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Supporting Information

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Preparation of the Elusive [(por)Fe(NO)(O-ligand)] Complex by Diffusion of Nitric Oxide into a Crystal of the Precursor**

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PART A: Density Functional Theory (DFT) Calculations

All geometry optimizations and frequency calculations were performed with the program package Gaussian 03[1] using the BP86[2-3] functional and TZVP[4-5] basis set. In Gaussian calculations, convergence was reached when the relative change in the density matrix between subsequent iterations was less that 1×10^{-8}. Molecular orbitals were obtained from BP86/TZVP single point calculations using ORCA.[6] Molecular orbitals were plotted with the program orca_plot included in the ORCA package and visualized using GaussView. Force constants in internal coordinates were extracted from the Gaussian output using a modified version of the program Redong (QCPE 628).[7-8]

References

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Table S1. Geometric and vibrational parameters of selected (P)Fe(NO)(X)$^{0/1+}$ complexes. All data is experimental unless otherwise indicated.

	Geometric Parameters [Å] [°]					Frequencies [cm^{-1}]	
Complex	**ΔFe-NO**	**ΔN-O**	**< Fe-X-O**	**ΔFe-X**	**ΔFe-Np**	***v*(N-O)**	***v*(Fe-NO)**
calc. (P)Fe(NO)(MeIm)$^{1+}$	1.644	1.147	180	2.018	2.022	1933	639
(OEP)Fe(NO)(MeIm)(ClO_4)	1.646	1.135	177	1.988	2.003	1921	-
(TPP)Fe(NO)(MeIm)(BF_4)	-	-	-	-	-	1896	580
calc. (P)Fe(NO)(OC(=O)CF_3)	1.637	1.155	175.8	1.936	2.025	1898	649
calc. (P)Fe(NO)(OC(=O)CH_3)	1.656	1.158	170.6	1.905	2.027	1871	644
(TPP)Fe(NO)(OC(=O)CF_3)	1.618	1.151	175.8	1.899	2.011	1907	-
calc. (P)Fe(NO)(NO_2)	1.676	1.158	165.4	2.067	2.025	1854	596
(TPP)Fe(NO)(NO_2)	1.671	1.144	169	1.998	1.996	1874	-
calc. (P)Fe(NO)(SPh)	1.685	1.162	164.4	2.343	2.027	1829	584
(OEP)Fe(NO)(SR-H_2)	1.671	1.187	160	2.356	2.01	1850	549

Table S2. Charge contributions of important molecular orbital of (P)Fe(NO)(OC(=O)CF_3) calculated with BP86/TZVP.

			Fe		N		O	$OC(=O)CF_3^-$
MO #	**label**	**energy**	**d**	**s**	**p**	**s**	**p**	**s+p**
<129>	π^*_y_d_{yz}	-0.15192	28.3	0	40.8	0	24.3	0.8
<128>	π^*_x_d_{xz} (LUMO)	-0.15303	31.8	0.5	36.1	0.1	21.9	3.0
<127>	A_{2u} (HOMO)	-0.19883	0.7	0.2	0.1	0	0	1.5
<125>	$OC(=O)CF_3^-$ (σ) + d_{z^2}_σ*	-0.2196	3.1	0.3	0.1	0	0.1	4.0
<115>	d_{yz}_π^*_y	-0.2998	46.9	0	3.6	0	10.6	3.0
<114>	d_{xz}_π^*_x	-0.30115	48.2	0	4.0	0	12.2	6.0
<71>	σ_{nb}_d_{z^2}	-0.53473	4.8	2.6	18.2	11.4	32.3	1.9

Table S3. BP86/TZVP calculated force constants and stretching frequencies of $(P)Fe(NO)(X)^{0/1+}$ complexes.

	Calculated Force Constants (mdyn/Å)			Calculated Frequencies (cm^{-1})	
Complex	N-O	Fe-NO	Fe-X[a]	ν(N-O)	ν(Fe-NO)
$(P)Fe(NO)(MeIm)^{1+}$	15.62	4.82	1.48	1933	639
$(P)Fe(NO)(OC(=O)CF_3)$	14.87	5.14	1.62	1898	649
$(P)Fe(NO)(OC(=O)CH_3)$	14.54	4.67	1.90	1871	644
$(P)Fe(NO)(NO_2)$	14.43	4.24	1.29	1854	596
(P)Fe(NO)(SPh)	14.03	3.99	1.16	1829	584

Table S4. Charge contributions of important molecular orbital of $(P)Fe(NO)(X)^{0/1+}$ calculated with BP86/TZVP.

		π-backbond							**dz^2/dxz_σ***						
		Fe		**N**		**O**	**X**		**Fe**		**N**		**O**	**X**	
Complex	**MO**	**d**	**s**	**p**	**s**	**p**	**s+p**	**MO**	**d**	**s**	**p**	**s**	**p**	**s+p**	**ref**
$(P)Fe(NO)(MeIm)^{1+}$	<124>π*_dyz	27	0	42	0	26	0	<122>	1	0.2	0.1	0	0	2	1
	<123> π*_dxz	27	0	42	0	26	0								
$(P)Fe(NO)(OC(=O)CF_3)$	<129> π*_dyz	28.3	0	40.8	0	24.3	0.8	<125>	3.1	0.3	0.1	0	0.1	4	tw
	<128> π*_dxz	31.8	0.5	36.1	0.1	21.9	3								
$(P)Fe(NO)(NO_2)$	<113> π*_dxz	27.5	0	41.5	0	24.6	0	*<108> + <109>*	*14.6*	*1.4*	*1*	*0.1*	*0.9*	*8*	tw
	<112> π*_dyz/dz^2	28.4	0.5	33.1	0.1	20.7	3.8								
(P)Fe(NO)(SPh)	<130> π*_dz^2/dxz	25.4	0	42.2	0	25	0.1	<124> + <127>	14.6	1.5	1.3	0	1.1	26.6	2
	<129> π*_dyz_pz(S)	31.8	0.8	28.3	0.2	17.4	10.8								

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Part B: X-ray Crystallographic Determination of (TPP)Fe(OC(=O)CF$_3$) (1)

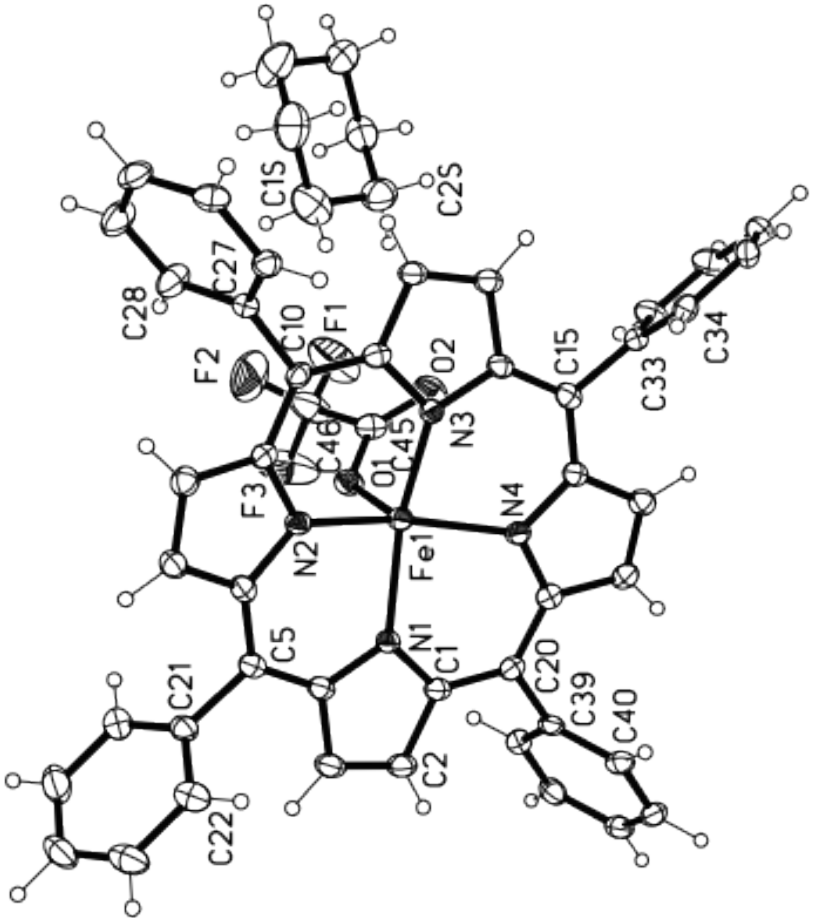

Figure S1. Molecular structure of (TPP)Fe(OC(=O)CF$_3$) (**1**).

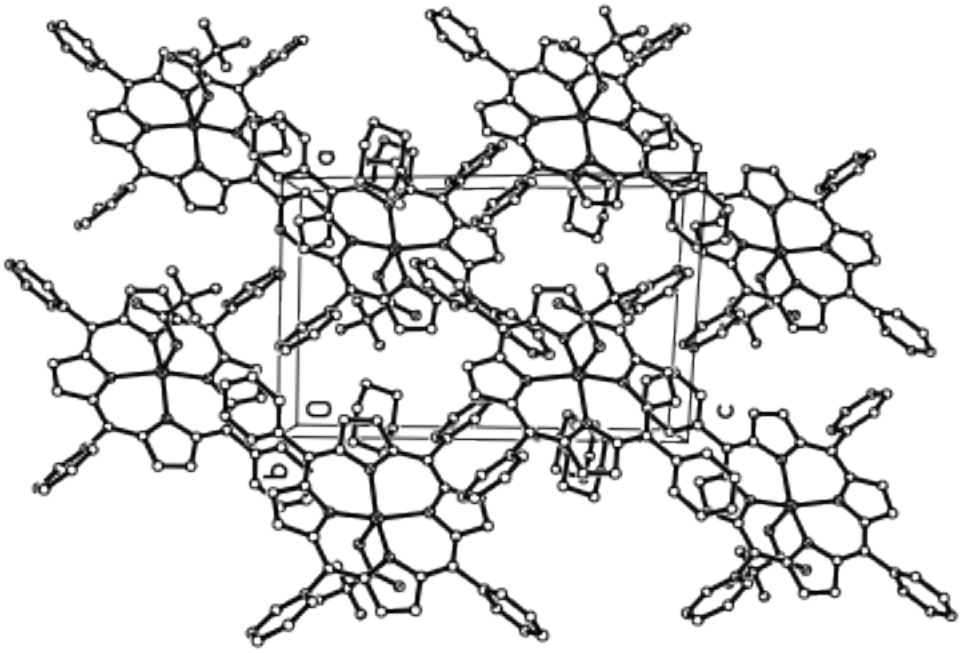

Figure S2. Crystal packing of (TPP)Fe(OC(=O)CF_3) (**1**), with displacement ellipsoids drawn at the 50% probability level.

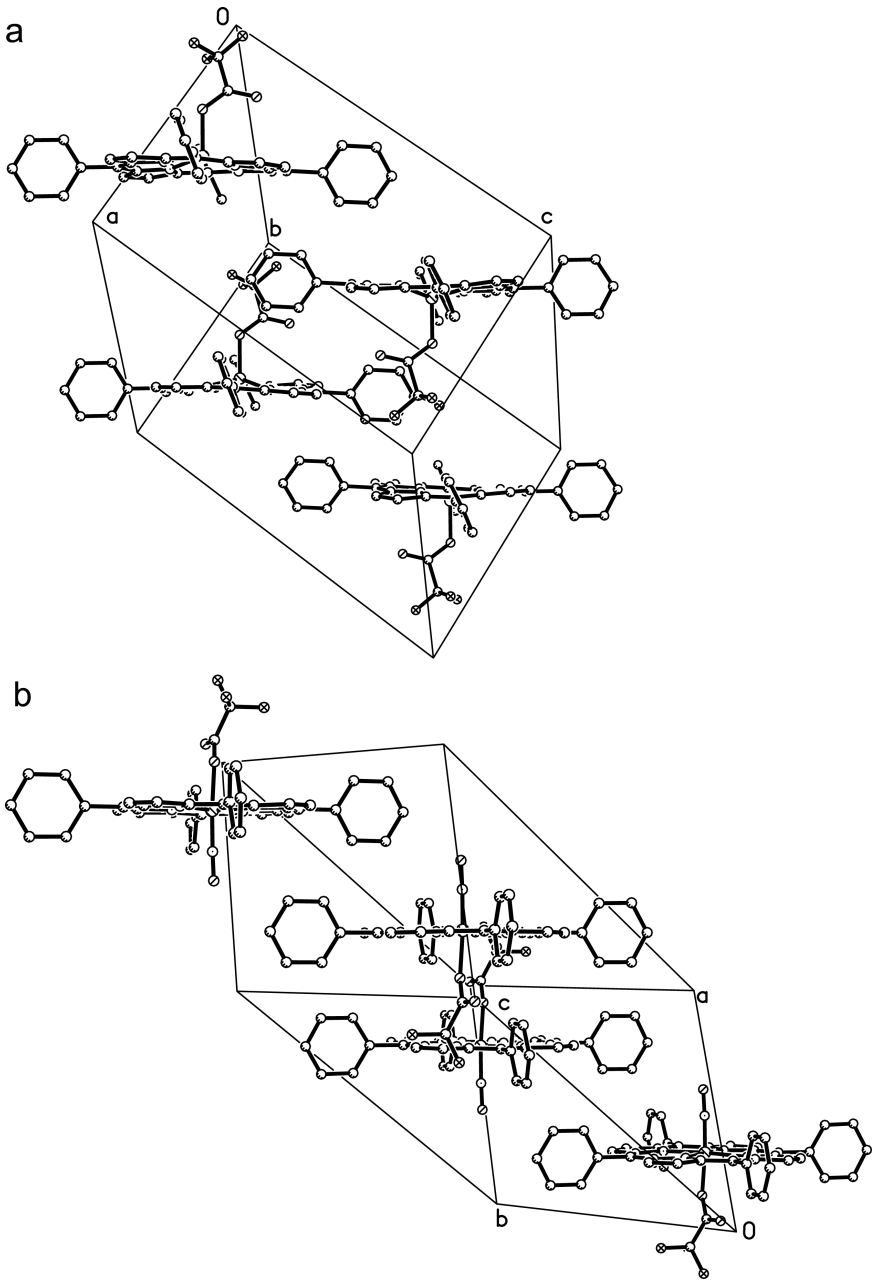

Figure S3. Comparison of the unit cell of (TPP)Fe(OC(=O)CF_3) (**1**; a) with that of (TPP)Fe(NO)(OC(=O)CF_3) (**2**; b)

Experimental

A black prism-shaped crystal of dimensions 0.30 x 0.30 x 0.26 mm was selected for structural analysis. Intensity data for this compound were collected using a diffractometer with a Bruker APEX ccd area detector (*1*) and graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The sample was cooled to 100(2) K. Cell parameters were determined from a non-linear least squares fit of 8966 peaks in the range $2.25 < \theta < 28.29°$. A total of 24156 data were measured in the range $1.86 < \theta < 28.31°$ using Φ and ω oscillation frames. The data were corrected for absorption by the Semi-empirical from equivalents method (*2*) giving minimum and maximum transmission factors of 0.8840 and 0.8983. The data were merged to form a set of 10322 independent data with R(int) = 0.0371 and a coverage of 100.0 %.

The Triclinic space group $P\bar{1}$ was determined by systematic absences and statistical tests and verified by subsequent refinement. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2 (*3*). Hydrogen atom positions of hydrogens bonded to carbons were initially determined by geometry and refined by a riding model. Hydrogens bonded to nitrogens and oxygens were located on a difference map, and their positions were refined independently. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atom displacement parameters were set to 1.2 (1.5 for methyl) times the isotropic equivalent displacement parameters of the bonded atoms. A total of 563 parameters were refined against 0 restraints and 10322 data to give $wR(F^2) = 0.1407$ and S = 0.986 for weights of $w = 1/[\sigma^2 (F^2) + (? P)2 + ? P]$, where $P = [Fo^2 + 2Fc^2] / 3$. The final R(F) was 0.0524 for the 7973 observed, $[F > 4\sigma(F)]$, data. The largest shift/s.u. was 0.000 in the final refinement cycle. The final difference map had maxima and minima of 0.564 and -0.513 e/Å^3, respectively. The absolute structure was determined by refinement of the Flack parameter (*4*). The polar axis restraints were taken from Flack and Schwarzenbach (*5*).

Note: In the difference map before this model, a large (>3 e-/Å^3) peak was located near (0.99 Å from the iron, across the TPP ring). In this model, this extra peak is modeled as disordered Fe (i.e., Fe1 in the Tables). Note that the trifluoroacetate bonded to this alternate Fe could not be located in the subsequent difference map.

References

(1) (a) Data Collection: SMART Software Reference Manual (2007). Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373, USA. (b) Data Reduction: SAINT

Software Reference Manual (2007). B ruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA.
(2) G. M. Sheldrick (2001). SADABS. Program for Empirical Absorption Correction of Area Detector Data. University of Göttingen, Germany.
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Table S5. Crystal data and structure refinement for **1**•(C_6H_{12})

Empirical formula	$C_{52}H_{40}F_3Fe_1N_4O_2$	
Formula weight	865.73	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	*a* = 11.2285(9) Å	α = 72.885(2)°
	b = 12.0522(9) Å	β = 82.233(2)°
	c = 17.1643(13) Å	γ = 70.680(2)°
Volume	2093.1(3) $Å^3$	
Z, Z'	2	
Density (calculated)	1.374 Mg/m3	
Wavelength	0.71073 Å	
Temperature	100(2) K	
F(000)	898	
Absorption coefficient	0.421 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8983 and 0.8840	
Theta range for data collection	1.86 to 28.31°	
Reflections collected	24156	
Independent reflections	10322 [R(int) = 0.0371]	
Data / restraints / parameters	10322 / 0 / 563	
wR(F2 all data)	wR2 = 0.1407	
R(F obsd data)	R1 = 0.0524	
Goodness-of-fit on F2	0.986	
Observed data [I > 2s(I)]	7973	
Largest and mean shift / s.u.	0.000and 0.000	
Largest diff. peak and hole	0.564 and -0.513 e/$Å^3$	

$wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$

$R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$

Table S6. Atomic coordinates and equivalent isotropic displacement parameters for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0.26209(3)	0.30443(3)	0.726616(19)	0.01530(10)
Fe(1')	0.1973(6)	0.2668(5)	0.7193(4)	0.01530(10)
F(1)	0.64297(19)	0.4450(2)	0.76183(14)	0.0734(7)
F(2)	0.5785(2)	0.3210(2)	0.85968(13)	0.0791(7)
F(3)	0.46639(19)	0.5069(2)	0.82427(17)	0.0887(9)
O(1)	0.36672(15)	0.37140(15)	0.76814(10)	0.0253(4)
O(2)	0.52313(17)	0.37749(16)	0.67049(11)	0.0332(4)
N(1)	0.08486(17)	0.41629(16)	0.74828(11)	0.0183(4)
N(2)	0.23232(17)	0.17847(16)	0.83318(11)	0.0185(4)
N(3)	0.39282(17)	0.16133(16)	0.69140(11)	0.0180(4)
N(4)	0.24192(17)	0.39711(16)	0.60553(11)	0.0187(4)
C(1)	0.0230(2)	0.52865(19)	0.69817(14)	0.0202(4)
C(2)	-0.0868(2)	0.5897(2)	0.74096(15)	0.0257(5)
C(3)	-0.0913(2)	0.5150(2)	0.81645(15)	0.0272(5)
C(4)	0.0147(2)	0.4063(2)	0.82117(14)	0.0207(5)
C(5)	0.0381(2)	0.3052(2)	0.88918(14)	0.0201(5)
C(6)	0.1375(2)	0.1978(2)	0.89275(13)	0.0196(4)
C(7)	0.1578(2)	0.0912(2)	0.96069(14)	0.0229(5)
C(8)	0.2656(2)	0.0080(2)	0.94329(14)	0.0236(5)
C(9)	0.3129(2)	0.06231(19)	0.86421(13)	0.0191(4)
C(10)	0.4236(2)	0.00525(19)	0.82462(13)	0.0190(4)
C(11)	0.4607(2)	0.05363(19)	0.74393(14)	0.0193(4)
C(12)	0.5745(2)	-0.0031(2)	0.70220(14)	0.0220(5)
C(13)	0.5743(2)	0.0676(2)	0.62538(14)	0.0212(5)
C(14)	0.4616(2)	0.17028(19)	0.61746(13)	0.0186(4)
C(15)	0.4295(2)	0.26527(19)	0.54664(14)	0.0194(4)
C(16)	0.3261(2)	0.37087(19)	0.54161(13)	0.0186(4)
C(17)	0.2946(2)	0.4698(2)	0.46913(14)	0.0222(5)
C(18)	0.1924(2)	0.5566(2)	0.48917(14)	0.0225(5)
C(19)	0.1588(2)	0.51157(19)	0.57342(13)	0.0194(4)
C(20)	0.0578(2)	0.57556(19)	0.61663(14)	0.0194(4)
C(21)	-0.0518(2)	0.3136(2)	0.96179(14)	0.0228(5)
C(22)	-0.1691(2)	0.2981(2)	0.96111(17)	0.0311(6)
C(23)	-0.2558(3)	0.3105(2)	1.02647(18)	0.0360(6)
C(24)	-0.2256(3)	0.3395(2)	1.09174(17)	0.0388(7)
C(25)	-0.1095(3)	0.3564(3)	1.09240(17)	0.0400(7)
C(26)	-0.0227(3)	0.3431(2)	1.02706(15)	0.0316(6)
C(27)	0.5059(2)	-0.11513(19)	0.87179(14)	0.0204(5)

C(28)	0.5674(3)	-0.1210(2)	0.93822(16)	0.0307(6)
C(29)	0.6389(3)	-0.2322(2)	0.98601(17)	0.0351(6)
C(30)	0.6511(2)	-0.3393(2)	0.96630(15)	0.0282(5)
C(31)	0.5922(2)	-0.3339(2)	0.89910(15)	0.0253(5)
C(32)	0.5195(2)	-0.2230(2)	0.85206(14)	0.0221(5)
C(33)	0.5128(2)	0.25403(19)	0.47176(13)	0.0189(4)
C(34)	0.5166(2)	0.1662(2)	0.43250(14)	0.0211(5)
C(35)	0.5966(2)	0.1533(2)	0.36469(13)	0.0233(5)
C(36)	0.6737(2)	0.2268(2)	0.33462(14)	0.0255(5)
C(37)	0.6693(2)	0.3152(2)	0.37272(16)	0.0294(6)
C(38)	0.5900(2)	0.3280(2)	0.44107(15)	0.0268(5)
C(39)	-0.0180(2)	0.7023(2)	0.57448(14)	0.0206(5)
C(40)	-0.0926(2)	0.7235(2)	0.51008(14)	0.0229(5)
C(41)	-0.1637(2)	0.8421(2)	0.47189(15)	0.0257(5)
C(42)	-0.1595(2)	0.9391(2)	0.49772(15)	0.0271(5)
C(43)	-0.0863(2)	0.9186(2)	0.56255(15)	0.0273(5)
C(44)	-0.0162(2)	0.8006(2)	0.60069(14)	0.0242(5)
C(45)	0.4737(2)	0.3855(2)	0.73635(16)	0.0259(5)
C(46)	0.5410(3)	0.4162(3)	0.7949(2)	0.0449(8)
C(1S)	0.7910(3)	0.0978(3)	0.7835(2)	0.0490(8)
C(2S)	0.8362(3)	0.1798(3)	0.70737(19)	0.0425(7)
C(3S)	0.9688(3)	0.1793(3)	0.71612(18)	0.0391(7)
C(4S)	1.0603(3)	0.0508(3)	0.73388(18)	0.0419(7)
C(5S)	1.0142(3)	-0.0320(3)	0.8087(2)	0.0581(9)
C(6S)	0.8817(3)	-0.0316(3)	0.8002(2)	0.0502(8)

Table S7. Bond lengths [Å] and angles [°] for **1**.

Fe(1)-O(1)	1.9319(16)
Fe(1)-N(3)	2.0477(18)
Fe(1)-N(4)	2.0523(19)
Fe(1)-N(1)	2.0581(18)
Fe(1)-N(2)	2.0733(18)
Fe(1')-N(2)	1.954(6)
Fe(1')-N(1)	1.985(6)
Fe(1')-N(3)	2.212(6)
Fe(1')-N(4)	2.232(6)
F(1)-C(46)	1.313(3)
F(2)-C(46)	1.336(4)
F(3)-C(46)	1.324(3)
O(1)-C(45)	1.294(3)
O(2)-C(45)	1.206(3)
N(1)-C(4)	1.381(3)
N(1)-C(1)	1.382(3)
N(2)-C(6)	1.384(3)
N(2)-C(9)	1.384(3)
N(3)-C(11)	1.386(3)
N(3)-C(14)	1.388(3)
N(4)-C(19)	1.385(3)
N(4)-C(16)	1.387(3)
C(1)-C(20)	1.401(3)
C(1)-C(2)	1.440(3)
C(2)-C(3)	1.348(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.439(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.397(3)
C(5)-C(6)	1.393(3)
C(5)-C(21)	1.500(3)
C(6)-C(7)	1.435(3)
C(7)-C(8)	1.355(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.437(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.400(3)
C(10)-C(11)	1.400(3)
C(10)-C(27)	1.496(3)
C(11)-C(12)	1.440(3)
C(12)-C(13)	1.343(3)
C(12)-H(12)	0.9500

C(13)-C(14)	1.436(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.394(3)
C(15)-C(16)	1.400(3)
C(15)-C(33)	1.496(3)
C(16)-C(17)	1.436(3)
C(17)-C(18)	1.357(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.433(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.401(3)
C(20)-C(39)	1.495(3)
C(21)-C(26)	1.378(4)
C(21)-C(22)	1.391(3)
C(22)-C(23)	1.392(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.380(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.386(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.393(4)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(28)	1.384(3)
C(27)-C(32)	1.393(3)
C(28)-C(29)	1.390(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.388(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.381(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.388(3)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(38)	1.392(3)
C(33)-C(34)	1.399(3)
C(34)-C(35)	1.384(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.385(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.389(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.388(3)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500

C(39)-C(40)	1.390(3)
C(39)-C(44)	1.393(3)
C(40)-C(41)	1.395(3)
C(40)-H(40)	0.9500
C(41)-C(42)	1.383(4)
C(41)-H(41)	0.9500
C(42)-C(43)	1.387(4)
C(42)-H(42)	0.9500
C(43)-C(44)	1.387(3)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-C(46)	1.526(4)
C(1S)-C(6S)	1.522(5)
C(1S)-C(2S)	1.527(4)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900
C(2S)-C(3S)	1.515(4)
C(2S)-H(2S1)	0.9900
C(2S)-H(2S2)	0.9900
C(3S)-C(4S)	1.517(4)
C(3S)-H(3S1)	0.9900
C(3S)-H(3S2)	0.9900
C(4S)-C(5S)	1.523(4)
C(4S)-H(4S1)	0.9900
C(4S)-H(4S2)	0.9900
C(5S)-C(6S)	1.512(5)
C(5S)-H(5S1)	0.9900
C(5S)-H(5S2)	0.9900
C(6S)-H(6SA)	0.9900
C(6S)-H(6SB)	0.9900

O(1)-Fe(1)-N(3)	102.21(7)
O(1)-Fe(1)-N(4)	105.86(7)
N(3)-Fe(1)-N(4)	88.21(7)
O(1)-Fe(1)-N(1)	100.93(7)
N(3)-Fe(1)-N(1)	156.78(7)
N(4)-Fe(1)-N(1)	87.39(7)
O(1)-Fe(1)-N(2)	98.90(7)
N(3)-Fe(1)-N(2)	87.20(7)
N(4)-Fe(1)-N(2)	155.23(7)
N(1)-Fe(1)-N(2)	87.31(7)
N(2)-Fe(1')-N(1)	92.8(3)
N(2)-Fe(1')-N(3)	85.8(2)
N(1)-Fe(1')-N(3)	146.7(3)
N(2)-Fe(1')-N(4)	148.6(3)

N(1)-Fe(1')-N(4)	84.4(2)
N(3)-Fe(1')-N(4)	79.9(2)
C(45)-O(1)-Fe(1)	126.38(16)
C(4)-N(1)-C(1)	105.62(17)
C(4)-N(1)-Fe(1')	119.7(2)
C(1)-N(1)-Fe(1')	129.7(2)
C(4)-N(1)-Fe(1)	126.87(15)
C(1)-N(1)-Fe(1)	126.46(14)
C(6)-N(2)-C(9)	105.71(17)
C(6)-N(2)-Fe(1')	119.3(2)
C(9)-N(2)-Fe(1')	128.5(2)
C(6)-N(2)-Fe(1)	127.35(14)
C(9)-N(2)-Fe(1)	126.46(14)
C(11)-N(3)-C(14)	105.78(17)
C(11)-N(3)-Fe(1)	125.23(14)
C(14)-N(3)-Fe(1)	125.13(14)
C(11)-N(3)-Fe(1')	123.5(2)
C(14)-N(3)-Fe(1')	129.4(2)
C(19)-N(4)-C(16)	105.43(18)
C(19)-N(4)-Fe(1)	126.83(14)
C(16)-N(4)-Fe(1)	126.34(14)
C(19)-N(4)-Fe(1')	122.9(2)
C(16)-N(4)-Fe(1')	128.1(2)
N(1)-C(1)-C(20)	125.6(2)
N(1)-C(1)-C(2)	109.99(19)
C(20)-C(1)-C(2)	124.3(2)
C(3)-C(2)-C(1)	107.1(2)
C(3)-C(2)-H(2)	126.4
C(1)-C(2)-H(2)	126.4
C(2)-C(3)-C(4)	107.3(2)
C(2)-C(3)-H(3)	126.3
C(4)-C(3)-H(3)	126.3
N(1)-C(4)-C(5)	126.1(2)
N(1)-C(4)-C(3)	109.92(19)
C(5)-C(4)-C(3)	123.9(2)
C(6)-C(5)-C(4)	124.1(2)
C(6)-C(5)-C(21)	118.75(19)
C(4)-C(5)-C(21)	117.12(19)
N(2)-C(6)-C(5)	125.7(2)
N(2)-C(6)-C(7)	109.95(19)
C(5)-C(6)-C(7)	124.3(2)
C(8)-C(7)-C(6)	107.3(2)
C(8)-C(7)-H(7)	126.4
C(6)-C(7)-H(7)	126.4
C(7)-C(8)-C(9)	107.2(2)

C(7)-C(8)-H(8)	126.4
C(9)-C(8)-H(8)	126.4
N(2)-C(9)-C(10)	125.4(2)
N(2)-C(9)-C(8)	109.82(19)
C(10)-C(9)-C(8)	124.8(2)
C(9)-C(10)-C(11)	124.0(2)
C(9)-C(10)-C(27)	117.48(19)
C(11)-C(10)-C(27)	118.55(19)
N(3)-C(11)-C(10)	125.5(2)
N(3)-C(11)-C(12)	109.56(19)
C(10)-C(11)-C(12)	124.9(2)
C(13)-C(12)-C(11)	107.4(2)
C(13)-C(12)-H(12)	126.3
C(11)-C(12)-H(12)	126.3
C(12)-C(13)-C(14)	107.8(2)
C(12)-C(13)-H(13)	126.1
C(14)-C(13)-H(13)	126.1
N(3)-C(14)-C(15)	126.0(2)
N(3)-C(14)-C(13)	109.44(19)
C(15)-C(14)-C(13)	124.6(2)
C(14)-C(15)-C(16)	124.3(2)
C(14)-C(15)-C(33)	117.57(19)
C(16)-C(15)-C(33)	118.17(19)
N(4)-C(16)-C(15)	125.5(2)
N(4)-C(16)-C(17)	110.20(19)
C(15)-C(16)-C(17)	124.3(2)
C(18)-C(17)-C(16)	106.9(2)
C(18)-C(17)-H(17)	126.6
C(16)-C(17)-H(17)	126.6
C(17)-C(18)-C(19)	107.5(2)
C(17)-C(18)-H(18)	126.2
C(19)-C(18)-H(18)	126.2
N(4)-C(19)-C(20)	125.4(2)
N(4)-C(19)-C(18)	109.99(19)
C(20)-C(19)-C(18)	124.6(2)
C(19)-C(20)-C(1)	124.0(2)
C(19)-C(20)-C(39)	118.86(19)
C(1)-C(20)-C(39)	117.12(19)
C(26)-C(21)-C(22)	119.6(2)
C(26)-C(21)-C(5)	120.8(2)
C(22)-C(21)-C(5)	119.4(2)
C(21)-C(22)-C(23)	120.3(3)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	119.7(3)

C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(23)-C(24)-C(25)	120.3(2)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.7(3)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(21)-C(26)-C(25)	120.3(3)
C(21)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(28)-C(27)-C(32)	118.7(2)
C(28)-C(27)-C(10)	119.7(2)
C(32)-C(27)-C(10)	121.6(2)
C(27)-C(28)-C(29)	121.1(2)
C(27)-C(28)-H(28)	119.5
C(29)-C(28)-H(28)	119.5
C(30)-C(29)-C(28)	119.8(2)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(31)-C(30)-C(29)	119.4(2)
C(31)-C(30)-H(30)	120.3
C(29)-C(30)-H(30)	120.3
C(30)-C(31)-C(32)	120.7(2)
C(30)-C(31)-H(31)	119.7
C(32)-C(31)-H(31)	119.7
C(31)-C(32)-C(27)	120.3(2)
C(31)-C(32)-H(32)	119.9
C(27)-C(32)-H(32)	119.9
C(38)-C(33)-C(34)	118.8(2)
C(38)-C(33)-C(15)	120.9(2)
C(34)-C(33)-C(15)	120.28(19)
C(35)-C(34)-C(33)	120.3(2)
C(35)-C(34)-H(34)	119.9
C(33)-C(34)-H(34)	119.9
C(34)-C(35)-C(36)	120.8(2)
C(34)-C(35)-H(35)	119.6
C(36)-C(35)-H(35)	119.6
C(35)-C(36)-C(37)	119.3(2)
C(35)-C(36)-H(36)	120.4
C(37)-C(36)-H(36)	120.4
C(38)-C(37)-C(36)	120.3(2)
C(38)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9
C(37)-C(38)-C(33)	120.7(2)

C(37)-C(38)-H(38)	119.7
C(33)-C(38)-H(38)	119.7
C(40)-C(39)-C(44)	119.2(2)
C(40)-C(39)-C(20)	120.8(2)
C(44)-C(39)-C(20)	119.9(2)
C(39)-C(40)-C(41)	120.2(2)
C(39)-C(40)-H(40)	119.9
C(41)-C(40)-H(40)	119.9
C(42)-C(41)-C(40)	120.0(2)
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(41)-C(42)-C(43)	120.2(2)
C(41)-C(42)-H(42)	119.9
C(43)-C(42)-H(42)	119.9
C(44)-C(43)-C(42)	119.7(2)
C(44)-C(43)-H(43)	120.1
C(42)-C(43)-H(43)	120.1
C(43)-C(44)-C(39)	120.7(2)
C(43)-C(44)-H(44)	119.6
C(39)-C(44)-H(44)	119.6
O(2)-C(45)-O(1)	129.6(2)
O(2)-C(45)-C(46)	119.3(2)
O(1)-C(45)-C(46)	111.1(2)
F(1)-C(46)-F(3)	108.0(3)
F(1)-C(46)-F(2)	106.2(3)
F(3)-C(46)-F(2)	106.0(3)
F(1)-C(46)-C(45)	113.1(2)
F(3)-C(46)-C(45)	112.2(2)
F(2)-C(46)-C(45)	110.9(2)
C(6S)-C(1S)-C(2S)	110.2(3)
C(6S)-C(1S)-H(1S1)	109.6
C(2S)-C(1S)-H(1S1)	109.6
C(6S)-C(1S)-H(1S2)	109.6
C(2S)-C(1S)-H(1S2)	109.6
H(1S1)-C(1S)-H(1S2)	108.1
C(3S)-C(2S)-C(1S)	111.1(3)
C(3S)-C(2S)-H(2S1)	109.4
C(1S)-C(2S)-H(2S1)	109.4
C(3S)-C(2S)-H(2S2)	109.4
C(1S)-C(2S)-H(2S2)	109.4
H(2S1)-C(2S)-H(2S2)	108.0
C(2S)-C(3S)-C(4S)	111.3(2)
C(2S)-C(3S)-H(3S1)	109.4
C(4S)-C(3S)-H(3S1)	109.4
C(2S)-C(3S)-H(3S2)	109.4

C(4S)-C(3S)-H(3S2)	109.4
H(3S1)-C(3S)-H(3S2)	108.0
C(3S)-C(4S)-C(5S)	110.6(3)
C(3S)-C(4S)-H(4S1)	109.5
C(5S)-C(4S)-H(4S1)	109.5
C(3S)-C(4S)-H(4S2)	109.5
C(5S)-C(4S)-H(4S2)	109.5
H(4S1)-C(4S)-H(4S2)	108.1
C(6S)-C(5S)-C(4S)	112.0(3)
C(6S)-C(5S)-H(5S1)	109.2
C(4S)-C(5S)-H(5S1)	109.2
C(6S)-C(5S)-H(5S2)	109.2
C(4S)-C(5S)-H(5S2)	109.2
H(5S1)-C(5S)-H(5S2)	107.9
C(5S)-C(6S)-C(1S)	110.5(3)
C(5S)-C(6S)-H(6SA)	109.5
C(1S)-C(6S)-H(6SA)	109.5
C(5S)-C(6S)-H(6SB)	109.5
C(1S)-C(6S)-H(6SB)	109.5
H(6SA)-C(6S)-H(6SB)	108.1

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U11 + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	13(1)	16(1)	16(1)	-5(1)	0(1)	-3(1)
Fe(1')	13(1)	16(1)	16(1)	-5(1)	0(1)	-3(1)
F(1)	47(1)	125(2)	94(2)	-75(2)	26(1)	-57(1)
F(2)	67(2)	126(2)	53(1)	-24(1)	-28(1)	-30(1)
F(3)	41(1)	121(2)	151(2)	-120(2)	4(1)	-16(1)
O(1)	20(1)	31(1)	28(1)	-12(1)	2(1)	-9(1)
O(2)	30(1)	40(1)	35(1)	-16(1)	7(1)	-16(1)
N(1)	16(1)	18(1)	18(1)	-4(1)	0(1)	-4(1)
N(2)	17(1)	18(1)	20(1)	-7(1)	-1(1)	-4(1)
N(3)	17(1)	19(1)	18(1)	-7(1)	-2(1)	-4(1)
N(4)	16(1)	19(1)	20(1)	-7(1)	-1(1)	-3(1)
C(1)	16(1)	20(1)	23(1)	-7(1)	-1(1)	-3(1)
C(2)	19(1)	23(1)	27(1)	-4(1)	1(1)	-1(1)
C(3)	21(1)	26(1)	28(1)	-7(1)	5(1)	-2(1)
C(4)	17(1)	24(1)	22(1)	-8(1)	2(1)	-5(1)
C(5)	18(1)	21(1)	21(1)	-8(1)	2(1)	-5(1)
C(6)	20(1)	21(1)	18(1)	-7(1)	1(1)	-6(1)
C(7)	24(1)	23(1)	21(1)	-5(1)	3(1)	-7(1)
C(8)	26(1)	21(1)	22(1)	-6(1)	-1(1)	-5(1)
C(9)	20(1)	19(1)	20(1)	-6(1)	-2(1)	-4(1)
C(10)	20(1)	18(1)	19(1)	-6(1)	-5(1)	-3(1)
C(11)	17(1)	19(1)	23(1)	-9(1)	-2(1)	-4(1)
C(12)	17(1)	23(1)	26(1)	-10(1)	-1(1)	-3(1)
C(13)	17(1)	23(1)	24(1)	-9(1)	-1(1)	-4(1)
C(14)	17(1)	20(1)	21(1)	-10(1)	0(1)	-5(1)
C(15)	19(1)	21(1)	22(1)	-10(1)	1(1)	-8(1)
C(16)	18(1)	20(1)	20(1)	-8(1)	-1(1)	-6(1)
C(17)	22(1)	23(1)	22(1)	-7(1)	0(1)	-7(1)
C(18)	22(1)	22(1)	22(1)	-4(1)	-3(1)	-6(1)
C(19)	19(1)	19(1)	20(1)	-5(1)	-2(1)	-6(1)
C(20)	18(1)	18(1)	22(1)	-6(1)	-3(1)	-3(1)
C(21)	21(1)	19(1)	23(1)	-3(1)	4(1)	-2(1)
C(22)	27(1)	30(1)	36(2)	-11(1)	5(1)	-8(1)
C(23)	26(1)	29(1)	45(2)	-6(1)	14(1)	-8(1)
C(24)	38(2)	30(1)	31(2)	0(1)	17(1)	-1(1)
C(25)	49(2)	40(2)	23(1)	-9(1)	3(1)	-3(1)
C(26)	30(1)	38(1)	25(1)	-8(1)	1(1)	-8(1)
C(27)	19(1)	20(1)	21(1)	-6(1)	-1(1)	-3(1)

C(28)	37(2)	23(1)	33(1)	-12(1)	-16(1)	-2(1)
C(29)	39(2)	32(1)	33(2)	-10(1)	-17(1)	-2(1)
C(30)	26(1)	21(1)	31(1)	-2(1)	-7(1)	-1(1)
C(31)	22(1)	20(1)	34(1)	-10(1)	0(1)	-4(1)
C(32)	22(1)	22(1)	23(1)	-7(1)	-3(1)	-5(1)
C(33)	17(1)	21(1)	18(1)	-6(1)	-1(1)	-3(1)
C(34)	24(1)	21(1)	20(1)	-4(1)	-3(1)	-9(1)
C(35)	27(1)	26(1)	17(1)	-8(1)	-3(1)	-6(1)
C(36)	22(1)	29(1)	21(1)	-6(1)	2(1)	-4(1)
C(37)	22(1)	28(1)	40(2)	-11(1)	8(1)	-12(1)
C(38)	25(1)	27(1)	35(1)	-17(1)	6(1)	-12(1)
C(39)	15(1)	21(1)	21(1)	-3(1)	3(1)	-4(1)
C(40)	18(1)	23(1)	26(1)	-5(1)	-1(1)	-6(1)
C(41)	17(1)	31(1)	23(1)	0(1)	-3(1)	-5(1)
C(42)	20(1)	25(1)	26(1)	-1(1)	5(1)	-1(1)
C(43)	30(1)	24(1)	26(1)	-8(1)	4(1)	-5(1)
C(44)	21(1)	24(1)	24(1)	-6(1)	-3(1)	-2(1)
C(45)	21(1)	24(1)	34(1)	-11(1)	-2(1)	-5(1)
C(46)	28(2)	67(2)	58(2)	-43(2)	8(1)	-19(1)
C(1S)	48(2)	62(2)	52(2)	-30(2)	8(2)	-27(2)
C(2S)	41(2)	38(2)	46(2)	-14(1)	-6(1)	-4(1)
C(3S)	49(2)	37(1)	33(2)	-11(1)	2(1)	-15(1)
C(4S)	38(2)	45(2)	39(2)	-7(1)	-7(1)	-9(1)
C(5S)	59(2)	53(2)	50(2)	10(2)	-16(2)	-16(2)
C(6S)	65(2)	51(2)	40(2)	-5(1)	-2(2)	-30(2)

Table S9. Hydrogen coordinates and isotropic displacement parameters for **1**.

	x	y	z	U(eq)
H(2)	-0.1451	0.6679	0.7199	0.031
H(3)	-0.1530	0.5312	0.8587	0.033
H(7)	0.1054	0.0808	1.0089	0.027
H(8)	0.3030	-0.0715	0.9771	0.028
H(12)	0.6379	-0.0769	0.7249	0.026
H(13)	0.6375	0.0524	0.5837	0.025
H(17)	0.3371	0.4737	0.4171	0.027
H(18)	0.1507	0.6333	0.4538	0.027
H(22)	-0.1900	0.2790	0.9158	0.037
H(23)	-0.3354	0.2990	1.0262	0.043
H(24)	-0.2847	0.3480	1.1364	0.047
H(25)	-0.0893	0.3770	1.1372	0.048
H(26)	0.0569	0.3545	1.0275	0.038
H(28)	0.5607	-0.0478	0.9514	0.037
H(29)	0.6792	-0.2349	1.0320	0.042
H(30)	0.6996	-0.4156	0.9988	0.034
H(31)	0.6015	-0.4069	0.8849	0.030
H(32)	0.4789	-0.2206	0.8062	0.027
H(34)	0.4642	0.1153	0.4524	0.025
H(35)	0.5986	0.0934	0.3385	0.028
H(36)	0.7290	0.2169	0.2884	0.031
H(37)	0.7207	0.3670	0.3519	0.035
H(38)	0.5885	0.3879	0.4672	0.032
H(40)	-0.0952	0.6570	0.4920	0.028
H(41)	-0.2150	0.8562	0.4281	0.031
H(42)	-0.2068	1.0199	0.4710	0.033
H(43)	-0.0844	0.9852	0.5807	0.033
H(44)	0.0337	0.7867	0.6452	0.029
H(1S1)	0.7858	0.1303	0.8309	0.059
H(1S2)	0.7055	0.0972	0.7755	0.059
H(2S1)	0.8347	0.1509	0.6593	0.051
H(2S2)	0.7780	0.2642	0.6983	0.051
H(3S1)	0.9686	0.2154	0.7610	0.047
H(3S2)	0.9971	0.2301	0.6651	0.047
H(4S1)	1.1446	0.0525	0.7434	0.050
H(4S2)	1.0684	0.0181	0.6862	0.050
H(5S1)	1.0723	-0.1164	0.8170	0.070
H(5S2)	1.0158	-0.0047	0.8574	0.070
H(6SA)	0.8537	-0.0830	0.8510	0.060
H(6SB)	0.8812	-0.0666	0.7548	0.060

Table S10. Torsion angles [°] for **1**.

N(3)-Fe(1)-O(1)-C(45)	41.2(2)
N(4)-Fe(1)-O(1)-C(45)	-50.5(2)
N(1)-Fe(1)-O(1)-C(45)	-140.83(19)
N(2)-Fe(1)-O(1)-C(45)	130.21(19)
N(2)-Fe(1')-N(1)-C(4)	-31.8(3)
N(3)-Fe(1')-N(1)-C(4)	-118.4(5)
N(4)-Fe(1')-N(1)-C(4)	179.56(18)
N(2)-Fe(1')-N(1)-C(1)	176.92(19)
N(3)-Fe(1')-N(1)-C(1)	90.3(6)
N(4)-Fe(1')-N(1)-C(1)	28.3(3)
O(1)-Fe(1)-N(1)-C(4)	-81.51(18)
N(3)-Fe(1)-N(1)-C(4)	93.5(2)
N(4)-Fe(1)-N(1)-C(4)	172.84(18)
N(2)-Fe(1)-N(1)-C(4)	17.04(18)
O(1)-Fe(1)-N(1)-C(1)	85.06(18)
N(3)-Fe(1)-N(1)-C(1)	-99.9(2)
N(4)-Fe(1)-N(1)-C(1)	-20.59(18)
N(2)-Fe(1)-N(1)-C(1)	-176.39(18)
N(1)-Fe(1')-N(2)-C(6)	35.9(3)
N(3)-Fe(1')-N(2)-C(6)	-177.36(17)
N(4)-Fe(1')-N(2)-C(6)	119.8(5)
N(1)-Fe(1')-N(2)-C(9)	-176.58(19)
N(3)-Fe(1')-N(2)-C(9)	-29.9(3)
N(4)-Fe(1')-N(2)-C(9)	-92.7(6)
O(1)-Fe(1)-N(2)-C(6)	87.97(18)
N(3)-Fe(1)-N(2)-C(6)	-170.11(19)
N(4)-Fe(1)-N(2)-C(6)	-90.5(2)
N(1)-Fe(1)-N(2)-C(6)	-12.68(18)
O(1)-Fe(1)-N(2)-C(9)	-82.94(18)
N(3)-Fe(1)-N(2)-C(9)	18.99(18)
N(4)-Fe(1)-N(2)-C(9)	98.6(2)
N(1)-Fe(1)-N(2)-C(9)	176.42(18)
O(1)-Fe(1)-N(3)-C(11)	71.61(18)
N(4)-Fe(1)-N(3)-C(11)	177.45(17)
N(1)-Fe(1)-N(3)-C(11)	-103.4(2)
N(2)-Fe(1)-N(3)-C(11)	-26.90(17)
O(1)-Fe(1)-N(3)-C(14)	-83.09(18)
N(4)-Fe(1)-N(3)-C(14)	22.75(17)
N(1)-Fe(1)-N(3)-C(14)	101.9(2)
N(2)-Fe(1)-N(3)-C(14)	178.40(18)
N(2)-Fe(1')-N(3)-C(11)	19.9(3)
N(1)-Fe(1')-N(3)-C(11)	108.5(5)
N(4)-Fe(1')-N(3)-C(11)	171.75(17)

N(2)-Fe(1')-N(3)-C(14)	-174.82(19)
N(1)-Fe(1')-N(3)-C(14)	-86.2(6)
N(4)-Fe(1')-N(3)-C(14)	-22.9(3)
O(1)-Fe(1)-N(4)-C(19)	-80.75(18)
N(3)-Fe(1)-N(4)-C(19)	177.06(18)
N(1)-Fe(1)-N(4)-C(19)	19.87(18)
N(2)-Fe(1)-N(4)-C(19)	97.7(2)
O(1)-Fe(1)-N(4)-C(16)	83.73(18)
N(3)-Fe(1)-N(4)-C(16)	-18.46(17)
N(1)-Fe(1)-N(4)-C(16)	-175.65(18)
N(2)-Fe(1)-N(4)-C(16)	-97.8(2)
N(2)-Fe(1')-N(4)-C(19)	-112.8(6)
N(1)-Fe(1')-N(4)-C(19)	-26.6(3)
N(3)-Fe(1')-N(4)-C(19)	-177.12(18)
N(2)-Fe(1')-N(4)-C(16)	91.6(6)
N(1)-Fe(1')-N(4)-C(16)	177.87(19)
N(3)-Fe(1')-N(4)-C(16)	27.3(3)
C(4)-N(1)-C(1)-C(20)	-177.2(2)
Fe(1')-N(1)-C(1)-C(20)	-22.9(4)
Fe(1)-N(1)-C(1)-C(20)	14.0(3)
C(4)-N(1)-C(1)-C(2)	0.5(2)
Fe(1')-N(1)-C(1)-C(2)	154.8(3)
Fe(1)-N(1)-C(1)-C(2)	-168.41(15)
N(1)-C(1)-C(2)-C(3)	0.1(3)
C(20)-C(1)-C(2)-C(3)	177.8(2)
C(1)-C(2)-C(3)-C(4)	-0.6(3)
C(1)-N(1)-C(4)-C(5)	176.9(2)
Fe(1')-N(1)-C(4)-C(5)	19.6(4)
Fe(1)-N(1)-C(4)-C(5)	-14.2(3)
C(1)-N(1)-C(4)-C(3)	-0.9(2)
Fe(1')-N(1)-C(4)-C(3)	-158.2(3)
Fe(1)-N(1)-C(4)-C(3)	167.96(16)
C(2)-C(3)-C(4)-N(1)	0.9(3)
C(2)-C(3)-C(4)-C(5)	-176.9(2)
N(1)-C(4)-C(5)-C(6)	-0.3(4)
C(3)-C(4)-C(5)-C(6)	177.2(2)
N(1)-C(4)-C(5)-C(21)	-179.1(2)
C(3)-C(4)-C(5)-C(21)	-1.6(3)
C(9)-N(2)-C(6)-C(5)	177.1(2)
Fe(1')-N(2)-C(6)-C(5)	-28.9(4)
Fe(1)-N(2)-C(6)-C(5)	4.7(3)
C(9)-N(2)-C(6)-C(7)	-1.5(2)
Fe(1')-N(2)-C(6)-C(7)	152.6(2)
Fe(1)-N(2)-C(6)-C(7)	-173.90(15)
C(4)-C(5)-C(6)-N(2)	5.4(4)

C(21)-C(5)-C(6)-N(2)	-175.9(2)
C(4)-C(5)-C(6)-C(7)	-176.3(2)
C(21)-C(5)-C(6)-C(7)	2.5(3)
N(2)-C(6)-C(7)-C(8)	1.0(3)
C(5)-C(6)-C(7)-C(8)	-177.6(2)
C(6)-C(7)-C(8)-C(9)	-0.1(3)
C(6)-N(2)-C(9)-C(10)	-179.1(2)
Fe(1')-N(2)-C(9)-C(10)	30.0(4)
Fe(1)-N(2)-C(9)-C(10)	-6.6(3)
C(6)-N(2)-C(9)-C(8)	1.4(2)
Fe(1')-N(2)-C(9)-C(8)	-149.5(3)
Fe(1)-N(2)-C(9)-C(8)	173.90(15)
C(7)-C(8)-C(9)-N(2)	-0.8(3)
C(7)-C(8)-C(9)-C(10)	179.7(2)
N(2)-C(9)-C(10)-C(11)	-7.1(4)
C(8)-C(9)-C(10)-C(11)	172.3(2)
N(2)-C(9)-C(10)-C(27)	173.4(2)
C(8)-C(9)-C(10)-C(27)	-7.2(3)
C(14)-N(3)-C(11)-C(10)	-177.2(2)
Fe(1)-N(3)-C(11)-C(10)	24.1(3)
Fe(1')-N(3)-C(11)-C(10)	-8.9(4)
C(14)-N(3)-C(11)-C(12)	1.4(2)
Fe(1)-N(3)-C(11)-C(12)	-157.34(15)
Fe(1')-N(3)-C(11)-C(12)	169.6(2)
C(9)-C(10)-C(11)-N(3)	-2.1(4)
C(27)-C(10)-C(11)-N(3)	177.43(19)
C(9)-C(10)-C(11)-C(12)	179.6(2)
C(27)-C(10)-C(11)-C(12)	-0.9(3)
N(3)-C(11)-C(12)-C(13)	-1.2(3)
C(10)-C(11)-C(12)-C(13)	177.4(2)
C(11)-C(12)-C(13)-C(14)	0.5(3)
C(11)-N(3)-C(14)-C(15)	-179.3(2)
Fe(1)-N(3)-C(14)-C(15)	-20.6(3)
Fe(1')-N(3)-C(14)-C(15)	13.4(4)
C(11)-N(3)-C(14)-C(13)	-1.0(2)
Fe(1)-N(3)-C(14)-C(13)	157.68(15)
Fe(1')-N(3)-C(14)-C(13)	-168.4(2)
C(12)-C(13)-C(14)-N(3)	0.3(3)
C(12)-C(13)-C(14)-C(15)	178.6(2)
N(3)-C(14)-C(15)-C(16)	4.6(4)
C(13)-C(14)-C(15)-C(16)	-173.4(2)
N(3)-C(14)-C(15)-C(33)	-176.54(19)
C(13)-C(14)-C(15)-C(33)	5.5(3)
C(19)-N(4)-C(16)-C(15)	178.0(2)
Fe(1)-N(4)-C(16)-C(15)	10.8(3)

Fe(1')-N(4)-C(16)-C(15)	-23.1(4)
C(19)-N(4)-C(16)-C(17)	-0.2(2)
Fe(1)-N(4)-C(16)-C(17)	-167.40(15)
Fe(1')-N(4)-C(16)-C(17)	158.6(3)
C(14)-C(15)-C(16)-N(4)	0.7(4)
C(33)-C(15)-C(16)-N(4)	-178.20(19)
C(14)-C(15)-C(16)-C(17)	178.7(2)
C(33)-C(15)-C(16)-C(17)	-0.2(3)
N(4)-C(16)-C(17)-C(18)	0.7(3)
C(15)-C(16)-C(17)-C(18)	-177.6(2)
C(16)-C(17)-C(18)-C(19)	-0.9(3)
C(16)-N(4)-C(19)-C(20)	-179.4(2)
Fe(1)-N(4)-C(19)-C(20)	-12.3(3)
Fe(1')-N(4)-C(19)-C(20)	20.4(3)
C(16)-N(4)-C(19)-C(18)	-0.3(2)
Fe(1)-N(4)-C(19)-C(18)	166.77(15)
Fe(1')-N(4)-C(19)-C(18)	-160.5(2)
C(17)-C(18)-C(19)-N(4)	0.8(3)
C(17)-C(18)-C(19)-C(20)	179.9(2)
N(4)-C(19)-C(20)-C(1)	-3.6(4)
C(18)-C(19)-C(20)-C(1)	177.5(2)
N(4)-C(19)-C(20)-C(39)	175.8(2)
C(18)-C(19)-C(20)-C(39)	-3.1(3)
N(1)-C(1)-C(20)-C(19)	2.7(4)
C(2)-C(1)-C(20)-C(19)	-174.6(2)
N(1)-C(1)-C(20)-C(39)	-176.7(2)
C(2)-C(1)-C(20)-C(39)	5.9(3)
C(6)-C(5)-C(21)-C(26)	82.5(3)
C(4)-C(5)-C(21)-C(26)	-98.6(3)
C(6)-C(5)-C(21)-C(22)	-101.2(3)
C(4)-C(5)-C(21)-C(22)	77.7(3)
C(26)-C(21)-C(22)-C(23)	-1.0(4)
C(5)-C(21)-C(22)-C(23)	-177.4(2)
C(21)-C(22)-C(23)-C(24)	0.7(4)
C(22)-C(23)-C(24)-C(25)	0.0(4)
C(23)-C(24)-C(25)-C(26)	-0.5(4)
C(22)-C(21)-C(26)-C(25)	0.6(4)
C(5)-C(21)-C(26)-C(25)	176.9(2)
C(24)-C(25)-C(26)-C(21)	0.1(4)
C(9)-C(10)-C(27)-C(28)	-66.9(3)
C(11)-C(10)-C(27)-C(28)	113.6(3)
C(9)-C(10)-C(27)-C(32)	111.1(3)
C(11)-C(10)-C(27)-C(32)	-68.4(3)
C(32)-C(27)-C(28)-C(29)	-1.7(4)
C(10)-C(27)-C(28)-C(29)	176.4(2)

C(27)-C(28)-C(29)-C(30)	1.2(4)
C(28)-C(29)-C(30)-C(31)	0.2(4)
C(29)-C(30)-C(31)-C(32)	-1.0(4)
C(30)-C(31)-C(32)-C(27)	0.5(4)
C(28)-C(27)-C(32)-C(31)	0.8(4)
C(10)-C(27)-C(32)-C(31)	-177.2(2)
C(14)-C(15)-C(33)-C(38)	-109.7(3)
C(16)-C(15)-C(33)-C(38)	69.3(3)
C(14)-C(15)-C(33)-C(34)	68.7(3)
C(16)-C(15)-C(33)-C(34)	-112.4(2)
C(38)-C(33)-C(34)-C(35)	0.3(3)
C(15)-C(33)-C(34)-C(35)	-178.0(2)
C(33)-C(34)-C(35)-C(36)	-0.1(3)
C(34)-C(35)-C(36)-C(37)	-0.7(4)
C(35)-C(36)-C(37)-C(38)	1.2(4)
C(36)-C(37)-C(38)-C(33)	-0.9(4)
C(34)-C(33)-C(38)-C(37)	0.1(4)
C(15)-C(33)-C(38)-C(37)	178.5(2)
C(19)-C(20)-C(39)-C(40)	66.9(3)
C(1)-C(20)-C(39)-C(40)	-113.6(2)
C(19)-C(20)-C(39)-C(44)	-114.3(2)
C(1)-C(20)-C(39)-C(44)	65.2(3)
C(44)-C(39)-C(40)-C(41)	0.6(3)
C(39)-C(40)-C(41)-C(42)	0.4(3)
C(40)-C(41)-C(42)-C(43)	-1.1(4)
C(41)-C(42)-C(43)-C(44)	0.8(4)
C(42)-C(43)-C(44)-C(39)	0.2(4)
C(40)-C(39)-C(44)-C(43)	-0.9(3)
C(20)-C(39)-C(44)-C(43)	-179.7(2)
Fe(1)-O(1)-C(45)-O(2)	11.5(4)
Fe(1)-O(1)-C(45)-C(46)	-168.30(18)
O(2)-C(45)-C(46)-F(1)	7.5(4)
O(1)-C(45)-C(46)-F(1)	-172.7(2)
O(2)-C(45)-C(46)-F(3)	130.0(3)
O(1)-C(45)-C(46)-F(3)	-50.2(4)
O(2)-C(45)-C(46)-F(2)	-111.7(3)
O(1)-C(45)-C(46)-F(2)	68.1(3)
C(6S)-C(1S)-C(2S)-C(3S)	-57.1(3)
C(1S)-C(2S)-C(3S)-C(4S)	56.6(3)
C(2S)-C(3S)-C(4S)-C(5S)	-54.9(3)
C(3S)-C(4S)-C(5S)-C(6S)	55.3(4)
C(4S)-C(5S)-C(6S)-C(1S)	-56.3(4)
C(2S)-C(1S)-C(6S)-C(5S)	56.7(4)

Symmetry transformations used to generate equivalent atoms:

Part C: X-ray determination of (TPP)Fe(NO)(OC(=O)CF_3) (2)

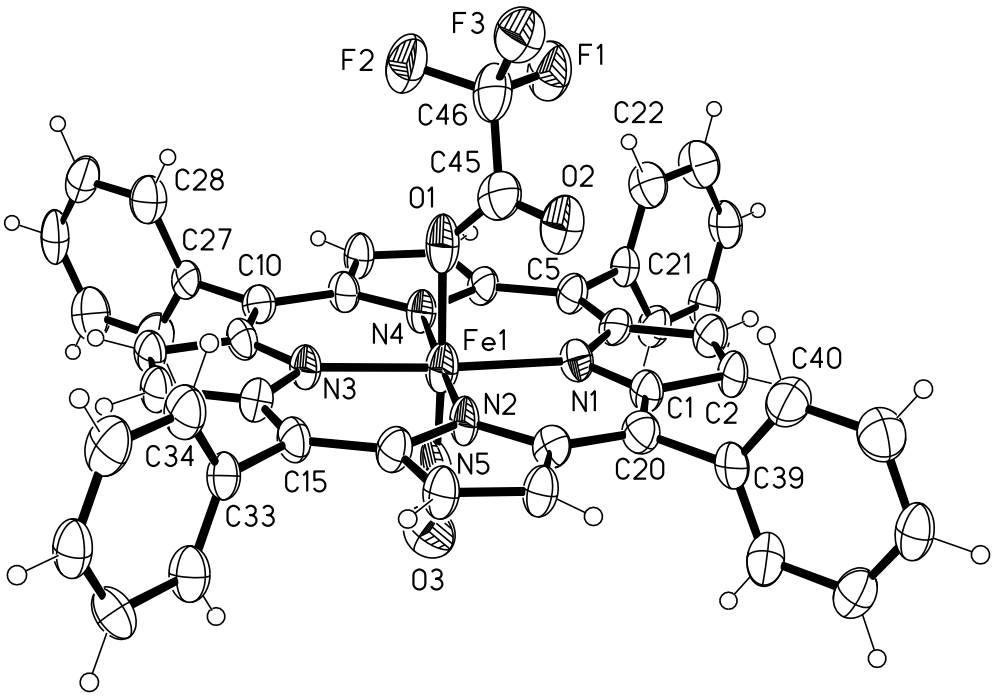

Figure S4. Molecular structure of (TPP)Fe(NO)(OC(=O)CF_3) (2).

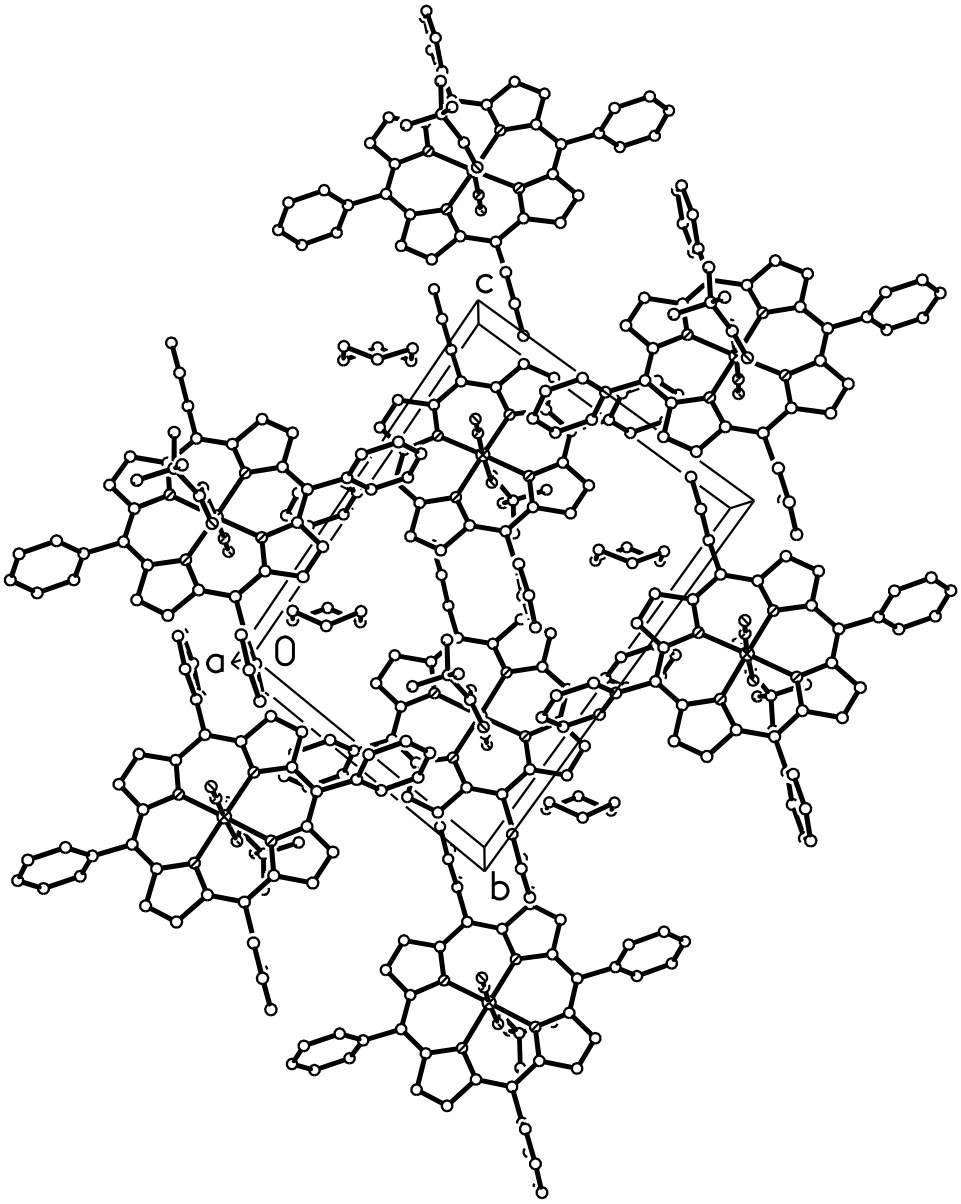

Figure S5. Crystal packing of (TPP)Fe(NO)(OC(=O)CF_3) **(2)**.

Comment

The intensity data were truncated at 0.9Å because data in higher resolution shells had R(int) > 0.25. The asymmetric unit of the cell contained one molecule of interest and one cyclohexane solvent molecule. The displacement ellipsoids were drawn at the 50% probability level.

Experimental

A black block-shaped crystal of dimensions 0.42 x 0.27 x 0.25 mm was selected for structural analysis. Intensity data for this compound were collected using a diffractometer with a Bruker APEX ccd area detector (1) and graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The sample was cooled to 100(2) K. Cell parameters were determined from a non-linear least squares fit of 9274 peaks in the range $2.53 < \theta < 27.34°$. A total of 15943 data were measured in the range $2.07 < \theta < 23.25°$ using ω oscillation frames. The data were corrected for absorption by the semi-empirical method (2) giving minimum and maximum transmission factors of 0.842 and 0.907. The data were merged to form a set of 6115 independent data with R(int) = 0.0565 and a coverage of 99.5 %.

The triclinic space group $P\bar{1}$ was determined by statistical tests and verified by subsequent refinement. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2 (3). Hydrogen atom positions were initially determined by geometry and refined by a riding model. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atom displacement parameters were set to 1.2 times the displacement parameters of the bonded atoms. A total of 577 parameters were refined against 0 restraints and 6115 data to give $wR(F^2) = 0.2494$ and S = 1.095 for weights of $w = 1/[\sigma^2 (F^2) + (0.0720\ P)^2 + 13.8000\ P]$, where $P = [F_o^2 + 2F_c^2] / 3$. The final $R(F)$ was 0.0812 for the 3525 observed, $[F > 4\sigma(F)]$, data. The largest shift/s.u. was 0.000 in the final refinement cycle. The final difference map had maxima and minima of 1.111 and -0.765 e/Å^3, respectively.

References

(1) (a) Data Collection: SMART Software Reference Manual (1998). Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA. (b) Data Reduction: SAINT Software Reference Manual (1998). Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373, USA.

(2) G. M. Sheldrick (2002). SADABS. Program for Empirical Absorption Correction of Area Detector Data. University of Göttingen, Germany.

(3) (a) G. M. Sheldrick (2000). SHELXTL Version 6.10 Reference Manual. Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA. (b) *International Tables for Crystallography, Vol C,* Tables 6.1.1.4, 4.2.6.8, and 4.2.4.2, Kluwer: Boston (1995).

Table S11. Crystal data and structure refinement for **2**·(C_6H_{12})

Empirical formula	$C_{46}H_{28}F_3FeN_5O_3$·(C_6H_{12})	
	$C_{52}H_{40}F_3FeN_5O_3$	
Formula weight	895.74	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.055(9) Å	α = 85.074(9)°
	b = 13.204(10) Å	β = 72.130(9)°
	c = 16.953(13) Å	γ = 65.693(8)°
Volume	2144(3) Å^3	
Z, Z'	2, 1	
Density (calculated)	1.387 Mg/m^3	
Wavelength	0.71073 Å	
Temperature	100(2) K	
F(000)	928	
Absorption coefficient	0.416 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.907 and 0.842	
Theta range for data collection	2.07 to 23.25°	
Reflections collected	15943	
Independent reflections	6115 [R(int) = 0.0565]	
Data / restraints / parameters	6115 / 0 / 577	
wR(F^2 all data)	$wR2$ = 0.2494	
R(F obsd data)	$R1$ = 0.0812	
Goodness-of-fit on F^2	1.095	
Observed data [I > 2σ(I)]	3525	
Largest and mean shift / s.u.	0.000and 0.000	
Largest diff. peak and hole	1.111 and -0.765 e/Å^3	

$wR2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$

$R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$

Table S12. Atomic coordinates and equivalent isotropic displacement parameters for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0.51519(12)	0.26891(9)	0.74273(6)	0.0387(4)
F(1)	0.0539(5)	0.4948(4)	0.7773(3)	0.0615(14)
F(2)	0.1637(5)	0.4903(4)	0.6464(3)	0.0600(13)
F(3)	0.0300(5)	0.4030(4)	0.6889(3)	0.0622(14)
O(1)	0.3544(6)	0.3402(4)	0.7068(3)	0.0444(14)
O(2)	0.2191(6)	0.2458(5)	0.7520(3)	0.0519(15)
O(3)	0.7527(7)	0.1918(5)	0.7925(4)	0.0596(16)
N(1)	0.3934(6)	0.2639(5)	0.8572(3)	0.0299(13)
N(2)	0.5346(6)	0.1174(5)	0.7151(3)	0.0326(14)
N(3)	0.6265(6)	0.2773(5)	0.6255(3)	0.0316(14)
N(4)	0.4857(6)	0.4255(5)	0.7681(3)	0.0308(14)
N(5)	0.6534(7)	0.2204(5)	0.7727(4)	0.0412(16)
C(1)	0.3621(7)	0.1773(5)	0.8907(4)	0.0299(16)
C(2)	0.2731(7)	0.2064(6)	0.9753(4)	0.0338(17)
C(3)	0.2536(7)	0.3109(6)	0.9920(4)	0.0348(17)
C(4)	0.3279(7)	0.3486(6)	0.9188(4)	0.0309(16)
C(5)	0.3339(7)	0.4516(6)	0.9125(4)	0.0331(17)
C(6)	0.4073(7)	0.4878(6)	0.8413(4)	0.0312(16)
C(7)	0.4113(7)	0.5943(6)	0.8348(4)	0.0362(18)
C(8)	0.4922(8)	0.5974(6)	0.7569(4)	0.0367(18)
C(9)	0.5376(7)	0.4913(6)	0.7157(4)	0.0308(16)
C(10)	0.6222(7)	0.4652(6)	0.6324(4)	0.0334(17)
C(11)	0.6608(7)	0.3637(6)	0.5927(4)	0.0324(17)
C(12)	0.7454(7)	0.3354(6)	0.5066(4)	0.0330(17)
C(13)	0.7614(7)	0.2329(6)	0.4891(4)	0.0341(17)
C(14)	0.6878(7)	0.1950(6)	0.5635(4)	0.0313(16)
C(15)	0.6826(7)	0.0919(6)	0.5686(4)	0.0342(17)
C(16)	0.6101(7)	0.0564(6)	0.6401(4)	0.0339(17)
C(17)	0.6019(8)	-0.0492(6)	0.6475(4)	0.0362(18)
C(18)	0.5263(7)	-0.0545(6)	0.7256(4)	0.0338(17)
C(19)	0.4854(7)	0.0488(5)	0.7678(4)	0.0290(16)
C(20)	0.4031(7)	0.0757(6)	0.8517(4)	0.0351(17)
C(21)	0.2582(7)	0.5288(6)	0.9880(4)	0.0323(17)
C(22)	0.1267(8)	0.6083(6)	0.9983(4)	0.043(2)
C(23)	0.0533(9)	0.6765(7)	1.0720(4)	0.048(2)
C(24)	0.1142(8)	0.6619(6)	1.1343(4)	0.043(2)
C(25)	0.2457(9)	0.5826(6)	1.1253(4)	0.043(2)
C(26)	0.3183(8)	0.5151(6)	1.0518(4)	0.0400(19)

C(27)	0.6691(7)	0.5491(6)	0.5866(4)	0.0291(16)
C(28)	0.5957(9)	0.6225(6)	0.5384(4)	0.045(2)
C(29)	0.6407(9)	0.7021(6)	0.4958(4)	0.045(2)
C(30)	0.7592(9)	0.7072(7)	0.5000(4)	0.047(2)
C(31)	0.8333(10)	0.6346(7)	0.5476(5)	0.056(2)
C(32)	0.7891(9)	0.5555(7)	0.5902(5)	0.051(2)
C(33)	0.7574(7)	0.0147(6)	0.4940(4)	0.0298(16)
C(34)	0.6950(8)	0.0159(6)	0.4332(4)	0.0418(19)
C(35)	0.7677(9)	-0.0531(6)	0.3613(4)	0.046(2)
C(36)	0.9036(8)	-0.1249(6)	0.3500(4)	0.0412(19)
C(37)	0.9689(8)	-0.1301(6)	0.4090(4)	0.0411(19)
C(38)	0.8933(8)	-0.0607(6)	0.4812(4)	0.0411(19)
C(39)	0.3591(7)	-0.0106(6)	0.8988(4)	0.0293(16)
C(40)	0.2332(9)	-0.0122(7)	0.9035(5)	0.045(2)
C(41)	0.1922(9)	-0.0916(7)	0.9503(5)	0.050(2)
C(42)	0.2762(8)	-0.1672(6)	0.9925(4)	0.0411(19)
C(43)	0.4010(9)	-0.1663(6)	0.9876(4)	0.044(2)
C(44)	0.4426(9)	-0.0879(7)	0.9414(4)	0.045(2)
C(45)	0.2418(9)	0.3261(7)	0.7226(4)	0.0421(19)
C(46)	0.1246(9)	0.4266(7)	0.7076(4)	0.049(2)
C(1S)	0.8333(10)	0.9255(8)	0.8085(5)	0.066(3)
C(2S)	0.8373(10)	0.8140(8)	0.7873(5)	0.069(3)
C(3S)	0.9697(10)	0.7546(8)	0.7144(5)	0.063(3)
C(4S)	1.0977(9)	0.7401(8)	0.7373(5)	0.059(2)
C(5S)	1.0936(10)	0.8499(8)	0.7593(6)	0.069(3)
C(6S)	0.9583(10)	0.9141(8)	0.8294(6)	0.067(3)

Table S13. Bond lengths [Å] and angles [°] for **2**.

Fe(1)-N(5)	1.618(8)	C(13)-H(13)	0.9500
Fe(1)-O(1)	1.899(6)	C(14)-C(15)	1.381(10)
Fe(1)-N(2)	2.004(6)	C(15)-C(16)	1.396(9)
Fe(1)-N(1)	2.008(5)	C(15)-C(33)	1.486(9)
Fe(1)-N(3)	2.013(5)	C(16)-C(17)	1.427(10)
Fe(1)-N(4)	2.019(6)	C(17)-C(18)	1.346(9)
F(1)-C(46)	1.361(9)	C(17)-H(17)	0.9500
F(2)-C(46)	1.358(9)	C(18)-C(19)	1.428(9)
F(3)-C(46)	1.335(9)	C(18)-H(18)	0.9500
O(1)-C(45)	1.278(9)	C(19)-C(20)	1.416(9)
O(2)-C(45)	1.220(9)	C(20)-C(39)	1.495(9)
O(3)-N(5)	1.151(8)	C(21)-C(22)	1.365(10)
N(1)-C(1)	1.358(8)	C(21)-C(26)	1.397(10)
N(1)-C(4)	1.391(8)	C(22)-C(23)	1.414(10)
N(2)-C(19)	1.372(8)	C(22)-H(22)	0.9500
N(2)-C(16)	1.390(8)	C(23)-C(24)	1.379(11)
N(3)-C(11)	1.368(9)	C(23)-H(23)	0.9500
N(3)-C(14)	1.377(8)	C(24)-C(25)	1.368(11)
N(4)-C(9)	1.355(8)	C(24)-H(24)	0.9500
N(4)-C(6)	1.377(8)	C(25)-C(26)	1.407(10)
C(1)-C(20)	1.382(9)	C(25)-H(25)	0.9500
C(1)-C(2)	1.445(9)	C(26)-H(26)	0.9500
C(2)-C(3)	1.346(10)	C(27)-C(28)	1.375(10)
C(2)-H(2)	0.9500	C(27)-C(32)	1.382(11)
C(3)-C(4)	1.437(9)	C(28)-C(29)	1.397(10)
C(3)-H(3)	0.9500	C(28)-H(28)	0.9500
C(4)-C(5)	1.382(10)	C(29)-C(30)	1.362(11)
C(5)-C(6)	1.402(9)	C(29)-H(29)	0.9500
C(5)-C(21)	1.497(9)	C(30)-C(31)	1.366(12)
C(6)-C(7)	1.419(10)	C(30)-H(30)	0.9500
C(7)-C(8)	1.357(9)	C(31)-C(32)	1.388(11)
C(7)-H(7)	0.9500	C(31)-H(31)	0.9500
C(8)-C(9)	1.442(9)	C(32)-H(32)	0.9500
C(8)-H(8)	0.9500	C(33)-C(38)	1.379(10)
C(9)-C(10)	1.411(9)	C(33)-C(34)	1.401(10)
C(10)-C(11)	1.392(9)	C(34)-C(35)	1.396(10)
C(10)-C(27)	1.477(10)	C(34)-H(34)	0.9500
C(11)-C(12)	1.454(9)	C(35)-C(36)	1.369(11)
C(12)-C(13)	1.338(9)	C(35)-H(35)	0.9500
C(12)-H(12)	0.9500	C(36)-C(37)	1.383(10)
C(13)-C(14)	1.448(9)	C(36)-H(36)	0.9500

C(37)-C(38)	1.405(10)	C(1S)-H(1S1)	0.9900
C(37)-H(37)	0.9500	C(1S)-H(1S2)	0.9900
C(38)-H(38)	0.9500	C(2S)-C(3S)	1.548(12)
C(39)-C(40)	1.379(10)	C(2S)-H(2S1)	0.9900
C(39)-C(44)	1.386(10)	C(2S)-H(2S2)	0.9900
C(40)-C(41)	1.400(11)	C(3S)-C(4S)	1.514(12)
C(40)-H(40)	0.9500	C(3S)-H(3S1)	0.9900
C(41)-C(42)	1.376(11)	C(3S)-H(3S2)	0.9900
C(41)-H(41)	0.9500	C(4S)-C(5S)	1.508(12)
C(42)-C(43)	1.362(11)	C(4S)-H(4S1)	0.9900
C(42)-H(42)	0.9500	C(4S)-H(4S2)	0.9900
C(43)-C(44)	1.388(10)	C(5S)-C(6S)	1.551(12)
C(43)-H(43)	0.9500	C(5S)-H(5S1)	0.9900
C(44)-H(44)	0.9500	C(5S)-H(5S2)	0.9900
C(45)-C(46)	1.494(12)	C(6S)-H(6S1)	0.9900
C(1S)-C(6S)	1.475(13)	C(6S)-H(6S2)	0.9900
C(1S)-C(2S)	1.525(13)		

N(5)-Fe(1)-O(1)	174.1(3)	C(6)-N(4)-Fe(1)	127.2(4)
N(5)-Fe(1)-N(2)	93.4(3)	O(3)-N(5)-Fe(1)	175.8(6)
O(1)-Fe(1)-N(2)	92.2(2)	N(1)-C(1)-C(20)	126.9(6)
N(5)-Fe(1)-N(1)	92.2(3)	N(1)-C(1)-C(2)	110.2(6)
O(1)-Fe(1)-N(1)	89.6(2)	C(20)-C(1)-C(2)	122.8(6)
N(2)-Fe(1)-N(1)	89.6(2)	C(3)-C(2)-C(1)	106.6(6)
N(5)-Fe(1)-N(3)	91.4(3)	C(3)-C(2)-H(2)	126.7
O(1)-Fe(1)-N(3)	86.8(2)	C(1)-C(2)-H(2)	126.7
N(2)-Fe(1)-N(3)	90.0(2)	C(2)-C(3)-C(4)	108.0(6)
N(1)-Fe(1)-N(3)	176.4(2)	C(2)-C(3)-H(3)	126.0
N(5)-Fe(1)-N(4)	90.0(3)	C(4)-C(3)-H(3)	126.0
O(1)-Fe(1)-N(4)	84.3(2)	C(5)-C(4)-N(1)	126.4(6)
N(2)-Fe(1)-N(4)	176.6(2)	C(5)-C(4)-C(3)	124.9(6)
N(1)-Fe(1)-N(4)	90.4(2)	N(1)-C(4)-C(3)	108.7(6)
N(3)-Fe(1)-N(4)	89.7(2)	C(4)-C(5)-C(6)	124.8(6)
C(45)-O(1)-Fe(1)	132.7(5)	C(4)-C(5)-C(21)	117.3(6)
C(1)-N(1)-C(4)	106.5(5)	C(6)-C(5)-C(21)	118.0(6)
C(1)-N(1)-Fe(1)	127.3(4)	N(4)-C(6)-C(5)	125.0(6)
C(4)-N(1)-Fe(1)	126.1(4)	N(4)-C(6)-C(7)	110.5(6)
C(19)-N(2)-C(16)	105.6(5)	C(5)-C(6)-C(7)	124.5(6)
C(19)-N(2)-Fe(1)	127.2(4)	C(8)-C(7)-C(6)	106.7(6)
C(16)-N(2)-Fe(1)	127.0(4)	C(8)-C(7)-H(7)	126.7
C(11)-N(3)-C(14)	106.6(5)	C(6)-C(7)-H(7)	126.7
C(11)-N(3)-Fe(1)	126.8(4)	C(7)-C(8)-C(9)	106.9(6)
C(14)-N(3)-Fe(1)	126.5(4)	C(7)-C(8)-H(8)	126.6
C(9)-N(4)-C(6)	106.1(5)	C(9)-C(8)-H(8)	126.6
C(9)-N(4)-Fe(1)	126.7(4)	N(4)-C(9)-C(10)	127.4(6)

N(4)-C(9)-C(8)	109.9(5)	C(25)-C(24)-H(24)	119.7
C(10)-C(9)-C(8)	122.7(6)	C(23)-C(24)-H(24)	119.7
C(11)-C(10)-C(9)	121.9(6)	C(24)-C(25)-C(26)	119.3(7)
C(11)-C(10)-C(27)	119.6(6)	C(24)-C(25)-H(25)	120.4
C(9)-C(10)-C(27)	118.5(6)	C(26)-C(25)-H(25)	120.4
N(3)-C(11)-C(10)	127.3(6)	C(21)-C(26)-C(25)	120.8(7)
N(3)-C(11)-C(12)	109.5(6)	C(21)-C(26)-H(26)	119.6
C(10)-C(11)-C(12)	123.2(6)	C(25)-C(26)-H(26)	119.6
C(13)-C(12)-C(11)	107.0(6)	C(28)-C(27)-C(32)	118.0(7)
C(13)-C(12)-H(12)	126.5	C(28)-C(27)-C(10)	121.0(7)
C(11)-C(12)-H(12)	126.5	C(32)-C(27)-C(10)	121.0(6)
C(12)-C(13)-C(14)	107.6(6)	C(27)-C(28)-C(29)	120.4(8)
C(12)-C(13)-H(13)	126.2	C(27)-C(28)-H(28)	119.8
C(14)-C(13)-H(13)	126.2	C(29)-C(28)-H(28)	119.8
N(3)-C(14)-C(15)	127.1(6)	C(30)-C(29)-C(28)	120.8(8)
N(3)-C(14)-C(13)	109.2(6)	C(30)-C(29)-H(29)	119.6
C(15)-C(14)-C(13)	123.7(6)	C(28)-C(29)-H(29)	119.6
C(14)-C(15)-C(16)	123.5(6)	C(29)-C(30)-C(31)	119.4(8)
C(14)-C(15)-C(33)	118.4(6)	C(29)-C(30)-H(30)	120.3
C(16)-C(15)-C(33)	118.2(6)	C(31)-C(30)-H(30)	120.3
N(2)-C(16)-C(15)	125.9(6)	C(30)-C(31)-C(32)	120.1(8)
N(2)-C(16)-C(17)	109.2(6)	C(30)-C(31)-H(31)	119.9
C(15)-C(16)-C(17)	124.9(6)	C(32)-C(31)-H(31)	119.9
C(18)-C(17)-C(16)	107.9(6)	C(27)-C(32)-C(31)	121.2(8)
C(18)-C(17)-H(17)	126.0	C(27)-C(32)-H(32)	119.4
C(16)-C(17)-H(17)	126.0	C(31)-C(32)-H(32)	119.4
C(17)-C(18)-C(19)	106.9(6)	C(38)-C(33)-C(34)	117.0(6)
C(17)-C(18)-H(18)	126.6	C(38)-C(33)-C(15)	120.8(6)
C(19)-C(18)-H(18)	126.6	C(34)-C(33)-C(15)	122.1(7)
N(2)-C(19)-C(20)	125.7(6)	C(35)-C(34)-C(33)	121.9(8)
N(2)-C(19)-C(18)	110.3(5)	C(35)-C(34)-H(34)	119.0
C(20)-C(19)-C(18)	123.9(6)	C(33)-C(34)-H(34)	119.0
C(1)-C(20)-C(19)	122.9(6)	C(36)-C(35)-C(34)	119.2(7)
C(1)-C(20)-C(39)	119.6(6)	C(36)-C(35)-H(35)	120.4
C(19)-C(20)-C(39)	117.6(6)	C(34)-C(35)-H(35)	120.4
C(22)-C(21)-C(26)	118.9(6)	C(35)-C(36)-C(37)	120.9(7)
C(22)-C(21)-C(5)	121.0(6)	C(35)-C(36)-H(36)	119.6
C(26)-C(21)-C(5)	119.9(7)	C(37)-C(36)-H(36)	119.6
C(21)-C(22)-C(23)	120.5(7)	C(36)-C(37)-C(38)	119.0(7)
C(21)-C(22)-H(22)	119.7	C(36)-C(37)-H(37)	120.5
C(23)-C(22)-H(22)	119.7	C(38)-C(37)-H(37)	120.5
C(24)-C(23)-C(22)	119.8(8)	C(33)-C(38)-C(37)	121.9(7)
C(24)-C(23)-H(23)	120.1	C(33)-C(38)-H(38)	119.0
C(22)-C(23)-H(23)	120.1	C(37)-C(38)-H(38)	119.0
C(25)-C(24)-C(23)	120.7(7)	C(40)-C(39)-C(44)	118.9(7)

C(40)-C(39)-C(20)	120.9(6)	H(1S1)-C(1S)-H(1S2)	107.8
C(44)-C(39)-C(20)	120.1(6)	C(1S)-C(2S)-C(3S)	108.9(8)
C(39)-C(40)-C(41)	119.8(7)	C(1S)-C(2S)-H(2S1)	109.9
C(39)-C(40)-H(40)	120.1	C(3S)-C(2S)-H(2S1)	109.9
C(41)-C(40)-H(40)	120.1	C(1S)-C(2S)-H(2S2)	109.9
C(42)-C(41)-C(40)	120.4(8)	C(3S)-C(2S)-H(2S2)	109.9
C(42)-C(41)-H(41)	119.8	H(2S1)-C(2S)-H(2S2)	108.3
C(40)-C(41)-H(41)	119.8	C(4S)-C(3S)-C(2S)	110.0(7)
C(43)-C(42)-C(41)	119.9(7)	C(4S)-C(3S)-H(3S1)	109.7
C(43)-C(42)-H(42)	120.1	C(2S)-C(3S)-H(3S1)	109.7
C(41)-C(42)-H(42)	120.1	C(4S)-C(3S)-H(3S2)	109.7
C(42)-C(43)-C(44)	120.2(8)	C(2S)-C(3S)-H(3S2)	109.7
C(42)-C(43)-H(43)	119.9	H(3S1)-C(3S)-H(3S2)	108.2
C(44)-C(43)-H(43)	119.9	C(5S)-C(4S)-C(3S)	111.9(8)
C(39)-C(44)-C(43)	120.8(7)	C(5S)-C(4S)-H(4S1)	109.2
C(39)-C(44)-H(44)	119.6	C(3S)-C(4S)-H(4S1)	109.2
C(43)-C(44)-H(44)	119.6	C(5S)-C(4S)-H(4S2)	109.2
O(2)-C(45)-O(1)	128.1(8)	C(3S)-C(4S)-H(4S2)	109.2
O(2)-C(45)-C(46)	118.8(8)	H(4S1)-C(4S)-H(4S2)	107.9
O(1)-C(45)-C(46)	112.9(7)	C(4S)-C(5S)-C(6S)	110.4(8)
F(3)-C(46)-F(2)	106.2(6)	C(4S)-C(5S)-H(5S1)	109.6
F(3)-C(46)-F(1)	105.5(7)	C(6S)-C(5S)-H(5S1)	109.6
F(2)-C(46)-F(1)	105.9(6)	C(4S)-C(5S)-H(5S2)	109.6
F(3)-C(46)-C(45)	113.5(7)	C(6S)-C(5S)-H(5S2)	109.6
F(2)-C(46)-C(45)	114.7(7)	H(5S1)-C(5S)-H(5S2)	108.1
F(1)-C(46)-C(45)	110.4(6)	C(1S)-C(6S)-C(5S)	111.8(8)
C(6S)-C(1S)-C(2S)	112.8(8)	C(1S)-C(6S)-H(6S1)	109.3
C(6S)-C(1S)-H(1S1)	109.0	C(5S)-C(6S)-H(6S1)	109.3
C(2S)-C(1S)-H(1S1)	109.0	C(1S)-C(6S)-H(6S2)	109.3
C(6S)-C(1S)-H(1S2)	109.0	C(5S)-C(6S)-H(6S2)	109.3
C(2S)-C(1S)-H(1S2)	109.0	H(6S1)-C(6S)-H(6S2)	107.9

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	52(1)	42(1)	20(1)	-5(1)	0(1)	-23(1)
F(1)	74(3)	51(3)	36(2)	-8(2)	5(2)	-16(3)
F(2)	76(4)	57(3)	33(2)	4(2)	-3(2)	-24(3)
F(3)	63(3)	76(4)	47(3)	7(2)	-16(2)	-28(3)
O(1)	62(4)	48(3)	22(2)	-7(2)	5(2)	-32(3)
O(2)	67(4)	52(4)	38(3)	2(3)	-8(3)	-31(3)
O(3)	60(4)	61(4)	54(4)	-14(3)	-13(3)	-21(3)
N(1)	35(3)	37(3)	18(3)	-6(2)	-4(2)	-17(3)
N(2)	43(4)	37(3)	13(3)	-5(2)	3(2)	-19(3)
N(3)	39(4)	35(3)	17(3)	-5(2)	-1(2)	-16(3)
N(4)	41(4)	36(3)	16(3)	-5(2)	-2(2)	-19(3)
N(5)	45(4)	49(4)	27(3)	-14(3)	11(3)	-29(4)
C(1)	35(4)	30(4)	19(3)	-5(3)	-1(3)	-12(3)
C(2)	43(4)	41(4)	13(3)	-3(3)	2(3)	-18(4)
C(3)	43(5)	37(4)	20(3)	-4(3)	-3(3)	-15(4)
C(4)	36(4)	37(4)	17(3)	2(3)	-8(3)	-12(3)
C(5)	41(4)	36(4)	20(3)	0(3)	-5(3)	-16(4)
C(6)	39(4)	34(4)	15(3)	-3(3)	-4(3)	-12(3)
C(7)	45(5)	33(4)	22(4)	-7(3)	4(3)	-16(4)
C(8)	49(5)	37(4)	22(4)	-4(3)	0(3)	-22(4)
C(9)	37(4)	32(4)	19(3)	-8(3)	-1(3)	-14(3)
C(10)	36(4)	37(4)	21(3)	-4(3)	-5(3)	-10(3)
C(11)	31(4)	40(4)	21(3)	-6(3)	1(3)	-13(3)
C(12)	39(4)	33(4)	21(3)	-6(3)	0(3)	-13(3)
C(13)	42(4)	36(4)	19(3)	-5(3)	0(3)	-16(4)
C(14)	38(4)	35(4)	24(3)	3(3)	-7(3)	-20(3)
C(15)	36(4)	40(4)	20(3)	-4(3)	0(3)	-13(4)
C(16)	43(5)	35(4)	21(4)	0(3)	-5(3)	-16(4)
C(17)	48(5)	43(4)	16(3)	-5(3)	-2(3)	-21(4)
C(18)	46(5)	38(4)	19(3)	-2(3)	-4(3)	-22(4)
C(19)	36(4)	35(4)	18(3)	-6(3)	-8(3)	-14(3)
C(20)	34(4)	46(5)	26(4)	2(3)	-9(3)	-17(4)
C(21)	37(4)	38(4)	22(3)	2(3)	-3(3)	-19(4)
C(22)	49(5)	53(5)	30(4)	-9(4)	-7(4)	-24(4)
C(23)	53(5)	48(5)	35(4)	-16(4)	-2(4)	-18(4)
C(24)	52(5)	46(5)	26(4)	-13(3)	4(4)	-23(4)

C(25)	62(6)	50(5)	17(3)	-5(3)	-3(3)	-29(5)
C(26)	50(5)	40(4)	25(4)	0(3)	-5(3)	-17(4)
C(27)	36(4)	33(4)	13(3)	-8(3)	-2(3)	-10(3)
C(28)	53(5)	47(5)	33(4)	-2(4)	-6(4)	-24(4)
C(29)	64(6)	32(4)	28(4)	3(3)	-4(4)	-15(4)
C(30)	66(6)	43(5)	25(4)	-7(3)	10(4)	-31(5)
C(31)	62(6)	65(6)	46(5)	-1(5)	-4(4)	-39(5)
C(32)	59(6)	54(5)	38(4)	5(4)	-10(4)	-25(5)
C(33)	35(4)	35(4)	25(3)	2(3)	-4(3)	-23(4)
C(34)	51(5)	43(5)	24(4)	-7(3)	-3(3)	-17(4)
C(35)	66(6)	47(5)	23(4)	-7(3)	-11(4)	-22(5)
C(36)	56(6)	39(4)	25(4)	-5(3)	0(4)	-23(4)
C(37)	36(4)	44(5)	35(4)	-14(3)	1(3)	-13(4)
C(38)	53(5)	45(5)	28(4)	-6(3)	-4(3)	-26(4)
C(39)	36(4)	34(4)	13(3)	-11(3)	3(3)	-14(3)
C(40)	50(5)	47(5)	44(4)	11(4)	-16(4)	-24(4)
C(41)	48(5)	56(5)	45(5)	2(4)	-10(4)	-23(4)
C(42)	58(6)	40(5)	23(4)	-4(3)	1(4)	-25(4)
C(43)	55(6)	44(5)	35(4)	8(4)	-13(4)	-22(4)
C(44)	51(5)	56(5)	34(4)	10(4)	-8(4)	-31(4)
C(45)	51(5)	49(5)	25(4)	-6(4)	-11(4)	-18(5)
C(46)	64(6)	67(6)	25(4)	-1(4)	-7(4)	-38(5)
C(1S)	71(7)	62(6)	45(5)	-10(4)	0(5)	-16(5)
C(2S)	78(7)	83(7)	48(5)	9(5)	-24(5)	-32(6)
C(3S)	78(7)	73(6)	32(4)	-1(4)	-6(4)	-31(6)
C(4S)	59(6)	69(6)	39(5)	3(4)	-7(4)	-22(5)
C(5S)	70(7)	76(7)	54(6)	1(5)	-4(5)	-33(6)
C(6S)	66(7)	72(7)	58(6)	-10(5)	-10(5)	-27(5)

Table S15. Hydrogen coordinates and isotropic displacement parameters for **2**.

	x	y	z	U(eq)
H(2)	0.2357	0.1608	1.0119	0.041
H(3)	0.2002	0.3524	1.0431	0.042
H(7)	0.3661	0.6522	0.8768	0.043
H(8)	0.5146	0.6579	0.7339	0.044
H(12)	0.7824	0.3811	0.4697	0.040
H(13)	0.8118	0.1924	0.4374	0.041
H(17)	0.6427	-0.1059	0.6047	0.043
H(18)	0.5043	-0.1153	0.7483	0.041
H(22)	0.0843	0.6179	0.9557	0.052
H(23)	-0.0378	0.7322	1.0785	0.057
H(24)	0.0643	0.7073	1.1839	0.052
H(25)	0.2875	0.5732	1.1682	0.051
H(26)	0.4094	0.4595	1.0454	0.048
H(28)	0.5138	0.6191	0.5339	0.054
H(29)	0.5881	0.7533	0.4636	0.054
H(30)	0.7900	0.7606	0.4701	0.057
H(31)	0.9152	0.6384	0.5516	0.067
H(32)	0.8423	0.5047	0.6223	0.061
H(34)	0.6005	0.0651	0.4411	0.050
H(35)	0.7234	-0.0502	0.3207	0.055
H(36)	0.9538	-0.1717	0.3010	0.049
H(37)	1.0633	-0.1800	0.4007	0.049
H(38)	0.9372	-0.0657	0.5225	0.049
H(40)	0.1743	0.0404	0.8750	0.054
H(41)	0.1060	-0.0932	0.9529	0.060
H(42)	0.2471	-0.2200	1.0250	0.049
H(43)	0.4598	-0.2194	1.0158	0.053
H(44)	0.5292	-0.0872	0.9389	0.054
H(1S1)	0.8245	0.9736	0.7606	0.080
H(1S2)	0.7501	0.9627	0.8562	0.080
H(2S1)	0.7535	0.8261	0.7714	0.082
H(2S2)	0.8385	0.7674	0.8362	0.082
H(3S1)	0.9751	0.6809	0.7013	0.076
H(3S2)	0.9653	0.7991	0.6645	0.076
H(4S1)	1.1045	0.6918	0.7852	0.071
H(4S2)	1.1815	0.7027	0.6901	0.071
H(5S1)	1.0981	0.8951	0.7096	0.082
H(5S2)	1.1754	0.8368	0.7777	0.082
H(6S1)	0.9611	0.8741	0.8814	0.080

H(6S2)	0.9529	0.9889	0.8390	0.080

Table S16. Torsion angles [°] for **2**.

N(5)-Fe(1)-O(1)-C(45)	-147(2)	N(2)-Fe(1)-N(4)-C(6)	91(4)
N(2)-Fe(1)-O(1)-C(45)	49.7(6)	N(1)-Fe(1)-N(4)-C(6)	0.2(6)
N(1)-Fe(1)-O(1)-C(45)	-39.9(6)	N(3)-Fe(1)-N(4)-C(6)	176.6(6)
N(3)-Fe(1)-O(1)-C(45)	139.6(6)	O(1)-Fe(1)-N(5)-O(3)	-12(9)
N(4)-Fe(1)-O(1)-C(45)	-130.3(6)	N(2)-Fe(1)-N(5)-O(3)	151(8)
N(5)-Fe(1)-N(1)-C(1)	-88.4(6)	N(1)-Fe(1)-N(5)-O(3)	-119(8)
O(1)-Fe(1)-N(1)-C(1)	97.2(6)	N(3)-Fe(1)-N(5)-O(3)	61(8)
N(2)-Fe(1)-N(1)-C(1)	4.9(6)	N(4)-Fe(1)-N(5)-O(3)	-29(8)
N(3)-Fe(1)-N(1)-C(1)	89(4)	C(4)-N(1)-C(1)-C(20)	178.9(7)
N(4)-Fe(1)-N(1)-C(1)	-178.5(6)	Fe(1)-N(1)-C(1)-C(20)	-2.9(10)
N(5)-Fe(1)-N(1)-C(4)	89.4(6)	C(4)-N(1)-C(1)-C(2)	0.8(8)
O(1)-Fe(1)-N(1)-C(4)	-85.0(5)	Fe(1)-N(1)-C(1)-C(2)	178.9(5)
N(2)-Fe(1)-N(1)-C(4)	-177.3(5)	N(1)-C(1)-C(2)-C(3)	-0.9(8)
N(3)-Fe(1)-N(1)-C(4)	-93(4)	C(20)-C(1)-C(2)-C(3)	-179.1(7)
N(4)-Fe(1)-N(1)-C(4)	-0.7(5)	C(1)-C(2)-C(3)-C(4)	0.6(8)
N(5)-Fe(1)-N(2)-C(19)	86.7(6)	C(1)-N(1)-C(4)-C(5)	178.5(7)
O(1)-Fe(1)-N(2)-C(19)	-95.1(6)	Fe(1)-N(1)-C(4)-C(5)	0.3(10)
N(1)-Fe(1)-N(2)-C(19)	-5.5(6)	C(1)-N(1)-C(4)-C(3)	-0.4(7)
N(3)-Fe(1)-N(2)-C(19)	178.1(6)	Fe(1)-N(1)-C(4)-C(3)	-178.6(4)
N(4)-Fe(1)-N(2)-C(19)	-96(4)	C(2)-C(3)-C(4)-C(5)	-179.1(7)
N(5)-Fe(1)-N(2)-C(16)	-87.8(6)	C(2)-C(3)-C(4)-N(1)	-0.1(8)
O(1)-Fe(1)-N(2)-C(16)	90.4(6)	N(1)-C(4)-C(5)-C(6)	0.7(12)
N(1)-Fe(1)-N(2)-C(16)	-180.0(6)	C(3)-C(4)-C(5)-C(6)	179.5(7)
N(3)-Fe(1)-N(2)-C(16)	3.6(6)	N(1)-C(4)-C(5)-C(21)	-178.2(6)
N(4)-Fe(1)-N(2)-C(16)	89(4)	C(3)-C(4)-C(5)-C(21)	0.6(10)
N(5)-Fe(1)-N(3)-C(11)	-86.9(6)	C(9)-N(4)-C(6)-C(5)	179.6(7)
O(1)-Fe(1)-N(3)-C(11)	87.4(6)	Fe(1)-N(4)-C(6)-C(5)	0.6(10)
N(2)-Fe(1)-N(3)-C(11)	179.7(6)	C(9)-N(4)-C(6)-C(7)	-0.6(8)
N(1)-Fe(1)-N(3)-C(11)	96(4)	Fe(1)-N(4)-C(6)-C(7)	-179.6(5)
N(4)-Fe(1)-N(3)-C(11)	3.1(6)	C(4)-C(5)-C(6)-N(4)	-1.3(12)
N(5)-Fe(1)-N(3)-C(14)	90.3(6)	C(21)-C(5)-C(6)-N(4)	177.7(6)
O(1)-Fe(1)-N(3)-C(14)	-95.4(6)	C(4)-C(5)-C(6)-C(7)	179.0(7)
N(2)-Fe(1)-N(3)-C(14)	-3.1(6)	C(21)-C(5)-C(6)-C(7)	-2.1(11)
N(1)-Fe(1)-N(3)-C(14)	-87(4)	N(4)-C(6)-C(7)-C(8)	0.3(8)
N(4)-Fe(1)-N(3)-C(14)	-179.7(6)	C(5)-C(6)-C(7)-C(8)	-179.9(7)
N(5)-Fe(1)-N(4)-C(9)	89.3(6)	C(6)-C(7)-C(8)-C(9)	0.1(8)
O(1)-Fe(1)-N(4)-C(9)	-89.0(6)	C(6)-N(4)-C(9)-C(10)	-178.6(7)
N(2)-Fe(1)-N(4)-C(9)	-88(4)	Fe(1)-N(4)-C(9)-C(10)	0.4(10)
N(1)-Fe(1)-N(4)-C(9)	-178.6(6)	C(6)-N(4)-C(9)-C(8)	0.6(8)
N(3)-Fe(1)-N(4)-C(9)	-2.2(6)	Fe(1)-N(4)-C(9)-C(8)	179.6(5)
N(5)-Fe(1)-N(4)-C(6)	-92.0(6)	C(7)-C(8)-C(9)-N(4)	-0.4(8)
O(1)-Fe(1)-N(4)-C(6)	89.8(6)	C(7)-C(8)-C(9)-C(10)	178.8(7)

N(4)-C(9)-C(10)-C(11)	1.6(12)	C(2)-C(1)-C(20)-C(39)	-2.4(10)
C(8)-C(9)-C(10)-C(11)	-177.6(7)	N(2)-C(19)-C(20)-C(1)	0.1(11)
N(4)-C(9)-C(10)-C(27)	-179.1(7)	C(18)-C(19)-C(20)-C(1)	-178.5(7)
C(8)-C(9)-C(10)-C(27)	1.8(10)	N(2)-C(19)-C(20)-C(39)	179.7(6)
C(14)-N(3)-C(11)-C(10)	180.0(7)	C(18)-C(19)-C(20)-C(39)	1.1(10)
Fe(1)-N(3)-C(11)-C(10)	-2.4(10)	C(4)-C(5)-C(21)-C(22)	-95.7(8)
C(14)-N(3)-C(11)-C(12)	0.7(8)	C(6)-C(5)-C(21)-C(22)	85.3(9)
Fe(1)-N(3)-C(11)-C(12)	178.3(5)	C(4)-C(5)-C(21)-C(26)	79.8(9)
C(9)-C(10)-C(11)-N(3)	-0.5(12)	C(6)-C(5)-C(21)-C(26)	-99.2(8)
C(27)-C(10)-C(11)-N(3)	-179.8(7)	C(26)-C(21)-C(22)-C(23)	0.7(11)
C(9)-C(10)-C(11)-C(12)	178.7(7)	C(5)-C(21)-C(22)-C(23)	176.3(7)
C(27)-C(10)-C(11)-C(12)	-0.6(11)	C(21)-C(22)-C(23)-C(24)	-0.7(12)
N(3)-C(11)-C(12)-C(13)	-0.4(8)	C(22)-C(23)-C(24)-C(25)	0.6(12)
C(10)-C(11)-C(12)-C(13)	-179.7(7)	C(23)-C(24)-C(25)-C(26)	-0.5(11)
C(11)-C(12)-C(13)-C(14)	-0.1(8)	C(22)-C(21)-C(26)-C(25)	-0.6(11)
C(11)-N(3)-C(14)-C(15)	179.2(7)	C(5)-C(21)-C(26)-C(25)	-176.3(7)
Fe(1)-N(3)-C(14)-C(15)	1.6(10)	C(24)-C(25)-C(26)-C(21)	0.5(11)
C(11)-N(3)-C(14)-C(13)	-0.7(8)	C(11)-C(10)-C(27)-C(28)	85.6(8)
Fe(1)-N(3)-C(14)-C(13)	-178.4(5)	C(9)-C(10)-C(27)-C(28)	-93.8(8)
C(12)-C(13)-C(14)-N(3)	0.5(8)	C(11)-C(10)-C(27)-C(32)	-93.6(8)
C(12)-C(13)-C(14)-C(15)	-179.5(7)	C(9)-C(10)-C(27)-C(32)	87.0(9)
N(3)-C(14)-C(15)-C(16)	0.8(12)	C(32)-C(27)-C(28)-C(29)	-1.3(10)
C(13)-C(14)-C(15)-C(16)	-179.2(7)	C(10)-C(27)-C(28)-C(29)	179.5(6)
N(3)-C(14)-C(15)-C(33)	-179.6(7)	C(27)-C(28)-C(29)-C(30)	1.3(11)
C(13)-C(14)-C(15)-C(33)	0.4(11)	C(28)-C(29)-C(30)-C(31)	-1.1(11)
C(19)-N(2)-C(16)-C(15)	-178.1(7)	C(29)-C(30)-C(31)-C(32)	1.0(12)
Fe(1)-N(2)-C(16)-C(15)	-2.7(10)	C(28)-C(27)-C(32)-C(31)	1.1(11)
C(19)-N(2)-C(16)-C(17)	2.0(8)	C(10)-C(27)-C(32)-C(31)	-179.6(7)
Fe(1)-N(2)-C(16)-C(17)	177.4(5)	C(30)-C(31)-C(32)-C(27)	-1.0(12)
C(14)-C(15)-C(16)-N(2)	-0.3(12)	C(14)-C(15)-C(33)-C(38)	91.2(8)
C(33)-C(15)-C(16)-N(2)	-179.8(7)	C(16)-C(15)-C(33)-C(38)	-89.2(9)
C(14)-C(15)-C(16)-C(17)	179.6(7)	C(14)-C(15)-C(33)-C(34)	-87.8(9)
C(33)-C(15)-C(16)-C(17)	0.1(11)	C(16)-C(15)-C(33)-C(34)	91.8(9)
N(2)-C(16)-C(17)-C(18)	-1.5(8)	C(38)-C(33)-C(34)-C(35)	-2.1(11)
C(15)-C(16)-C(17)-C(18)	178.5(7)	C(15)-C(33)-C(34)-C(35)	176.9(7)
C(16)-C(17)-C(18)-C(19)	0.5(8)	C(33)-C(34)-C(35)-C(36)	0.6(11)
C(16)-N(2)-C(19)-C(20)	179.6(7)	C(34)-C(35)-C(36)-C(37)	0.4(11)
Fe(1)-N(2)-C(19)-C(20)	4.2(10)	C(35)-C(36)-C(37)-C(38)	0.2(11)
C(16)-N(2)-C(19)-C(18)	-1.7(8)	C(34)-C(33)-C(38)-C(37)	2.7(10)
Fe(1)-N(2)-C(19)-C(18)	-177.1(5)	C(15)-C(33)-C(38)-C(37)	-176.3(7)
C(17)-C(18)-C(19)-N(2)	0.8(8)	C(36)-C(37)-C(38)-C(33)	-1.8(11)
C(17)-C(18)-C(19)-C(20)	179.5(7)	C(1)-C(20)-C(39)-C(40)	86.5(8)
N(1)-C(1)-C(20)-C(19)	-0.7(12)	C(19)-C(20)-C(39)-C(40)	-93.1(8)
C(2)-C(1)-C(20)-C(19)	177.2(7)	C(1)-C(20)-C(39)-C(44)	-90.9(8)
N(1)-C(1)-C(20)-C(39)	179.7(6)	C(19)-C(20)-C(39)-C(44)	89.5(8)

C(44)-C(39)-C(40)-C(41)	-0.4(10)	O(1)-C(45)-C(46)-F(3)	153.0(6)
C(20)-C(39)-C(40)-C(41)	-177.8(6)	O(2)-C(45)-C(46)-F(2)	-153.8(6)
C(39)-C(40)-C(41)-C(42)	0.8(11)	O(1)-C(45)-C(46)-F(2)	30.6(9)
C(40)-C(41)-C(42)-C(43)	-1.2(11)	O(2)-C(45)-C(46)-F(1)	86.7(8)
C(41)-C(42)-C(43)-C(44)	1.3(11)	O(1)-C(45)-C(46)-F(1)	-88.9(7)
C(40)-C(39)-C(44)-C(43)	0.5(10)	C(6S)-C(1S)-C(2S)-C(3S)	-57.2(10)
C(20)-C(39)-C(44)-C(43)	177.9(6)	C(1S)-C(2S)-C(3S)-C(4S)	57.4(10)
C(42)-C(43)-C(44)-C(39)	-0.9(11)	C(2S)-C(3S)-C(4S)-C(5S)	-58.4(10)
Fe(1)-O(1)-C(45)-O(2)	-17.5(11)	C(3S)-C(4S)-C(5S)-C(6S)	55.2(10)
Fe(1)-O(1)-C(45)-C(46)	157.6(5)	C(2S)-C(1S)-C(6S)-C(5S)	55.3(11)
O(2)-C(45)-C(46)-F(3)	-31.4(9)	C(4S)-C(5S)-C(6S)-C(1S)	-53.2(11)