-N(3)-C(8)-C(9)	-163.1(4)
C(12)-N(3)-C(8)-C(7)	176.4(5)
Fe(1)-N(3)-C(8)-C(7)	13.0(6)
N(4)-C(7)-C(8)-N(3)	18.3(6)
N(4)-C(7)-C(8)-C(9)	-165.5(5)
N(3)-C(8)-C(9)-C(10)	2.1(8)
C(7)-C(8)-C(9)-C(10)	-173.8(5)
C(8)-C(9)-C(10)-C(11)	-2.5(9)
C(9)-C(10)-C(11)-C(12)	0.3(10)
C(8)-N(3)-C(12)-C(11)	-2.6(8)
Fe(1)-N(3)-C(12)-C(11)	158.5(4)
C(8)-N(3)-C(12)-N(1)	176.8(5)
Fe(1)-N(3)-C(12)-N(1)	-22.1(7)
C(10)-C(11)-C(12)-N(3)	2.3(9)
C(10)-C(11)-C(12)-N(1)	-177.1(6)
C(13)-N(1)-C(12)-N(3)	20.5(9)
C(13)-N(1)-C(12)-C(11)	-160.1(6)
Fe(1)-O(1)-C(13)-N(1)	-10.9(8)
Fe(1)-O(1)-C(13)-C(14)	171.3(4)
C(12)-N(1)-C(13)-O(1)	-3.5(9)
C(12)-N(1)-C(13)-C(14)	174.4(5)
O(1)-C(13)-C(14)-C(15)	-3.8(7)
N(1)-C(13)-C(14)-C(15)	178.3(5)

O(1)-C(13)-C(14)-C(17)	116.2(5)
N(1)-C(13)-C(14)-C(17)	-61.7(6)
O(1)-C(13)-C(14)-C(16)	-124.0(5)
N(1)-C(13)-C(14)-C(16)	58.1(6)
C(7)-N(4)-C(18)-C(19)	69.8(5)
C(6)-N(4)-C(18)-C(19)	-168.2(4)
Fe(1)-N(4)-C(18)-C(19)	-48.7(4)
N(4)-C(18)-C(19)-C(24)	68.2(5)
N(4)-C(18)-C(19)-C(20)	-111.0(5)
C(24)-C(19)-C(20)-C(21)	1.1(7)
C(18)-C(19)-C(20)-C(21)	-179.7(4)
C(19)-C(20)-C(21)-C(22)	2.8(7)
C(19)-C(20)-C(21)-C(25)	-177.2(5)
C(20)-C(21)-C(22)-C(23)	-3.4(7)
C(25)-C(21)-C(22)-C(23)	176.6(5)
C(21)-C(22)-C(23)-C(24)	0.1(7)
C(21)-C(22)-C(23)-C(26)	177.7(4)
Fe(2)-O(5)-C(24)-C(19)	119.6(4)
Fe(1)-O(5)-C(24)-C(19)	-63.6(4)
Fe(2)-O(5)-C(24)-C(23)	-59.3(4)
Fe(1)-O(5)-C(24)-C(23)	117.6(3)
C(20)-C(19)-C(24)-O(5)	176.6(4)
C(18)-C(19)-C(24)-O(5)	-2.6(6)
C(20)-C(19)-C(24)-C(23)	-4.5(6)
C(18)-C(19)-C(24)-C(23)	176.3(4)
C(22)-C(23)-C(24)-O(5)	-177.2(4)
C(26)-C(23)-C(24)-O(5)	5.2(6)
C(22)-C(23)-C(24)-C(19)	4.0(6)
C(26)-C(23)-C(24)-C(19)	-173.7(4)
C(22)-C(23)-C(26)-N(8)	-113.2(5)
C(24)-C(23)-C(26)-N(8)	64.4(5)
C(33)-N(8)-C(26)-C(23)	179.2(4)
C(27)-N(8)-C(26)-C(23)	56.2(5)
Fe(2)-N(8)-C(26)-C(23)	-64.0(4)
C(33)-N(8)-C(27)-C(28)	144.6(5)
C(26)-N(8)-C(27)-C(28)	-91.9(5)
Fe(2)-N(8)-C(27)-C(28)	28.5(5)
C(32)-N(7)-C(28)-C(29)	0.1(6)
Fe(2)-N(7)-C(28)-C(29)	-161.9(3)
C(32)-N(7)-C(28)-C(27)	-176.0(4)
Fe(2)-N(7)-C(28)-C(27)	22.0(5)
N(8)-C(27)-C(28)-N(7)	-34.6(6)
N(8)-C(27)-C(28)-C(29)	149.3(4)
N(7)-C(28)-C(29)-C(30)	-0.7(7)
C(27)-C(28)-C(29)-C(30)	175.1(4)
C(28)-C(29)-C(30)-C(31)	0.4(7)

C(29)-C(30)-C(31)-C(32)	0.6(7)
C(28)-N(7)-C(32)-C(31)	1.0(7)
Fe(2)-N(7)-C(32)-C(31)	161.1(4)
C(30)-C(31)-C(32)-N(7)	-1.4(7)
C(26)-N(8)-C(33)-C(34)	163.1(4)
C(27)-N(8)-C(33)-C(34)	-73.7(5)
Fe(2)-N(8)-C(33)-C(34)	44.3(4)
C(38)-N(6)-C(34)-C(35)	1.8(7)
Fe(2)-N(6)-C(34)-C(35)	-177.5(4)
C(38)-N(6)-C(34)-C(33)	-176.5(4)
Fe(2)-N(6)-C(34)-C(33)	4.2(5)
N(8)-C(33)-C(34)-N(6)	-33.8(6)
N(8)-C(33)-C(34)-C(35)	147.9(5)
N(6)-C(34)-C(35)-C(36)	-2.2(8)
C(33)-C(34)-C(35)-C(36)	176.0(5)
C(34)-C(35)-C(36)-C(37)	0.0(9)
C(35)-C(36)-C(37)-C(38)	2.3(9)
C(34)-N(6)-C(38)-N(5)	-178.9(4)
Fe(2)-N(6)-C(38)-N(5)	0.3(6)
C(34)-N(6)-C(38)-C(37)	0.6(7)
Fe(2)-N(6)-C(38)-C(37)	179.8(4)
C(39)-N(5)-C(38)-N(6)	-0.1(8)
C(39)-N(5)-C(38)-C(37)	-179.6(5)
C(36)-C(37)-C(38)-N(6)	-2.7(8)
C(36)-C(37)-C(38)-N(5)	176.8(5)
Fe(2)-O(3)-C(39)-N(5)	6.8(7)
Fe(2)-O(3)-C(39)-C(40)	-174.4(3)
C(38)-N(5)-C(39)-O(3)	-3.3(8)
C(38)-N(5)-C(39)-C(40)	177.8(5)
O(3)-C(39)-C(40)-C(43)	24.7(6)
N(5)-C(39)-C(40)-C(43)	-156.4(5)
O(3)-C(39)-C(40)-C(41)	146.6(5)
N(5)-C(39)-C(40)-C(41)	-34.5(7)
O(3)-C(39)-C(40)-C(42)	-93.6(6)
N(5)-C(39)-C(40)-C(42)	85.3(6)
C(50)-N(10)-C(46)-C(47)	-2.8(6)
Fe(3)-N(10)-C(46)-C(47)	171.6(3)
C(50)-N(10)-C(46)-N(9)	176.7(4)
Fe(3)-N(10)-C(46)-N(9)	-8.9(6)
C(58)-N(9)-C(46)-N(10)	15.5(7)
C(58)-N(9)-C(46)-C(47)	-165.0(5)
N(10)-C(46)-C(47)-C(48)	2.9(7)
N(9)-C(46)-C(47)-C(48)	-176.6(4)
C(46)-C(47)-C(48)-C(49)	-0.3(7)
C(47)-C(48)-C(49)-C(50)	-2.3(7)
C(46)-N(10)-C(50)-C(49)	0.0(6)

Fe(3)-N(10)-C(50)-C(49)	-175.2(3)
C(46)-N(10)-C(50)-C(51)	177.6(4)
Fe(3)-N(10)-C(50)-C(51)	2.4(5)
C(48)-C(49)-C(50)-N(10)	2.5(7)
C(48)-C(49)-C(50)-C(51)	-174.9(4)
C(52)-N(12)-C(51)-C(50)	73.5(5)
C(63)-N(12)-C(51)-C(50)	-163.7(4)
Fe(3)-N(12)-C(51)-C(50)	-45.1(4)
N(10)-C(50)-C(51)-N(12)	29.4(5)
C(49)-C(50)-C(51)-N(12)	-153.0(4)
C(51)-N(12)-C(52)-C(53)	-145.3(4)
C(63)-N(12)-C(52)-C(53)	91.8(4)
Fe(3)-N(12)-C(52)-C(53)	-28.4(4)
C(57)-N(11)-C(53)-C(54)	-0.9(6)
Fe(3)-N(11)-C(53)-C(54)	161.8(3)
C(57)-N(11)-C(53)-C(52)	176.1(4)
Fe(3)-N(11)-C(53)-C(52)	-21.1(4)
N(12)-C(52)-C(53)-N(11)	34.0(5)
N(12)-C(52)-C(53)-C(54)	-148.9(4)
N(11)-C(53)-C(54)-C(55)	2.1(6)
C(52)-C(53)-C(54)-C(55)	-174.9(4)
C(53)-C(54)-C(55)-C(56)	-1.2(6)
C(54)-C(55)-C(56)-C(57)	-0.7(6)
C(53)-N(11)-C(57)-C(56)	-1.1(6)
Fe(3)-N(11)-C(57)-C(56)	-162.1(3)
C(55)-C(56)-C(57)-N(11)	1.9(7)
Fe(3)-O(6)-C(58)-N(9)	-19.9(7)
Fe(3)-O(6)-C(58)-C(59)	158.4(4)
C(46)-N(9)-C(58)-O(6)	-1.6(8)
C(46)-N(9)-C(58)-C(59)	-180.0(5)
O(6)-C(58)-C(59)-C(61)	-107.6(5)
N(9)-C(58)-C(59)-C(61)	70.8(6)
O(6)-C(58)-C(59)-C(60)	11.6(7)
N(9)-C(58)-C(59)-C(60)	-170.1(5)
O(6)-C(58)-C(59)-C(62)	131.9(5)
N(9)-C(58)-C(59)-C(62)	-49.7(6)
C(51)-N(12)-C(63)-C(64)	179.9(4)
C(52)-N(12)-C(63)-C(64)	-57.4(5)
Fe(3)-N(12)-C(63)-C(64)	62.9(4)
N(12)-C(63)-C(64)-C(69)	-65.2(5)
N(12)-C(63)-C(64)-C(65)	113.7(4)
C(69)-C(64)-C(65)-C(66)	0.7(6)
C(63)-C(64)-C(65)-C(66)	-178.3(4)
C(64)-C(65)-C(66)-C(67)	1.5(7)
C(64)-C(65)-C(66)-C(70)	-177.0(4)
C(65)-C(66)-C(67)-C(68)	-2.5(7)

C(70)-C(66)-C(67)-C(68)	175.9(4)
C(66)-C(67)-C(68)-C(69)	1.3(6)
C(66)-C(67)-C(68)-C(71)	-173.2(4)
Fe(3)-O(10)-C(69)-C(68)	-123.4(3)
Fe(4)-O(10)-C(69)-C(68)	57.6(4)
Fe(3)-O(10)-C(69)-C(64)	57.5(4)
Fe(4)-O(10)-C(69)-C(64)	-121.6(3)
C(67)-C(68)-C(69)-O(10)	-178.2(4)
C(71)-C(68)-C(69)-O(10)	-3.6(6)
C(67)-C(68)-C(69)-C(64)	1.0(6)
C(71)-C(68)-C(69)-C(64)	175.5(4)
C(65)-C(64)-C(69)-O(10)	177.3(4)
C(63)-C(64)-C(69)-O(10)	-3.8(6)
C(65)-C(64)-C(69)-C(68)	-1.9(6)
C(63)-C(64)-C(69)-C(68)	177.0(4)
C(78)-N(16)-C(71)-C(68)	-177.2(5)
C(72)-N(16)-C(71)-C(68)	-55.3(5)
Fe(4)-N(16)-C(71)-C(68)	63.5(4)
C(67)-C(68)-C(71)-N(16)	110.1(5)
C(69)-C(68)-C(71)-N(16)	-64.4(5)
C(78)-N(16)-C(72)-C(73)	-148.9(5)
C(71)-N(16)-C(72)-C(73)	88.5(5)
Fe(4)-N(16)-C(72)-C(73)	-32.9(5)
C(77)-N(15)-C(73)-C(74)	0.3(6)
Fe(4)-N(15)-C(73)-C(74)	156.2(4)
C(77)-N(15)-C(73)-C(72)	179.2(4)
Fe(4)-N(15)-C(73)-C(72)	-24.9(5)
N(16)-C(72)-C(73)-N(15)	40.4(6)
N(16)-C(72)-C(73)-C(74)	-140.7(5)
N(15)-C(73)-C(74)-C(75)	-2.2(7)
C(72)-C(73)-C(74)-C(75)	179.0(4)
C(73)-C(74)-C(75)-C(76)	3.0(7)
C(74)-C(75)-C(76)-C(77)	-2.0(7)
C(73)-N(15)-C(77)-C(76)	0.7(7)
Fe(4)-N(15)-C(77)-C(76)	-152.9(4)
C(75)-C(76)-C(77)-N(15)	0.1(7)
C(71)-N(16)-C(78)-C(79)	-167.1(5)
C(72)-N(16)-C(78)-C(79)	70.4(6)
Fe(4)-N(16)-C(78)-C(79)	-45.4(5)
C(83)-N(14)-C(79)-C(80)	1.9(9)
Fe(4)-N(14)-C(79)-C(80)	-176.6(6)
C(83)-N(14)-C(79)-C(78)	-177.7(5)
Fe(4)-N(14)-C(79)-C(78)	3.8(7)
N(16)-C(78)-C(79)-N(14)	28.3(8)
N(16)-C(78)-C(79)-C(80)	-151.3(6)
N(14)-C(79)-C(80)-C(81)	-1.7(11)

C(78)-C(79)-C(80)-C(81)	177.9(7)
C(79)-C(80)-C(81)-C(82)	0.4(13)
C(80)-C(81)-C(82)-C(83)	0.6(12)
C(79)-N(14)-C(83)-C(82)	-0.9(9)
Fe(4)-N(14)-C(83)-C(82)	177.4(5)
C(79)-N(14)-C(83)-N(13)	177.0(6)
Fe(4)-N(14)-C(83)-N(13)	-4.7(8)
C(81)-C(82)-C(83)-N(14)	-0.4(11)
C(81)-C(82)-C(83)-N(13)	-178.4(7)
C(84)-N(13)-C(83)-N(14)	19.2(10)
C(84)-N(13)-C(83)-C(82)	-162.8(7)
Fe(4)-O(8)-C(84)-N(13)	-16.0(10)
Fe(4)-O(8)-C(84)-C(85)	163.1(5)
C(83)-N(13)-C(84)-O(8)	-9.8(11)
C(83)-N(13)-C(84)-C(85)	171.0(6)
O(8)-C(84)-C(85)-C(86)	-95.0(8)
N(13)-C(84)-C(85)-C(86)	84.2(7)
O(8)-C(84)-C(85)-C(88)	23.0(9)
N(13)-C(84)-C(85)-C(88)	-157.8(7)
O(8)-C(84)-C(85)-C(87)	143.0(7)
N(13)-C(84)-C(85)-C(87)	-37.8(9)
O(19)-S(3)-C(93)-F(9)	-52.6(6)
O(17)-S(3)-C(93)-F(9)	-177.9(5)
O(18)-S(3)-C(93)-F(9)	66.6(6)
O(19)-S(3)-C(93)-F(7)	-177.3(6)
O(17)-S(3)-C(93)-F(7)	57.4(7)
O(18)-S(3)-C(93)-F(7)	-58.1(7)
O(19)-S(3)-C(93)-F(8)	63.2(7)
O(17)-S(3)-C(93)-F(8)	-62.1(6)
O(18)-S(3)-C(93)-F(8)	-177.6(6)
O(21)-S(4)-C(94)-F(12)	-172.4(4)
O(20)-S(4)-C(94)-F(12)	67.2(4)
O(22)-S(4)-C(94)-F(12)	-52.9(4)
O(21)-S(4)-C(94)-F(10)	-52.5(5)
O(20)-S(4)-C(94)-F(10)	-173.0(4)
O(22)-S(4)-C(94)-F(10)	67.0(4)
O(21)-S(4)-C(94)-F(11)	68.2(4)
O(20)-S(4)-C(94)-F(11)	-52.2(4)
O(22)-S(4)-C(94)-F(11)	-172.3(4)
O(25)-S(5)-C(95)-F(13)	64.6(6)
O(23)-S(5)-C(95)-F(13)	-55.2(6)
O(24)-S(5)-C(95)-F(13)	-174.0(5)
O(25)-S(5)-C(95)-F(14)	-177.4(6)
O(23)-S(5)-C(95)-F(14)	62.8(6)
O(24)-S(5)-C(95)-F(14)	-56.0(6)
O(25)-S(5)-C(95)-F(15)	-56.0(6)

O(23)-S(5)-C(95)-F(15)	-175.8(5)
O(24)-S(5)-C(95)-F(15)	65.4(6)
F(2)-C(91)-S(1)-O(11)	177.6(12)
F(3)-C(91)-S(1)-O(11)	55.9(10)
F(1)-C(91)-S(1)-O(11)	-62.9(10)
F(2)-C(91)-S(1)-O(12)	-61.9(10)
F(3)-C(91)-S(1)-O(12)	176.4(6)
F(1)-C(91)-S(1)-O(12)	57.6(7)
F(2)-C(91)-S(1)-O(13)	58.7(9)
F(3)-C(91)-S(1)-O(13)	-63.0(6)
F(1)-C(91)-S(1)-O(13)	178.2(6)
F(3A)-C(91A)-S(1A)-O(12A)	-63.7(19)
F(1A)-C(91A)-S(1A)-O(12A)	172.4(19)
F(2A)-C(91A)-S(1A)-O(12A)	54(2)
F(3A)-C(91A)-S(1A)-O(13A)	175.6(18)
F(1A)-C(91A)-S(1A)-O(13A)	51.7(19)
F(2A)-C(91A)-S(1A)-O(13A)	-67(2)
F(3A)-C(91A)-S(1A)-O(11A)	58(2)
F(1A)-C(91A)-S(1A)-O(11A)	-66(2)
F(2A)-C(91A)-S(1A)-O(11A)	176(2)
F(4)-C(92)-S(2)-O(16)	173.9(6)
F(6)-C(92)-S(2)-O(16)	-64.8(6)
F(5)-C(92)-S(2)-O(16)	53.8(6)
F(4)-C(92)-S(2)-O(14)	55.6(7)
F(6)-C(92)-S(2)-O(14)	176.9(6)
F(5)-C(92)-S(2)-O(14)	-64.4(7)
F(4)-C(92)-S(2)-O(15)	-64.8(7)
F(6)-C(92)-S(2)-O(15)	56.5(6)
F(5)-C(92)-S(2)-O(15)	175.1(6)

Symmetry transformations used to generate equivalent atoms:

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

Table S7. Hydrogen bonds for **0** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(29)	0.95	1.80	2.663(7)	149.4
O(4)-H(4O)...O(1)	0.95	2.60	3.352(4)	136.1
O(31)-H(31A)...O(14)	0.84	2.37	2.942(13)	125.9
O(30)-H(30A)...O(31)#1	0.84	2.40	3.191(14)	157.3
O(4)-H(4O)...O(24)#2	0.95	2.15	2.720(5)	117.1
O(7)-H(7)...O(8)	0.95	2.56	3.271(5)	131.3
O(7)-H(7)...O(17)	0.95	2.30	2.956(7)	125.6
O(9A ^b)-H(9O2 ^b)...O(7)	0.95	2.52	3.223(11)	131.1
N(1)-H(1A)...O(19)	0.88	2.12	2.988(6)	168.8
N(5)-H(5A)...O(12 ^a)#2	0.88	2.30	2.882(8)	124.1
N(5)-H(5A)...O(12A ^b)#2	0.88	2.09	2.903(17)	153.8
N(9)-H(9A)...O(11A ^b)#3	0.88	2.05	2.881(17)	157.3
N(13)-H(13A)...O(22)	0.88	2.04	2.869(6)	157.7
O(29)-H(29O)...O(25)	0.92(2)	1.92(4)	2.779(9)	156(5)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, y, -z+1/2$ #2 $x, y+1, z$ #3 $x-1/2, -y+1, z-1/2$

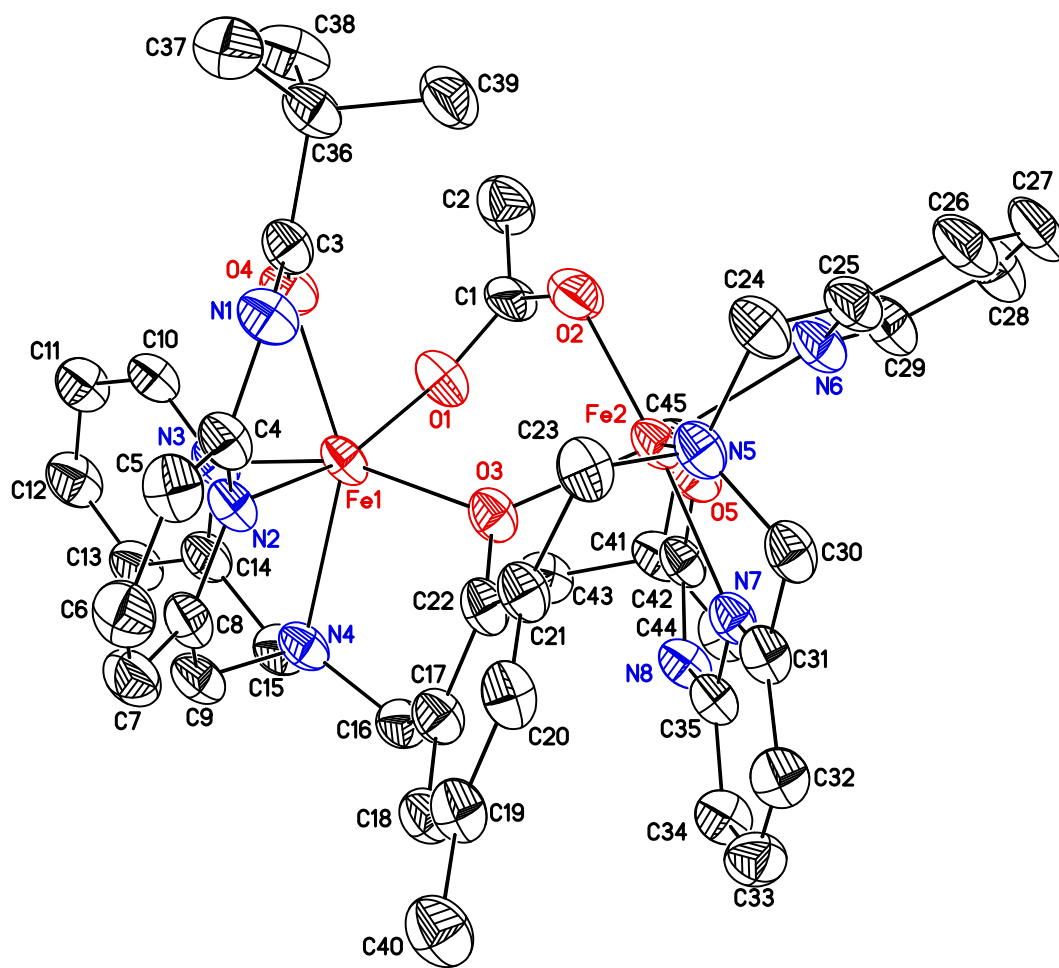


Figure S24. Crystal structure of complex **1** with ellipsoids drawn at 50% probability and atomic labeling scheme as indicated. Solvent molecules and hydrogen atoms are omitted for clarity.

Table S8. Crystal data and structure refinement for complex **1** (CCDC #2084745).

Identification Code	hd2135
Empirical formula	C ₄₉ H ₅₈ C ₁₄ F ₆ Fe ₂ N ₈ O ₁₁ S ₂
Formula weight	1366.65
Temperature	85(2) K
Wavelength	1.54184 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.2466(4) Å alpha = 101.362(4) deg. b = 12.2933(6) Å beta = 91.443(3) deg. c = 20.4907(10) Å gamma = 99.817(3) deg.
Volume	2974.6(2) Å ³
Z, Calculated density	2, 1.526 Mg/m ³
Absorption coefficient	6.929 mm ⁻¹
F(000)	1404
Crystal size	0.150 x 0.070 x 0.020 mm
Theta range for data collection	2.203 to 70.138 deg.
Limiting indices	-14<=h<=14, -14<=k<=14, -24<=l<=24
Reflections collected / unique	44463 / 10747 [R(int) = 0.0713]
Completeness to theta = 67.684	97.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.67427
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10747 / 1 / 754
Goodness-of-fit on F ²	1.082
Final R indices [I>2sigma(I)]	R1 = 0.0734, wR2 = 0.2015
R indices (all data)	R1 = 0.0808, wR2 = 0.2131
Extinction coefficient	0.00064(15)
Largest diff. peak and hole	1.365 and -0.919 e x Å ⁻³

Table S9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	1507(1)	7049(1)	6896(1)	30(1)
Fe(2)	2276(1)	5888(1)	8311(1)	32(1)
O(1)	439(3)	7119(3)	7680(2)	44(1)
O(2)	584(3)	5496(3)	7997(2)	46(1)
O(3)	2632(2)	6520(2)	7459(1)	34(1)
O(4)	284(2)	5675(2)	6366(2)	38(1)
O(5)	1876(2)	7141(2)	9066(2)	37(1)
O(6)	4187(3)	1660(3)	8391(2)	59(1)
O(7)	4572(3)	807(3)	9323(2)	57(1)
O(8)	5911(3)	971(3)	8479(2)	48(1)
O(9)	2989(3)	1768(3)	6352(2)	55(1)
O(10)	2221(3)	2501(3)	5473(2)	55(1)
O(11)	4215(3)	2904(3)	5737(2)	44(1)
N(1)	1446(3)	4618(3)	5811(2)	36(1)
N(2)	2346(3)	6517(3)	5990(2)	31(1)
N(3)	640(3)	8248(3)	6551(2)	34(1)
N(4)	2822(3)	8572(3)	6882(2)	33(1)
N(5)	3275(3)	4567(3)	7934(2)	34(1)
N(6)	1953(3)	4696(3)	8976(2)	40(1)
N(7)	3943(3)	6688(3)	8731(2)	32(1)
N(8)	3444(3)	8465(3)	9141(2)	34(1)
C(1)	19(4)	6274(4)	7931(3)	56(2)
C(2)	-1157(4)	6083(5)	8040(3)	54(1)
C(3)	476(3)	4740(3)	6083(2)	33(1)
C(4)	2305(3)	5449(4)	5682(2)	34(1)
C(5)	3059(4)	5096(4)	5222(2)	40(1)
C(6)	3883(4)	5915(5)	5071(2)	46(1)
C(7)	3929(4)	7028(4)	5373(2)	43(1)
C(8)	3166(4)	7305(4)	5840(2)	36(1)
C(9)	3164(4)	8489(4)	6191(2)	38(1)
C(10)	-357(4)	7999(4)	6228(2)	37(1)
C(11)	-883(4)	8795(4)	6035(3)	44(1)
C(12)	-350(4)	9908(4)	6182(3)	49(1)
C(13)	686(4)	10184(4)	6527(3)	42(1)
C(14)	1154(4)	9339(4)	6704(2)	38(1)
C(15)	2273(4)	9560(3)	7080(2)	40(1)
C(16)	3794(3)	8646(3)	7353(2)	35(1)
C(17)	4304(4)	7605(3)	7188(2)	36(1)

C(18)	5366(4)	7638(4)	6964(2)	37(1)
C(19)	5819(4)	6662(4)	6784(2)	40(1)
C(20)	5192(4)	5648(4)	6855(2)	38(1)
C(21)	4134(4)	5582(3)	7096(2)	35(1)
C(22)	3680(4)	6569(3)	7252(2)	33(1)
C(23)	3477(4)	4500(4)	7216(2)	38(1)
C(24)	2610(4)	3496(3)	8044(2)	43(1)
C(25)	2223(4)	3672(4)	8745(2)	40(1)
C(26)	2163(4)	2863(4)	9128(3)	51(1)
C(27)	1782(4)	3096(4)	9765(3)	53(1)
C(28)	1474(5)	4111(5)	9994(3)	54(1)
C(29)	1580(4)	4905(4)	9588(2)	44(1)
C(30)	4331(4)	4829(4)	8339(2)	36(1)
C(31)	4740(4)	6073(4)	8550(2)	35(1)
C(32)	5850(4)	6549(4)	8572(2)	40(1)
C(33)	6149(4)	7707(4)	8777(2)	45(1)
C(34)	5354(4)	8347(4)	8968(2)	40(1)
C(35)	4262(3)	7808(3)	8941(2)	33(1)
C(36)	-390(4)	3681(4)	6055(2)	38(1)
C(37)	-464(4)	2872(4)	5391(3)	51(1)
C(38)	-1520(4)	4041(4)	6190(3)	54(1)
C(39)	-57(5)	3127(4)	6624(3)	49(1)
C(40)	6964(4)	6735(4)	6518(3)	49(1)
C(41)	2354(4)	8122(3)	9223(2)	35(1)
C(42)	1696(4)	9046(4)	9516(3)	42(1)
C(43)	1499(4)	9679(4)	8958(3)	46(1)
C(44)	2301(5)	9843(4)	10119(3)	50(1)
C(45)	555(4)	8461(4)	9684(3)	53(1)
C(46)	5665(4)	2771(4)	9304(2)	44(1)
C(47)	3297(4)	910(4)	5141(2)	38(1)
C(48)	8371(7)	668(9)	7917(4)	97(3)
C(49)	4355(5)	8023(5)	2971(3)	59(1)
S(1)	5013(1)	1400(1)	8815(1)	43(1)
S(2)	3174(1)	2165(1)	5742(1)	39(1)
Cl(1)	9472(2)	1766(2)	8270(1)	114(1)
Cl(2)	8723(2)	-689(2)	7934(1)	86(1)
Cl(3)	3738(1)	9089(1)	3446(1)	69(1)
Cl(4)	3396(2)	6811(1)	2631(1)	75(1)
F(1)	4943(3)	3258(2)	9690(2)	58(1)
F(2)	6510(3)	2688(3)	9696(2)	56(1)
F(3)	6058(3)	3481(2)	8916(2)	55(1)
F(4)	4129(2)	436(2)	5322(2)	52(1)
F(5)	3504(2)	1148(2)	4537(1)	47(1)
F(6)	2376(2)	127(2)	5064(1)	46(1)

Table S10. Bond lengths [\AA] and angles [deg] for **1**.

Fe(1)-O(3)	2.042(3)
Fe(1)-O(1)	2.094(3)
Fe(1)-O(4)	2.148(3)
Fe(1)-N(3)	2.170(4)
Fe(1)-N(2)	2.186(3)
Fe(1)-N(4)	2.257(3)
Fe(2)-O(3)	2.073(3)
Fe(2)-O(5)	2.088(3)
Fe(2)-O(2)	2.100(3)
Fe(2)-N(7)	2.184(4)
Fe(2)-N(6)	2.185(4)
Fe(2)-N(5)	2.228(3)
O(1)-C(1)	1.284(5)
O(2)-C(1)	1.299(6)
O(3)-C(22)	1.357(5)
O(4)-C(3)	1.245(5)
O(5)-C(41)	1.224(5)
O(6)-S(1)	1.434(4)
O(7)-S(1)	1.448(3)
O(8)-S(1)	1.433(3)
O(9)-S(2)	1.439(4)
O(10)-S(2)	1.434(4)
O(11)-S(2)	1.435(3)
N(1)-C(3)	1.344(5)
N(1)-C(4)	1.406(5)
N(1)-H(1N)	0.79(4)
N(2)-C(4)	1.332(5)
N(2)-C(8)	1.357(5)
N(3)-C(10)	1.332(6)
N(3)-C(14)	1.354(6)
N(4)-C(9)	1.476(6)
N(4)-C(15)	1.480(5)
N(4)-C(16)	1.491(6)
N(5)-C(30)	1.471(6)
N(5)-C(24)	1.485(5)
N(5)-C(23)	1.488(6)
N(6)-C(29)	1.339(6)
N(6)-C(25)	1.354(6)
N(7)-C(35)	1.345(5)
N(7)-C(31)	1.349(5)
N(8)-C(41)	1.355(6)
N(8)-C(35)	1.411(5)
N(8)-H(8N)	0.79(4)

C(1)-C(2)	1.449(7)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-C(36)	1.523(6)
C(4)-C(5)	1.396(6)
C(5)-C(6)	1.386(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.377(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.388(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.492(6)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.372(7)
C(10)-H(10)	0.9500
C(11)-C(12)	1.382(7)
C(11)-H(11)	0.9500
C(12)-C(13)	1.392(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.371(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.510(6)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.502(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.386(6)
C(17)-C(22)	1.401(6)
C(18)-C(19)	1.396(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.385(6)
C(19)-C(40)	1.512(6)
C(20)-C(21)	1.394(6)
C(20)-H(20)	0.9500
C(21)-C(22)	1.404(6)
C(21)-C(23)	1.500(6)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.511(7)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.377(6)
C(26)-C(27)	1.391(8)

C(26)-H(26)	0.9500
C(27)-C(28)	1.363(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.393(7)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-C(31)	1.499(6)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(32)	1.381(6)
C(32)-C(33)	1.384(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.372(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.382(6)
C(34)-H(34)	0.9500
C(36)-C(37)	1.508(7)
C(36)-C(38)	1.539(7)
C(36)-C(39)	1.542(7)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(42)	1.538(6)
C(42)-C(44)	1.506(7)
C(42)-C(45)	1.538(6)
C(42)-C(43)	1.539(7)
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-F(2)	1.324(6)
C(46)-F(3)	1.331(5)

C(46)-F(1)	1.340(6)
C(46)-S(1)	1.822(5)
C(47)-F(4)	1.335(5)
C(47)-F(6)	1.337(5)
C(47)-F(5)	1.347(5)
C(47)-S(2)	1.805(5)
C(48)-Cl(1)	1.763(10)
C(48)-Cl(2)	1.799(10)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-Cl(4)	1.743(6)
C(49)-Cl(3)	1.763(6)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
O(3)-Fe(1)-O(1)	90.02(13)
O(3)-Fe(1)-O(4)	112.25(12)
O(1)-Fe(1)-O(4)	86.24(12)
O(3)-Fe(1)-N(3)	156.79(13)
O(1)-Fe(1)-N(3)	86.37(13)
O(4)-Fe(1)-N(3)	90.41(13)
O(3)-Fe(1)-N(2)	91.15(12)
O(1)-Fe(1)-N(2)	164.27(13)
O(4)-Fe(1)-N(2)	78.80(12)
N(3)-Fe(1)-N(2)	98.48(13)
O(3)-Fe(1)-N(4)	87.14(12)
O(1)-Fe(1)-N(4)	118.53(13)
O(4)-Fe(1)-N(4)	149.32(12)
N(3)-Fe(1)-N(4)	74.62(13)
N(2)-Fe(1)-N(4)	77.20(13)
O(3)-Fe(2)-O(5)	110.48(11)
O(3)-Fe(2)-O(2)	89.91(12)
O(5)-Fe(2)-O(2)	87.49(13)
O(3)-Fe(2)-N(7)	88.79(12)
O(5)-Fe(2)-N(7)	80.40(12)
O(2)-Fe(2)-N(7)	166.51(13)
O(3)-Fe(2)-N(6)	160.54(13)
O(5)-Fe(2)-N(6)	88.86(13)
O(2)-Fe(2)-N(6)	88.69(14)
N(7)-Fe(2)-N(6)	96.94(14)
O(3)-Fe(2)-N(5)	87.50(12)
O(5)-Fe(2)-N(5)	151.27(13)
O(2)-Fe(2)-N(5)	115.66(14)
N(7)-Fe(2)-N(5)	77.70(13)
N(6)-Fe(2)-N(5)	75.67(13)
C(1)-O(1)-Fe(1)	125.0(4)
C(1)-O(2)-Fe(2)	121.7(3)

C(22)-O(3)-Fe(1)	117.4(2)
C(22)-O(3)-Fe(2)	118.0(2)
Fe(1)-O(3)-Fe(2)	124.61(14)
C(3)-O(4)-Fe(1)	125.1(3)
C(41)-O(5)-Fe(2)	126.8(3)
C(3)-N(1)-C(4)	129.1(4)
C(3)-N(1)-H(1N)	113(4)
C(4)-N(1)-H(1N)	117(4)
C(4)-N(2)-C(8)	117.6(3)
C(4)-N(2)-Fe(1)	124.7(3)
C(8)-N(2)-Fe(1)	115.6(3)
C(10)-N(3)-C(14)	118.5(4)
C(10)-N(3)-Fe(1)	125.5(3)
C(14)-N(3)-Fe(1)	115.9(3)
C(9)-N(4)-C(15)	110.3(3)
C(9)-N(4)-C(16)	110.9(3)
C(15)-N(4)-C(16)	110.4(3)
C(9)-N(4)-Fe(1)	107.5(2)
C(15)-N(4)-Fe(1)	105.6(2)
C(16)-N(4)-Fe(1)	112.0(2)
C(30)-N(5)-C(24)	109.9(3)
C(30)-N(5)-C(23)	110.7(3)
C(24)-N(5)-C(23)	110.9(3)
C(30)-N(5)-Fe(2)	108.2(2)
C(24)-N(5)-Fe(2)	105.2(3)
C(23)-N(5)-Fe(2)	111.7(3)
C(29)-N(6)-C(25)	118.3(4)
C(29)-N(6)-Fe(2)	126.5(3)
C(25)-N(6)-Fe(2)	115.1(3)
C(35)-N(7)-C(31)	117.6(4)
C(35)-N(7)-Fe(2)	123.7(3)
C(31)-N(7)-Fe(2)	114.6(3)
C(41)-N(8)-C(35)	129.0(4)
C(41)-N(8)-H(8N)	119(4)
C(35)-N(8)-H(8N)	112(4)
O(1)-C(1)-O(2)	121.1(5)
O(1)-C(1)-C(2)	119.5(5)
O(2)-C(1)-C(2)	118.6(4)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
O(4)-C(3)-N(1)	122.2(4)
O(4)-C(3)-C(36)	120.0(4)

N(1)-C(3)-C(36)	117.8(4)
N(2)-C(4)-C(5)	123.9(4)
N(2)-C(4)-N(1)	119.0(4)
C(5)-C(4)-N(1)	117.0(4)
C(6)-C(5)-C(4)	117.5(4)
C(6)-C(5)-H(5)	121.3
C(4)-C(5)-H(5)	121.3
C(7)-C(6)-C(5)	119.6(4)
C(7)-C(6)-H(6)	120.2
C(5)-C(6)-H(6)	120.2
C(6)-C(7)-C(8)	119.2(4)
C(6)-C(7)-H(7)	120.4
C(8)-C(7)-H(7)	120.4
N(2)-C(8)-C(7)	122.0(4)
N(2)-C(8)-C(9)	115.4(4)
C(7)-C(8)-C(9)	122.5(4)
N(4)-C(9)-C(8)	113.0(3)
N(4)-C(9)-H(9A)	109.0
C(8)-C(9)-H(9A)	109.0
N(4)-C(9)-H(9B)	109.0
C(8)-C(9)-H(9B)	109.0
H(9A)-C(9)-H(9B)	107.8
N(3)-C(10)-C(11)	123.2(4)
N(3)-C(10)-H(10)	118.4
C(11)-C(10)-H(10)	118.4
C(10)-C(11)-C(12)	118.3(5)
C(10)-C(11)-H(11)	120.8
C(12)-C(11)-H(11)	120.8
C(11)-C(12)-C(13)	119.3(4)
C(11)-C(12)-H(12)	120.4
C(13)-C(12)-H(12)	120.4
C(14)-C(13)-C(12)	118.8(4)
C(14)-C(13)-H(13)	120.6
C(12)-C(13)-H(13)	120.6
N(3)-C(14)-C(13)	121.9(4)
N(3)-C(14)-C(15)	115.6(4)
C(13)-C(14)-C(15)	122.5(4)
N(4)-C(15)-C(14)	109.4(4)
N(4)-C(15)-H(15A)	109.8
C(14)-C(15)-H(15A)	109.8
N(4)-C(15)-H(15B)	109.8
C(14)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.2
N(4)-C(16)-C(17)	110.8(3)
N(4)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16A)	109.5

N(4)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	108.1
C(18)-C(17)-C(22)	119.2(4)
C(18)-C(17)-C(16)	121.9(4)
C(22)-C(17)-C(16)	118.9(4)
C(17)-C(18)-C(19)	121.7(4)
C(17)-C(18)-H(18)	119.1
C(19)-C(18)-H(18)	119.1
C(20)-C(19)-C(18)	118.2(4)
C(20)-C(19)-C(40)	122.0(4)
C(18)-C(19)-C(40)	119.8(4)
C(19)-C(20)-C(21)	121.9(4)
C(19)-C(20)-H(20)	119.1
C(21)-C(20)-H(20)	119.1
C(20)-C(21)-C(22)	118.9(4)
C(20)-C(21)-C(23)	122.3(4)
C(22)-C(21)-C(23)	118.8(4)
O(3)-C(22)-C(17)	119.9(4)
O(3)-C(22)-C(21)	120.1(4)
C(17)-C(22)-C(21)	120.0(4)
N(5)-C(23)-C(21)	111.5(3)
N(5)-C(23)-H(23A)	109.3
C(21)-C(23)-H(23A)	109.3
N(5)-C(23)-H(23B)	109.3
C(21)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	108.0
N(5)-C(24)-C(25)	109.3(4)
N(5)-C(24)-H(24A)	109.8
C(25)-C(24)-H(24A)	109.8
N(5)-C(24)-H(24B)	109.8
C(25)-C(24)-H(24B)	109.8
H(24A)-C(24)-H(24B)	108.3
N(6)-C(25)-C(26)	122.1(5)
N(6)-C(25)-C(24)	115.0(4)
C(26)-C(25)-C(24)	122.9(4)
C(25)-C(26)-C(27)	118.7(5)
C(25)-C(26)-H(26)	120.6
C(27)-C(26)-H(26)	120.6
C(28)-C(27)-C(26)	119.6(4)
C(28)-C(27)-H(27)	120.2
C(26)-C(27)-H(27)	120.2
C(27)-C(28)-C(29)	118.9(5)
C(27)-C(28)-H(28)	120.5
C(29)-C(28)-H(28)	120.5
N(6)-C(29)-C(28)	122.2(4)

N(6)-C(29)-H(29)	118.9
C(28)-C(29)-H(29)	118.9
N(5)-C(30)-C(31)	112.2(3)
N(5)-C(30)-H(30A)	109.2
C(31)-C(30)-H(30A)	109.2
N(5)-C(30)-H(30B)	109.2
C(31)-C(30)-H(30B)	109.2
H(30A)-C(30)-H(30B)	107.9
N(7)-C(31)-C(32)	122.7(4)
N(7)-C(31)-C(30)	114.8(4)
C(32)-C(31)-C(30)	122.5(4)
C(31)-C(32)-C(33)	118.3(4)
C(31)-C(32)-H(32)	120.8
C(33)-C(32)-H(32)	120.8
C(34)-C(33)-C(32)	119.9(4)
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(33)-C(34)-C(35)	118.3(4)
C(33)-C(34)-H(34)	120.8
C(35)-C(34)-H(34)	120.8
N(7)-C(35)-C(34)	123.1(4)
N(7)-C(35)-N(8)	118.5(4)
C(34)-C(35)-N(8)	118.4(4)
C(37)-C(36)-C(3)	112.4(4)
C(37)-C(36)-C(38)	110.0(4)
C(3)-C(36)-C(38)	108.1(4)
C(37)-C(36)-C(39)	110.8(4)
C(3)-C(36)-C(39)	106.7(4)
C(38)-C(36)-C(39)	108.7(4)
C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(36)-C(38)-H(38A)	109.5
C(36)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(36)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(36)-C(39)-H(39A)	109.5
C(36)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(36)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5

H(39B)-C(39)-H(39C)	109.5
C(19)-C(40)-H(40A)	109.5
C(19)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(19)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(5)-C(41)-N(8)	123.9(4)
O(5)-C(41)-C(42)	119.5(4)
N(8)-C(41)-C(42)	116.6(4)
C(44)-C(42)-C(45)	111.4(4)
C(44)-C(42)-C(41)	112.1(4)
C(45)-C(42)-C(41)	107.8(4)
C(44)-C(42)-C(43)	110.9(4)
C(45)-C(42)-C(43)	107.5(4)
C(41)-C(42)-C(43)	106.9(4)
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(42)-C(44)-H(44A)	109.5
C(42)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(42)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(42)-C(45)-H(45A)	109.5
C(42)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(42)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
F(2)-C(46)-F(3)	107.2(4)
F(2)-C(46)-F(1)	107.7(4)
F(3)-C(46)-F(1)	106.9(4)
F(2)-C(46)-S(1)	111.6(3)
F(3)-C(46)-S(1)	111.8(3)
F(1)-C(46)-S(1)	111.5(3)
F(4)-C(47)-F(6)	107.1(4)
F(4)-C(47)-F(5)	107.1(3)
F(6)-C(47)-F(5)	107.2(4)
F(4)-C(47)-S(2)	111.5(3)
F(6)-C(47)-S(2)	112.5(3)
F(5)-C(47)-S(2)	111.2(3)

Cl(1)-C(48)-Cl(2)	111.0(5)
Cl(1)-C(48)-H(48A)	109.4
Cl(2)-C(48)-H(48A)	109.4
Cl(1)-C(48)-H(48B)	109.4
Cl(2)-C(48)-H(48B)	109.4
H(48A)-C(48)-H(48B)	108.0
Cl(4)-C(49)-Cl(3)	112.9(3)
Cl(4)-C(49)-H(49A)	109.0
Cl(3)-C(49)-H(49A)	109.0
Cl(4)-C(49)-H(49B)	109.0
Cl(3)-C(49)-H(49B)	109.0
H(49A)-C(49)-H(49B)	107.8
O(8)-S(1)-O(6)	115.2(2)
O(8)-S(1)-O(7)	114.7(2)
O(6)-S(1)-O(7)	114.6(3)
O(8)-S(1)-C(46)	103.8(2)
O(6)-S(1)-C(46)	103.8(2)
O(7)-S(1)-C(46)	102.5(2)
O(10)-S(2)-O(11)	115.9(2)
O(10)-S(2)-O(9)	113.7(2)
O(11)-S(2)-O(9)	114.9(2)
O(10)-S(2)-C(47)	102.4(2)
O(11)-S(2)-C(47)	104.0(2)
O(9)-S(2)-C(47)	103.7(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z

Table S11. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	34(1)	27(1)	36(1)	15(1)	12(1)	11(1)
Fe(2)	35(1)	26(1)	42(1)	16(1)	11(1)	11(1)
O(1)	51(2)	41(2)	44(2)	17(1)	17(1)	10(1)
O(2)	44(2)	39(2)	57(2)	22(1)	4(1)	2(1)
O(3)	38(2)	29(1)	40(2)	15(1)	7(1)	13(1)
O(4)	36(2)	35(2)	44(2)	10(1)	14(1)	8(1)
O(5)	39(2)	33(2)	44(2)	13(1)	13(1)	12(1)
O(6)	50(2)	62(2)	66(2)	7(2)	4(2)	21(2)
O(7)	78(3)	36(2)	58(2)	12(2)	32(2)	2(2)
O(8)	51(2)	48(2)	52(2)	15(2)	19(2)	19(2)
O(9)	67(2)	53(2)	42(2)	11(2)	22(2)	-2(2)
O(10)	44(2)	42(2)	78(2)	-3(2)	-2(2)	22(2)
O(11)	42(2)	42(2)	47(2)	11(1)	14(1)	2(1)
N(1)	39(2)	27(2)	46(2)	10(2)	12(2)	11(2)
N(2)	32(2)	31(2)	36(2)	16(1)	12(1)	11(1)
N(3)	39(2)	29(2)	39(2)	14(1)	12(1)	13(1)
N(4)	37(2)	24(2)	43(2)	15(1)	9(1)	8(1)
N(5)	42(2)	28(2)	38(2)	12(1)	9(2)	11(1)
N(6)	46(2)	29(2)	51(2)	18(2)	10(2)	10(2)
N(7)	34(2)	30(2)	36(2)	14(1)	9(1)	11(1)
N(8)	39(2)	25(2)	44(2)	9(1)	15(2)	12(1)
C(1)	43(3)	42(3)	92(4)	49(3)	-20(2)	-7(2)
C(2)	46(3)	65(3)	56(3)	24(2)	17(2)	11(2)
C(3)	37(2)	31(2)	37(2)	12(2)	8(2)	11(2)
C(4)	36(2)	34(2)	38(2)	14(2)	11(2)	12(2)
C(5)	42(2)	45(2)	38(2)	9(2)	12(2)	19(2)
C(6)	38(2)	64(3)	39(2)	11(2)	16(2)	15(2)
C(7)	35(2)	55(3)	44(2)	21(2)	13(2)	7(2)
C(8)	39(2)	40(2)	37(2)	19(2)	9(2)	10(2)
C(9)	38(2)	32(2)	48(2)	19(2)	11(2)	7(2)
C(10)	38(2)	35(2)	43(2)	15(2)	14(2)	7(2)
C(11)	38(2)	45(3)	57(3)	22(2)	8(2)	17(2)
C(12)	47(3)	41(2)	68(3)	27(2)	9(2)	18(2)
C(13)	44(2)	31(2)	58(3)	21(2)	7(2)	11(2)
C(14)	40(2)	34(2)	45(2)	16(2)	10(2)	12(2)
C(15)	44(2)	23(2)	54(3)	12(2)	4(2)	10(2)
C(16)	35(2)	27(2)	45(2)	12(2)	2(2)	8(2)
C(17)	41(2)	30(2)	41(2)	12(2)	6(2)	12(2)

C(18)	38(2)	35(2)	41(2)	13(2)	7(2)	9(2)
C(19)	44(2)	41(2)	39(2)	14(2)	10(2)	15(2)
C(20)	46(2)	38(2)	36(2)	12(2)	11(2)	21(2)
C(21)	42(2)	31(2)	37(2)	12(2)	9(2)	14(2)
C(22)	40(2)	32(2)	34(2)	13(2)	9(2)	14(2)
C(23)	47(2)	31(2)	41(2)	10(2)	8(2)	17(2)
C(24)	55(3)	23(2)	54(3)	14(2)	10(2)	12(2)
C(25)	40(2)	30(2)	56(3)	18(2)	9(2)	9(2)
C(26)	50(3)	38(2)	75(3)	32(2)	18(2)	12(2)
C(27)	54(3)	47(3)	73(3)	41(3)	20(3)	13(2)
C(28)	60(3)	54(3)	61(3)	33(2)	25(2)	18(2)
C(29)	50(3)	38(2)	54(3)	23(2)	18(2)	16(2)
C(30)	41(2)	35(2)	41(2)	16(2)	11(2)	17(2)
C(31)	37(2)	38(2)	37(2)	14(2)	13(2)	17(2)
C(32)	40(2)	42(2)	41(2)	9(2)	10(2)	15(2)
C(33)	35(2)	51(3)	50(3)	11(2)	8(2)	8(2)
C(34)	42(2)	35(2)	47(2)	9(2)	10(2)	11(2)
C(35)	39(2)	30(2)	34(2)	11(2)	10(2)	9(2)
C(36)	40(2)	30(2)	50(2)	16(2)	11(2)	9(2)
C(37)	50(3)	46(3)	55(3)	9(2)	6(2)	5(2)
C(38)	43(3)	39(2)	84(4)	17(2)	20(2)	8(2)
C(39)	68(3)	34(2)	49(3)	18(2)	5(2)	5(2)
C(40)	51(3)	52(3)	51(3)	17(2)	18(2)	19(2)
C(41)	39(2)	31(2)	40(2)	16(2)	13(2)	14(2)
C(42)	42(2)	30(2)	61(3)	13(2)	20(2)	16(2)
C(43)	46(2)	33(2)	63(3)	13(2)	8(2)	14(2)
C(44)	56(3)	51(3)	49(3)	11(2)	15(2)	19(2)
C(45)	49(3)	41(3)	74(3)	15(2)	26(2)	14(2)
C(46)	53(3)	40(2)	45(2)	21(2)	10(2)	10(2)
C(47)	39(2)	41(2)	40(2)	16(2)	9(2)	17(2)
C(48)	75(5)	156(8)	67(4)	22(5)	23(4)	38(5)
C(49)	60(3)	65(3)	58(3)	14(3)	16(3)	22(3)
S(1)	47(1)	37(1)	46(1)	11(1)	16(1)	11(1)
S(2)	40(1)	35(1)	44(1)	8(1)	14(1)	10(1)
Cl(1)	114(2)	104(2)	116(2)	24(1)	-1(1)	-2(1)
Cl(2)	74(1)	109(1)	73(1)	15(1)	16(1)	11(1)
Cl(3)	86(1)	63(1)	62(1)	5(1)	8(1)	29(1)
Cl(4)	86(1)	54(1)	83(1)	12(1)	44(1)	3(1)
F(1)	73(2)	41(2)	61(2)	7(1)	20(2)	14(1)
F(2)	64(2)	51(2)	56(2)	22(1)	-3(1)	10(1)
F(3)	65(2)	46(2)	61(2)	32(1)	10(1)	9(1)
F(4)	56(2)	49(2)	62(2)	16(1)	9(1)	30(1)
F(5)	58(2)	45(1)	41(1)	12(1)	13(1)	15(1)
F(6)	51(2)	33(1)	55(2)	12(1)	10(1)	7(1)

Table S12. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.

	x	y	z	U(eq)
H(1N)	1500(40)	3980(40)	5670(30)	43
H(8N)	3710(40)	9100(40)	9270(30)	41
H(2A)	-1324	6708	8377	81
H(2B)	-1358	5375	8196	81
H(2C)	-1584	6037	7622	81
H(5)	3010	4322	5021	48
H(6)	4413	5710	4761	55
H(7)	4477	7600	5264	52
H(9A)	3918	8937	6198	45
H(9B)	2652	8821	5939	45
H(10)	-723	7234	6128	45
H(11)	-1594	8586	5805	52
H(12)	-688	10478	6050	58
H(13)	1063	10945	6638	51
H(15A)	2740	10239	6977	47
H(15B)	2178	9697	7566	47
H(16A)	3551	8737	7815	42
H(16B)	4355	9316	7327	42
H(18)	5796	8344	6933	45
H(20)	5491	4977	6735	45
H(23A)	2757	4330	6953	45
H(23B)	3886	3877	7061	45
H(24A)	3068	2897	7978	51
H(24B)	1961	3255	7718	51
H(26)	2379	2158	8960	61
H(27)	1735	2551	10039	64
H(28)	1191	4274	10423	65
H(29)	1380	5618	9752	53
H(30A)	4897	4480	8079	44
H(30B)	4229	4496	8741	44
H(32)	6394	6092	8450	48
H(33)	6905	8057	8785	54
H(34)	5548	9142	9115	49
H(37A)	-535	3279	5031	76
H(37B)	-1114	2274	5366	76
H(37C)	209	2538	5346	76
H(38A)	-1730	4417	5838	81
H(38B)	-1466	4563	6623	81
H(38C)	-2084	3374	6195	81

H(39A)	-627	2474	6648	74
H(39B)	13	3675	7048	74
H(39C)	656	2881	6539	74
H(40A)	6955	6978	6091	73
H(40B)	7184	5993	6454	73
H(40C)	7497	7281	6838	73
H(43A)	1039	10244	9116	69
H(43B)	1119	9142	8568	69
H(43C)	2214	10052	8836	69
H(44A)	1813	10349	10328	76
H(44B)	2966	10290	9984	76
H(44C)	2518	9411	10440	76
H(45A)	655	8011	10019	80
H(45B)	173	7966	9279	80
H(45C)	110	9031	9860	80
H(48A)	8198	716	7450	116
H(48B)	7700	755	8168	116
H(49A)	4739	8318	2606	71
H(49B)	4920	7823	3259	71

Table S13. Torsion angles [deg] for **1**.

Fe(1)-O(1)-C(1)-O(2)	36.9(7)
Fe(1)-O(1)-C(1)-C(2)	-132.9(5)
Fe(2)-O(2)-C(1)-O(1)	40.4(7)
Fe(2)-O(2)-C(1)-C(2)	-149.7(4)
Fe(1)-O(4)-C(3)-N(1)	-31.2(6)
Fe(1)-O(4)-C(3)-C(36)	147.1(3)
C(4)-N(1)-C(3)-O(4)	-12.2(7)
C(4)-N(1)-C(3)-C(36)	169.6(4)
C(8)-N(2)-C(4)-C(5)	0.8(6)
Fe(1)-N(2)-C(4)-C(5)	-161.9(3)
C(8)-N(2)-C(4)-N(1)	-178.1(4)
Fe(1)-N(2)-C(4)-N(1)	19.2(6)
C(3)-N(1)-C(4)-N(2)	17.7(7)
C(3)-N(1)-C(4)-C(5)	-161.2(4)
N(2)-C(4)-C(5)-C(6)	-1.4(7)
N(1)-C(4)-C(5)-C(6)	177.4(4)
C(4)-C(5)-C(6)-C(7)	0.0(7)
C(5)-C(6)-C(7)-C(8)	1.8(7)
C(4)-N(2)-C(8)-C(7)	1.2(6)
Fe(1)-N(2)-C(8)-C(7)	165.5(4)
C(4)-N(2)-C(8)-C(9)	179.1(4)
Fe(1)-N(2)-C(8)-C(9)	-16.6(5)
C(6)-C(7)-C(8)-N(2)	-2.6(7)
C(6)-C(7)-C(8)-C(9)	179.7(4)
C(15)-N(4)-C(9)-C(8)	-150.2(4)
C(16)-N(4)-C(9)-C(8)	87.2(4)
Fe(1)-N(4)-C(9)-C(8)	-35.5(4)
N(2)-C(8)-C(9)-N(4)	36.2(5)
C(7)-C(8)-C(9)-N(4)	-146.0(4)
C(14)-N(3)-C(10)-C(11)	1.1(6)
Fe(1)-N(3)-C(10)-C(11)	178.3(3)
N(3)-C(10)-C(11)-C(12)	-0.1(7)
C(10)-C(11)-C(12)-C(13)	-0.8(7)
C(11)-C(12)-C(13)-C(14)	0.7(7)
C(10)-N(3)-C(14)-C(13)	-1.2(6)
Fe(1)-N(3)-C(14)-C(13)	-178.7(3)
C(10)-N(3)-C(14)-C(15)	179.0(4)
Fe(1)-N(3)-C(14)-C(15)	1.5(5)
C(12)-C(13)-C(14)-N(3)	0.3(7)
C(12)-C(13)-C(14)-C(15)	-179.9(4)
C(9)-N(4)-C(15)-C(14)	70.4(4)
C(16)-N(4)-C(15)-C(14)	-166.7(3)
Fe(1)-N(4)-C(15)-C(14)	-45.4(4)
N(3)-C(14)-C(15)-N(4)	31.0(5)

C(13)-C(14)-C(15)-N(4)	-148.8(4)
C(9)-N(4)-C(16)-C(17)	-61.8(4)
C(15)-N(4)-C(16)-C(17)	175.6(3)
Fe(1)-N(4)-C(16)-C(17)	58.2(4)
N(4)-C(16)-C(17)-C(18)	114.3(4)
N(4)-C(16)-C(17)-C(22)	-64.7(5)
C(22)-C(17)-C(18)-C(19)	1.7(7)
C(16)-C(17)-C(18)-C(19)	-177.2(4)
C(17)-C(18)-C(19)-C(20)	-2.1(7)
C(17)-C(18)-C(19)-C(40)	177.7(4)
C(18)-C(19)-C(20)-C(21)	0.2(7)
C(40)-C(19)-C(20)-C(21)	-179.6(4)
C(19)-C(20)-C(21)-C(22)	2.0(7)
C(19)-C(20)-C(21)-C(23)	-176.0(4)
Fe(1)-O(3)-C(22)-C(17)	59.4(5)
Fe(2)-O(3)-C(22)-C(17)	-121.8(4)
Fe(1)-O(3)-C(22)-C(21)	-120.0(4)
Fe(2)-O(3)-C(22)-C(21)	58.9(5)
C(18)-C(17)-C(22)-O(3)	-178.8(4)
C(16)-C(17)-C(22)-O(3)	0.1(6)
C(18)-C(17)-C(22)-C(21)	0.5(6)
C(16)-C(17)-C(22)-C(21)	179.5(4)
C(20)-C(21)-C(22)-O(3)	177.0(4)
C(23)-C(21)-C(22)-O(3)	-4.9(6)
C(20)-C(21)-C(22)-C(17)	-2.3(6)
C(23)-C(21)-C(22)-C(17)	175.7(4)
C(30)-N(5)-C(23)-C(21)	-58.5(4)
C(24)-N(5)-C(23)-C(21)	179.2(4)
Fe(2)-N(5)-C(23)-C(21)	62.1(4)
C(20)-C(21)-C(23)-N(5)	116.1(4)
C(22)-C(21)-C(23)-N(5)	-61.9(5)
C(30)-N(5)-C(24)-C(25)	68.8(5)
C(23)-N(5)-C(24)-C(25)	-168.5(4)
Fe(2)-N(5)-C(24)-C(25)	-47.5(4)
C(29)-N(6)-C(25)-C(26)	-2.4(7)
Fe(2)-N(6)-C(25)-C(26)	174.1(4)
C(29)-N(6)-C(25)-C(24)	178.6(4)
Fe(2)-N(6)-C(25)-C(24)	-4.9(5)
N(5)-C(24)-C(25)-N(6)	36.4(6)
N(5)-C(24)-C(25)-C(26)	-142.6(5)
N(6)-C(25)-C(26)-C(27)	2.0(8)
C(24)-C(25)-C(26)-C(27)	-179.1(5)
C(25)-C(26)-C(27)-C(28)	0.2(8)
C(26)-C(27)-C(28)-C(29)	-1.8(9)
C(25)-N(6)-C(29)-C(28)	0.7(7)
Fe(2)-N(6)-C(29)-C(28)	-175.4(4)

C(27)-C(28)-C(29)-N(6)	1.4(8)
C(24)-N(5)-C(30)-C(31)	-149.2(3)
C(23)-N(5)-C(30)-C(31)	87.9(4)
Fe(2)-N(5)-C(30)-C(31)	-34.8(4)
C(35)-N(7)-C(31)-C(32)	0.0(6)
Fe(2)-N(7)-C(31)-C(32)	158.1(4)
C(35)-N(7)-C(31)-C(30)	178.4(4)
Fe(2)-N(7)-C(31)-C(30)	-23.5(4)
N(5)-C(30)-C(31)-N(7)	40.1(5)
N(5)-C(30)-C(31)-C(32)	-141.4(4)
N(7)-C(31)-C(32)-C(33)	-1.3(7)
C(30)-C(31)-C(32)-C(33)	-179.6(4)
C(31)-C(32)-C(33)-C(34)	1.7(7)
C(32)-C(33)-C(34)-C(35)	-0.8(7)
C(31)-N(7)-C(35)-C(34)	1.1(6)
Fe(2)-N(7)-C(35)-C(34)	-154.9(3)
C(31)-N(7)-C(35)-N(8)	-179.2(4)
Fe(2)-N(7)-C(35)-N(8)	24.8(5)
C(33)-C(34)-C(35)-N(7)	-0.6(7)
C(33)-C(34)-C(35)-N(8)	179.6(4)
C(41)-N(8)-C(35)-N(7)	7.7(7)
C(41)-N(8)-C(35)-C(34)	-172.6(4)
O(4)-C(3)-C(36)-C(37)	140.5(4)
N(1)-C(3)-C(36)-C(37)	-41.2(6)
O(4)-C(3)-C(36)-C(38)	18.9(6)
N(1)-C(3)-C(36)-C(38)	-162.8(4)
O(4)-C(3)-C(36)-C(39)	-97.9(5)
N(1)-C(3)-C(36)-C(39)	80.4(5)
Fe(2)-O(5)-C(41)-N(8)	-28.4(6)
Fe(2)-O(5)-C(41)-C(42)	150.1(3)
C(35)-N(8)-C(41)-O(5)	-7.5(7)
C(35)-N(8)-C(41)-C(42)	174.0(4)
O(5)-C(41)-C(42)-C(44)	134.5(4)
N(8)-C(41)-C(42)-C(44)	-46.9(5)
O(5)-C(41)-C(42)-C(45)	11.5(6)
N(8)-C(41)-C(42)-C(45)	-169.9(4)
O(5)-C(41)-C(42)-C(43)	-103.8(5)
N(8)-C(41)-C(42)-C(43)	74.8(5)
F(2)-C(46)-S(1)-O(8)	-55.1(4)
F(3)-C(46)-S(1)-O(8)	64.9(4)
F(1)-C(46)-S(1)-O(8)	-175.5(3)
F(2)-C(46)-S(1)-O(6)	-175.8(3)
F(3)-C(46)-S(1)-O(6)	-55.9(4)
F(1)-C(46)-S(1)-O(6)	63.7(4)
F(2)-C(46)-S(1)-O(7)	64.6(4)
F(3)-C(46)-S(1)-O(7)	-175.4(4)

F(1)-C(46)-S(1)-O(7)	-55.8(4)
F(4)-C(47)-S(2)-O(10)	-177.5(3)
F(6)-C(47)-S(2)-O(10)	-57.2(4)
F(5)-C(47)-S(2)-O(10)	63.1(3)
F(4)-C(47)-S(2)-O(11)	61.5(3)
F(6)-C(47)-S(2)-O(11)	-178.2(3)
F(5)-C(47)-S(2)-O(11)	-58.0(3)
F(4)-C(47)-S(2)-O(9)	-59.0(4)
F(6)-C(47)-S(2)-O(9)	61.3(4)
F(5)-C(47)-S(2)-O(9)	-178.5(3)

Table S14. Hydrogen bonds for **1** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(10)	0.79(4)	2.13(4)	2.884(5)	159(5)
N(8)-H(8N)...O(7)#1	0.79(4)	2.16(4)	2.921(5)	163(5)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z

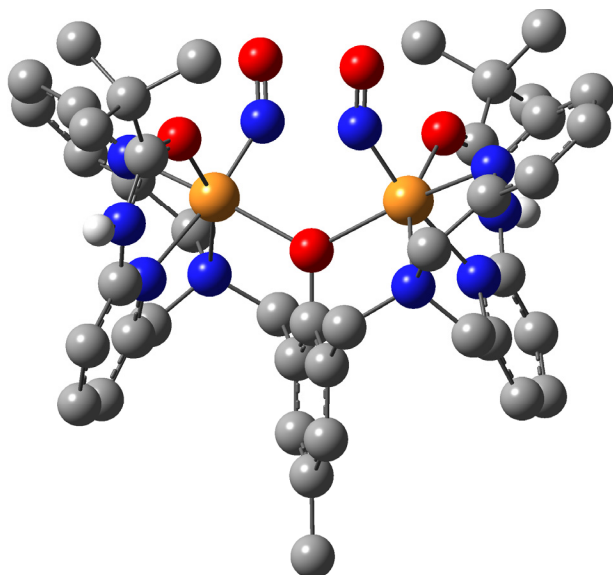


Figure S25. DFT-optimized structure of $0(\text{NO})_2$ using BP86/TZVP with hydrogen atoms (except for amide N-H groups) omitted for clarity.

Table S15. DFT-optimized coordinates (Å) of $0(\text{NO})_2$ using BP86/TZVP.

	X	Y	Z
Fe	1.834685	-0.399305	-0.466709
Fe	-1.836122	-0.39619	0.470844
O	0.000932	0.571816	0.002757
O	2.288433	-1.57514	1.181601
O	-2.2874	-1.579403	-1.173365
N	3.188617	-0.082051	2.712337
H	3.531481	0.001948	3.673014
N	3.043971	1.056911	0.58998
N	3.528075	-1.13819	-1.592349
N	2.112942	1.10028	-2.084708
N	-2.117741	1.111649	2.080665
N	-3.532419	-1.128681	1.595863
N	-3.040254	1.056527	-0.596697
N	-3.18176	-0.092639	-2.713622
H	-3.52292	-0.013012	-3.67527
C	2.779194	-1.338898	2.349279
C	3.355141	1.08072	1.92277
C	3.909667	2.216117	2.553622
H	4.144801	2.19554	3.621359

C	4.174193	3.35586	1.78547
H	4.603452	4.24598	2.251471
C	3.907864	3.326357	0.404104
H	4.138221	4.187044	-0.227636
C	3.358935	2.166939	-0.16314
C	3.226821	2.026892	-1.662172
H	3.103171	3.018475	-2.134868
H	4.176226	1.60314	-2.040624
C	4.421411	-2.07182	-1.149721
H	4.293549	-2.414294	-0.122111
C	5.434723	-2.576366	-1.978923
H	6.131885	-3.322925	-1.592833
C	5.532656	-2.106892	-3.302386
H	6.314499	-2.480588	-3.968178
C	4.609051	-1.146619	-3.760009
H	4.660934	-0.763838	-4.78278
C	3.610067	-0.687943	-2.88638
C	2.53363	0.297052	-3.290132
H	2.882461	0.955291	-4.11001
H	1.637583	-0.240547	-3.65354
C	0.837493	1.880509	-2.370418
H	0.078608	1.129717	-2.65541
H	1.011281	2.551129	-3.235618
C	0.396941	2.672695	-1.164272
C	0.381308	4.083584	-1.15591
H	0.670767	4.625939	-2.06392
C	-0.005279	4.819466	-0.010792
C	-0.39194	4.089547	1.138997
H	-0.691703	4.636661	2.040943
C	-0.397798	2.679189	1.157998
C	0.001706	1.968136	-0.000765
C	-0.843115	1.89326	2.366483
H	-0.085155	1.144045	2.657844
H	-1.019837	2.568364	3.227571
C	-2.54239	0.315004	3.289058
H	-2.893479	0.977765	4.104315
H	-1.647653	-0.220907	3.658132
C	-3.61793	-0.671742	2.887322
C	-4.619466	-1.125677	3.760508
H	-4.674089	-0.737604	4.781138

C	-5.542025	-2.08808	3.305283
H	-6.325832	-2.458127	3.970804
C	-5.440466	-2.564444	1.984558
H	-6.136709	-3.312848	1.600387
C	-4.424713	-2.064441	1.155601
H	-4.294023	-2.412277	0.130157
C	-3.229948	2.036524	1.649983
H	-3.108909	3.029699	2.120006
H	-4.180932	1.613577	2.025337
C	-3.354808	2.171146	0.149911
C	-3.897114	3.329814	-0.425074
H	-4.12671	4.194541	0.201336
C	-4.157481	3.353734	-1.807694
H	-4.58093	4.243477	-2.279661
C	-3.894501	2.209174	-2.569182
H	-4.125654	2.18418	-3.637702
C	-3.346516	1.07488	-1.930672
C	2.945617	-2.482262	3.364137
C	3.552863	-2.013139	4.71154
H	4.57648	-1.607402	4.60077
H	3.638813	-2.883475	5.382771
H	2.909198	-1.281852	5.238473
C	3.891573	-3.539467	2.705899
H	4.894781	-3.120289	2.509163
H	3.460238	-3.923118	1.766801
H	4.012984	-4.387666	3.400452
C	1.548375	-3.127103	3.609703
H	1.670276	-3.996679	4.277095
H	1.098448	-3.471688	2.666147
H	0.858552	-2.41719	4.101142
C	0.010717	6.334992	-0.008495
H	0.955134	6.726681	0.41505
H	-0.808648	6.751666	0.601435
H	-0.083155	6.744912	-1.027643
C	-2.776113	-1.348444	-2.342994
C	-2.943769	-2.496882	-3.351998
C	-1.547253	-3.144737	-3.593778
H	-1.669979	-4.017318	-4.257086
H	-1.098248	-3.485377	-2.648358
H	-0.856267	-2.438057	-4.088274

C	-3.549859	-2.033899	-4.702042
H	-3.637054	-2.907638	-5.368679
H	-2.904817	-1.306537	-5.232734
H	-4.572789	-1.625814	-4.593676
C	-3.891298	-3.549537	-2.688857
H	-4.894187	-3.128235	-2.495058
H	-3.461016	-3.928693	-1.747456
H	-4.013158	-4.401276	-3.378977
N	-0.980232	-1.749878	1.156968
O	-1.058632	-2.943128	1.360937
N	0.976418	-1.755716	-1.144538
O	1.053805	-2.950183	-1.341723

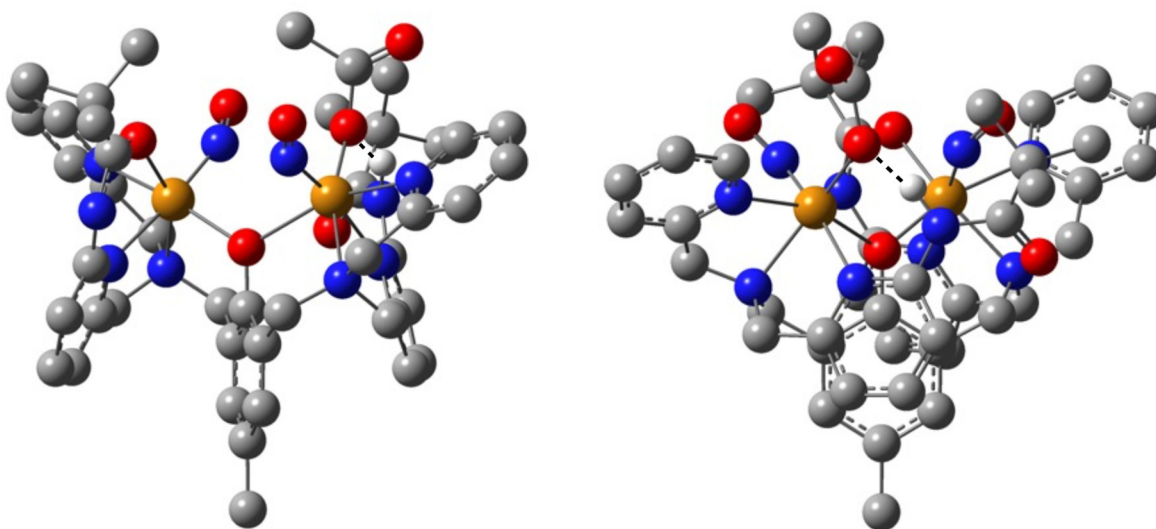


Figure S26. DFT-optimized structure of **1(NO)₂** using BP86/TZVP with hydrogen atoms (except for the hydrogen bonding amide N-H group) omitted for clarity. Hydrogen bonds are shown with dashed lines. The structure is shown in two different orientations for clarity.

Table S16. DFT-optimized coordinates (Å) of **1(NO)₂** using BP86/TZVP.

	X	Y	Z
Fe	-1.89043600	-0.69640300	-0.55018600
Fe	1.87933800	0.25664400	-0.28445600
O	0.12868000	-0.43871800	0.63493800
O	-0.79270600	4.17093500	1.16315400
O	2.32163800	-1.12132600	-1.86475800
N	-2.23939200	2.68479900	0.18151200
H	-2.40378700	2.22320400	-0.72953800
N	-2.64685300	0.56743300	1.14355200

N	-3.90585000	-1.45495100	-1.08457100
N	-2.39736400	-2.25573200	0.98442000
N	2.35858000	1.46143800	1.50298500
N	3.68098100	1.45418800	-0.82275300
N	3.04081700	-1.19029000	0.86251100
N	2.86864800	-3.00737500	-0.67282900
H	3.04175600	-4.00654300	-0.78461300
C	-1.52635500	3.89705300	0.21175600
C	-2.51523700	1.91413400	1.30746300
C	-2.74087000	2.53608600	2.55440900
H	-2.62566100	3.61391200	2.64160600
C	-3.12190800	1.76436600	3.63903400
H	-3.31684500	2.23487100	4.60446100
C	-3.27871100	0.38399200	3.47390500
H	-3.58680000	-0.25435600	4.30251100
C	-3.03681800	-0.16918700	2.22144300
C	-3.30303700	-1.63614100	1.99175700
H	-3.25675900	-2.18506100	2.94701000
H	-4.33269400	-1.73591800	1.61308400
C	-4.80762500	-0.81308400	-1.85785300
H	-4.52488800	0.17976900	-2.21630800
C	-6.02273500	-1.40171800	-2.21414900
H	-6.72053300	-0.84974300	-2.84456600
C	-6.31598600	-2.68647100	-1.75421500
H	-7.25850000	-3.17074400	-2.01604000
C	-5.38683700	-3.34271200	-0.94063700
H	-5.58939700	-4.34064800	-0.54704800
C	-4.18953900	-2.69786600	-0.62855100
C	-3.12680300	-3.32042800	0.24787300
H	-3.57769900	-4.04950500	0.94566100
H	-2.39810600	-3.87261700	-0.36744600
C	-1.14950600	-2.82351900	1.59963000
H	-0.50302200	-3.12178700	0.75849400
H	-1.41176100	-3.73226200	2.17209600
C	-0.46057900	-1.84347000	2.50662400
C	-0.43146000	-2.07233400	3.88915200
H	-0.85735700	-3.00514600	4.27309900
C	0.11094800	-1.14909800	4.79482000
C	0.61857400	0.04177400	4.25576200
H	1.01549400	0.80468500	4.93344800
C	0.62700300	0.30193700	2.87862400
C	0.10846000	-0.65948800	1.97143400
C	1.14066900	1.61871600	2.36652600
H	0.38426400	2.14792400	1.76595700
H	1.39289700	2.27494200	3.21918200
C	2.83244300	2.78437900	1.01984300

H	3.28188600	3.37243800	1.84027900
H	1.95368200	3.35124300	0.66943900
C	3.82454600	2.59346600	-0.10544800
C	4.81764000	3.52985700	-0.40565100
H	4.91563000	4.43362900	0.19867600
C	5.67144100	3.29094900	-1.48502100
H	6.45083800	4.01054200	-1.74174800
C	5.51489600	2.11638000	-2.22695900
H	6.16159700	1.89173900	-3.07574900
C	4.50743300	1.22440300	-1.86392900
H	4.33377400	0.29858500	-2.41405100
C	3.45002400	0.76565700	2.24462300
H	3.42602200	1.04158400	3.31173600
H	4.41301200	1.11775400	1.83990600
C	3.42183800	-0.73334100	2.08458300
C	3.87635700	-1.58171000	3.09308200
H	4.16580100	-1.17433200	4.06201400
C	3.94564200	-2.95381700	2.83836300
H	4.29014500	-3.64570000	3.60862300
C	3.58986500	-3.42929800	1.58143900
H	3.66172800	-4.49196300	1.34224600
C	3.14909700	-2.51054300	0.61430300
C	-1.80126600	4.89464700	-0.92890100
C	-2.19924900	4.23389300	-2.25970500
H	-1.39475800	3.59392600	-2.65169800
H	-2.38461000	5.01772500	-3.00846400
H	-3.12134400	3.63907200	-2.18918900
C	-0.56279800	5.78722500	-1.13059400
H	0.28879700	5.20731900	-1.51919800
H	-0.25776600	6.26276500	-0.18955800
H	-0.79194700	6.57578200	-1.86187400
C	-2.98580600	5.76187300	-0.41469000
H	-3.22829900	6.52293400	-1.17142200
H	-2.72399200	6.27910500	0.51949900
H	-3.88822100	5.15539600	-0.24522800
C	0.09997300	-1.40263700	6.28291100
H	-0.82219300	-1.01489600	6.74631200
H	0.94391600	-0.90842500	6.78465700
H	0.15045100	-2.47690800	6.51013900
C	2.61274500	-2.33798400	-1.83939600
C	2.78667400	-3.14462400	-3.14019400
C	1.88228500	-2.55586800	-4.23885500
H	2.08522300	-3.07209300	-5.18768000
H	2.07320800	-1.48509900	-4.38412400
H	0.81796900	-2.69117000	-4.00139900
C	2.47198600	-4.64551400	-2.95409300

H	2.53313500	-5.14451300	-3.93129500
H	1.45661700	-4.81278200	-2.56444700
H	3.19994300	-5.16963300	-2.31039200
C	4.27755600	-2.97666600	-3.54937700
H	4.96614700	-3.36409200	-2.78311400
H	4.52172400	-1.92243600	-3.74361200
H	4.45716000	-3.53784700	-4.47792100
N	1.03754900	1.39748100	-1.31187100
O	1.03344000	2.40629000	-1.90479900
N	-1.21271900	-1.85698900	-1.65400200
O	-1.36979900	-2.58459700	-2.57060600
O	-1.98781100	0.80270600	-1.79773600
C	-2.14676900	0.85910000	-3.13711200
O	-3.22187300	1.17814300	-3.62979000
C	-0.92901300	0.57478800	-3.99565600
H	-0.14683400	0.02236800	-3.46168100
H	-1.23913200	0.02939200	-4.89647700
H	-0.50982900	1.53689600	-4.32968800

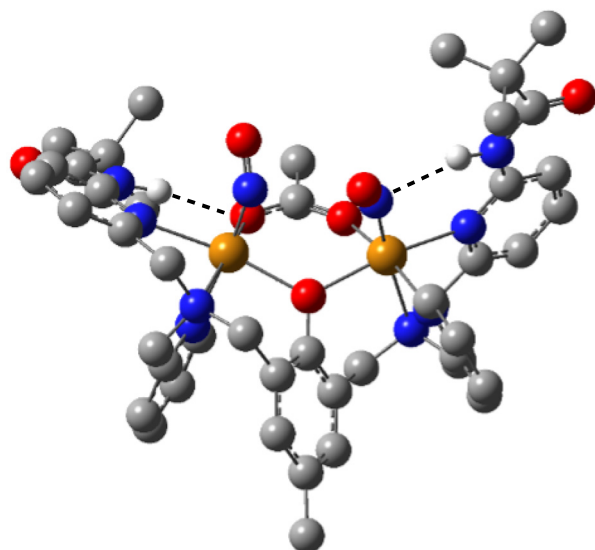


Figure S27. DFT-optimized structure of **2(NO)₂** using BP86/TZVP with hydrogen atoms (except for amide N-H groups) omitted for clarity. Hydrogen bonds are shown with dashed lines.

Table S17. DFT-optimized coordinates (Å) of **2(NO)₂** using BP86/TZVP.

	X	Y	Z
Fe	-1.86645700	0.06316500	-0.30133800
Fe	1.71952400	-0.00285200	0.64784200
O	-0.07774000	1.07697500	0.20810000
O	-0.65038400	-1.25976200	-1.37948600
O	1.56247000	-1.34506800	-0.90007200

O	-6.61180100	-3.30889000	0.17347600
O	6.64216200	-2.82231700	-0.19791800
N	-3.04207700	1.71251600	0.48967700
N	-2.05973000	1.37625500	-2.06278100
N	-3.57612600	-0.86871900	-1.53682100
N	2.86884600	1.31227900	-0.63642000
N	2.21858500	1.68245600	2.03617400
N	3.63061400	-0.63199700	1.68936600
N	-4.62146900	-2.14597700	0.12811800
H	-3.81340100	-1.87897000	0.68834000
N	4.46796700	-2.09773300	0.05084600
H	3.56954900	-1.97670200	-0.42704600
C	-3.30908700	1.93866100	1.79618300
H	-2.93613600	1.20244300	2.50904000
C	-4.02330300	3.04709500	2.23919600
H	-4.22083600	3.17364900	3.30400100
C	-4.46887500	3.97951300	1.29743800
H	-5.03090000	4.86193900	1.60851900
C	0.49619600	-1.78704400	-1.48199100
C	-4.18027300	3.76229800	-0.04853200
H	-4.50493800	4.47044300	-0.81296200
C	0.62859500	-3.02145300	-2.34477100
H	-0.22635400	-3.11236600	-3.02398800
H	0.64180100	-3.90670200	-1.68902800
H	1.56959900	-3.01711600	-2.90805600
C	-3.46671400	2.61893500	-0.42366700
C	-3.21699000	2.29558400	-1.87106900
H	-4.11753300	1.79595500	-2.26437500
H	-3.08217500	3.22011000	-2.45732800
C	3.00334000	1.16098900	-1.97288800
H	2.55244900	0.26062100	-2.39116900
C	3.68546000	2.07561900	-2.77009600
H	3.77657400	1.90273100	-3.84292300
C	4.24368500	3.20580800	-2.16454000
H	4.78368700	3.94651700	-2.75710700
C	4.10469100	3.36855400	-0.78663600
H	4.53054300	4.23663500	-0.28013100
C	3.41597900	2.40017300	-0.04773900
C	3.33824100	2.48155300	1.45853600
H	4.28493600	2.08669900	1.86161500
H	3.27049500	3.53330500	1.78155200
C	-0.79827900	2.14308900	-2.32770700
H	-0.92572300	2.74551600	-3.24568100
H	-0.02127800	1.38716300	-2.52162200
C	-0.38135900	3.02567800	-1.18326800
C	-0.30286300	4.41832000	-1.31477600

H	-0.59485300	4.87607700	-2.26543600
C	0.15776900	5.24237300	-0.27441700
C	0.19337700	6.74384900	-0.42022900
H	0.31143700	7.04538500	-1.47046700
H	1.01683600	7.18786300	0.15674600
H	-0.74068500	7.19980000	-0.05241300
C	0.57653000	4.61400800	0.91099200
H	0.95989400	5.22837200	1.73201700
C	0.51757600	3.22495000	1.07659400
C	0.00855900	2.42112000	0.03209500
C	1.02213600	2.54478900	2.32047800
H	1.28663400	3.29520900	3.08760100
H	0.25366400	1.87846200	2.74277700
C	-4.57360600	-1.73965600	-1.19873400
C	-5.49589500	-2.21613500	-2.15946800
H	-6.28087600	-2.89451500	-1.83510900
C	-5.37949500	-1.79437100	-3.47333500
H	-6.08758300	-2.15425900	-4.22198600
C	-4.35502900	-0.90870100	-3.82910200
H	-4.24116500	-0.55250200	-4.85381300
C	-3.47816200	-0.48170100	-2.83945200
C	-2.33610000	0.44210200	-3.18607500
H	-1.42243000	-0.14724800	-3.35367100
H	-2.56255400	0.99528200	-4.11511900
C	4.57620400	-1.54346400	1.32239500
C	5.61000500	-1.91515800	2.21420600
H	6.34648200	-2.64522400	1.89220200
C	5.67870200	-1.31817500	3.46197100
H	6.47325400	-1.60162500	4.15440100
C	4.73293700	-0.35028800	3.82188600
H	4.77695100	0.15896400	4.78553200
C	3.72119800	-0.05105800	2.91936500
C	2.66144600	0.97233000	3.26240600
H	1.77540000	0.48439900	3.70132500
H	3.05457900	1.67629400	4.01829200
C	-5.60822400	-2.94470400	0.76349700
C	-5.31525900	-3.29379900	2.24057600
C	-6.42353900	-4.24173300	2.73320500
H	-7.41489300	-3.77689100	2.65190900
H	-6.24295800	-4.49741400	3.78754300
H	-6.44404200	-5.17204700	2.14942200
C	-3.94475100	-4.00015200	2.36519000
H	-3.90498000	-4.90517900	1.74113200
H	-3.78731000	-4.30615400	3.41006400
H	-3.09588200	-3.35581800	2.08692600
C	-5.33977700	-1.99772300	3.08675100

H	-4.54626600	-1.28897400	2.80263900
H	-5.18894400	-2.25107900	4.14672600
H	-6.30840200	-1.48421000	2.99681800
C	5.51082900	-2.76177900	-0.65066200
C	5.10660700	-3.41522900	-1.99028900
C	6.37240100	-4.00101500	-2.64062600
H	7.11615400	-3.21960400	-2.84888900
H	6.10340600	-4.48760900	-3.58981100
H	6.84829100	-4.74651800	-1.99043900
C	4.10314800	-4.55656500	-1.69588500
H	4.55227400	-5.31479900	-1.03780200
H	3.82457300	-5.05406400	-2.63730300
H	3.18184700	-4.19399100	-1.21591000
C	4.48539900	-2.36831800	-2.94190300
H	3.55229300	-1.93782400	-2.54649500
H	4.25144900	-2.84556500	-3.90576600
H	5.19005400	-1.54632200	-3.13922800
N	-1.91892900	-0.81024000	1.20935400
O	-1.88983800	-0.74000200	2.38718900
N	0.96166700	-1.16093800	1.72872700
O	1.01041400	-2.25556400	2.14752500