Supplementary Material for

Steric and Electronic Control Over the Reactivity of a Thiolate–Ligated Fe(II) Complex with Dioxygen and Superoxide. Reversible μ-oxo Dimer Formation.

Roslyn M. Theisen, Jason Shearer, Werner Kaminsky,[§] and Julie A. Kovacs*

Supplementary Figures:

Figure S–1. Electronic absorption spectrum of dimeric $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**) in MeCN at ambient temperature.

Figure S–2. Electronic absorption spectrum of dimeric $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**) in MeOH at ambient temperature.

Figure S–3. Electronic absorption spectrum showing the intermediate (with λ_{max}= 460 nm) that forms in the reaction between $[(Fe^{II}(S^{Me2}N_4(tren))]^{+}$ (**1**) and dioxygen at low temperatures (–78 ˚C) in MeOH. Upon warming to ambient temperature this intermediate converts to the μ–oxo dimer, which has λ_{max}= 500 nm in MeOH.

Figure S–4. Electronic absorption spectrum showing that the μ-oxo bridge of dimeric $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**) is cleaved upon the addition of 2 equiv of $HCl_{(aq)}$ in MeCN to cleanly afford monomeric $[(Fe^{III}(S^{Me2}N_4(tren))(Cl)]^{+}$ (**7**).

Figure S–5. Electronic absorption spectrum showing that the μ-oxo bridge of dimeric $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**) is cleaved upon the addition of 2 equiv of LutNHCl in MeCN to cleanly afford monomeric $[(Fe^{III}(S^{Me2}N_4(tren))(Cl)]^{+}$ (**7**).

Figure S–6. Electronic absorption spectrum showing that the μ-oxo bridge of dimeric $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**) is cleaved upon the addition of 2 equiv of anhydrous HBF_4 in MeCN to cleanly afford monomeric $[(Fe^{III}(S^{Me2}N_4(tren))(MeCN)]^{+2}$ (**4**).

Figure S–7. $1/\chi$ versus temperature (SQUID) plot for $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**) showing the negative x-intercept, characteristic of an antiferromagnetically coupled system, and the estimated coupling constant J= –28 cm^{-1}.

Figure S–8. μ_{eff} versus temperature plot for $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)]^{2+}$ (**3**).

Figure S–9. ^1H NMR spectrum of $[Fe^{II}(S^{Me2}N_4(tren–Et_4))]^{+}$ (**5**) in CD_3CN.

Figure S–10. Electronic Absorption spectrum of $[Fe^{II}(S^{Me2}N_4(tren–Et_4))]^{+}$ (**5**) in MeCN at ambient temperature.

Supplementary Tables:

Table S-1. Crystal Data for $[Fe^{II}(S^{Me2}N_4(tren–Et_4))](PF_6)$ (**5**)

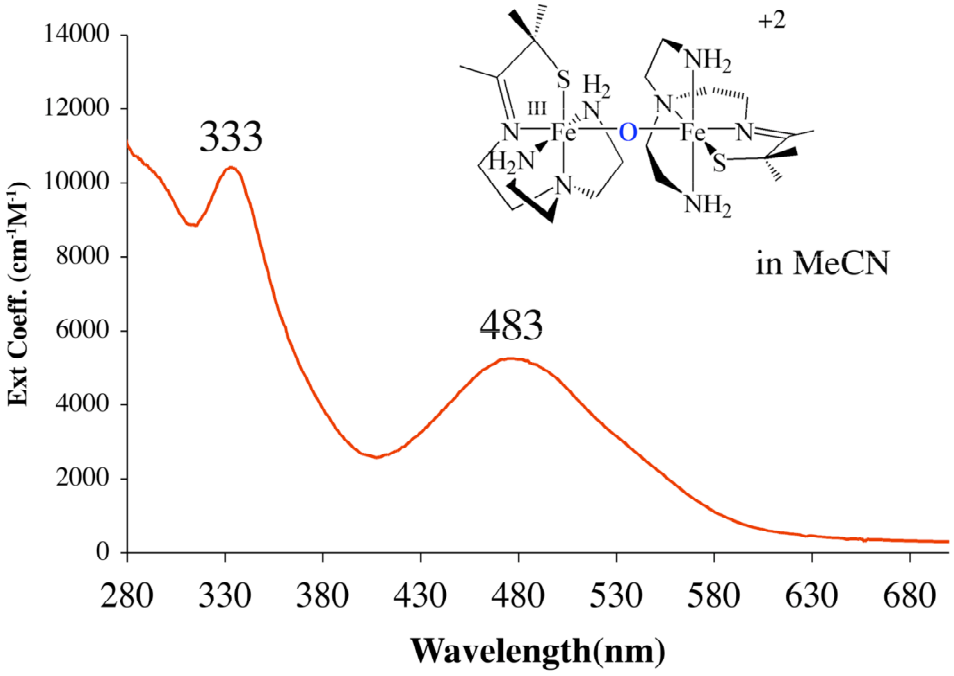

Figure S–1.

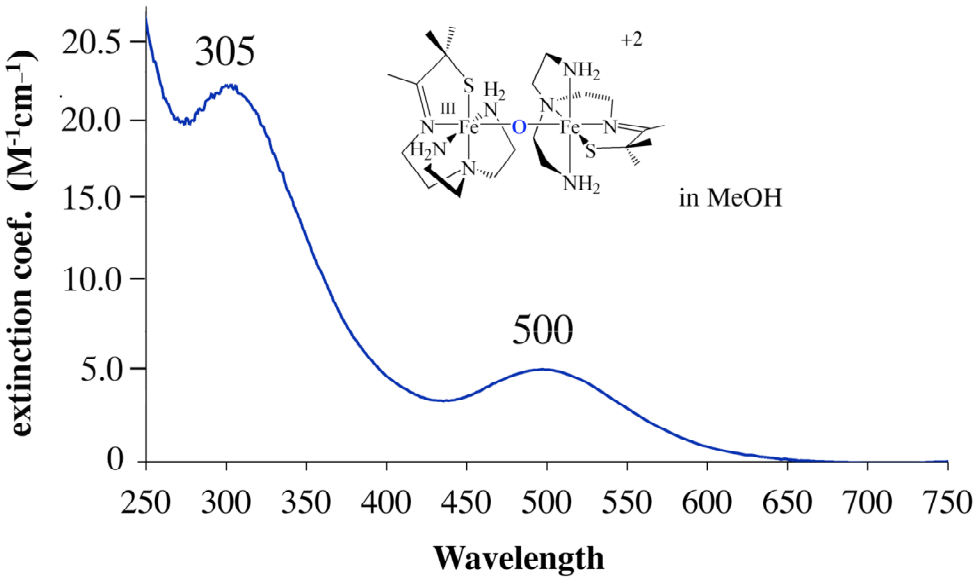

Figure S–2.

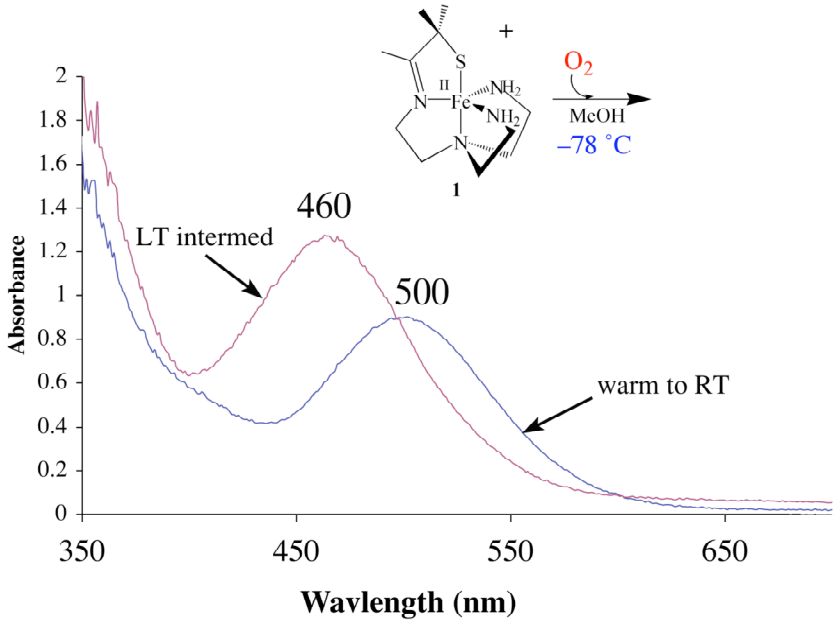

Figure S–3.

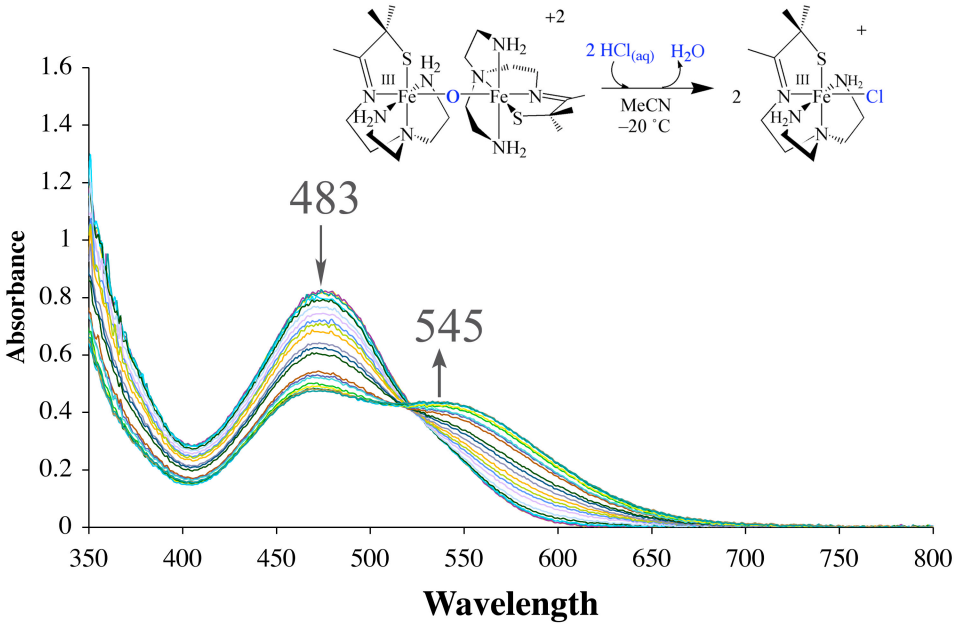

Figure S–4.

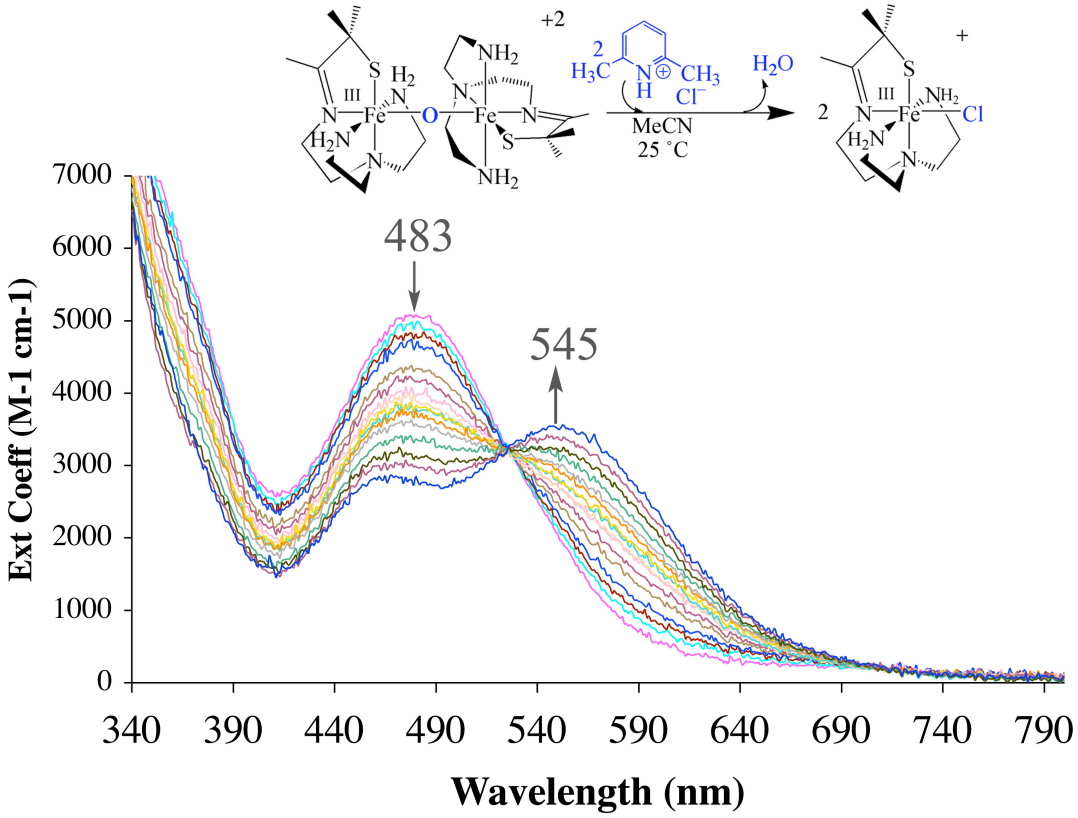

Figure S–5.

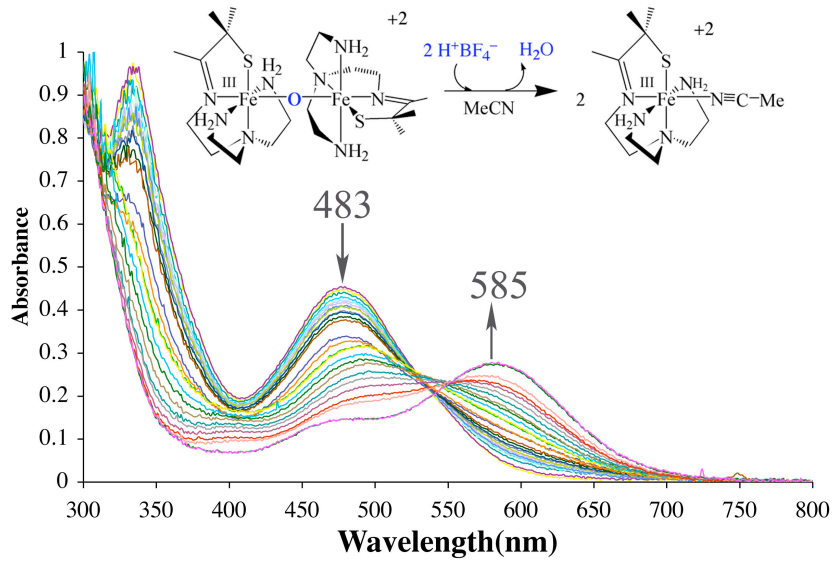

Figure S–6.

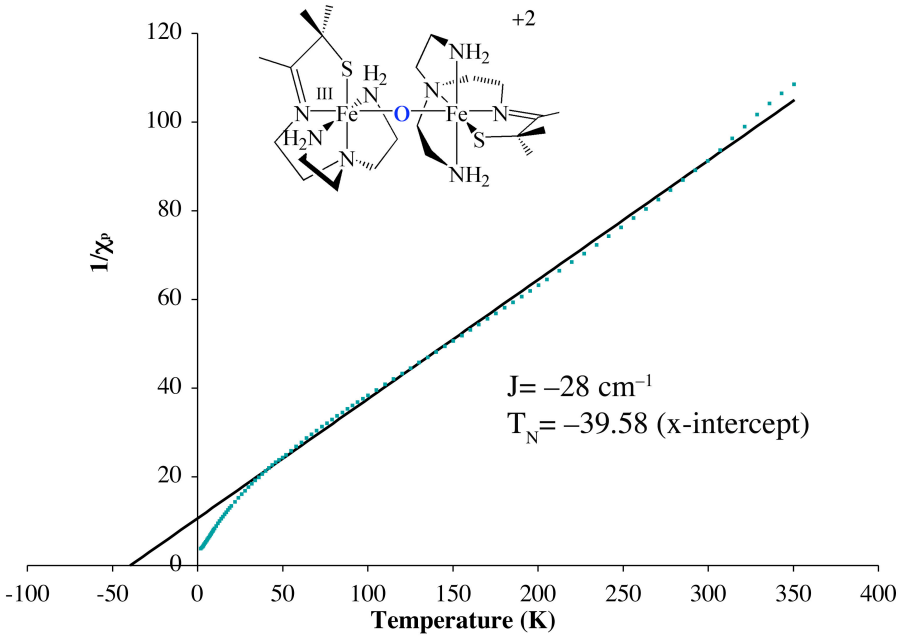

Figure S–7.

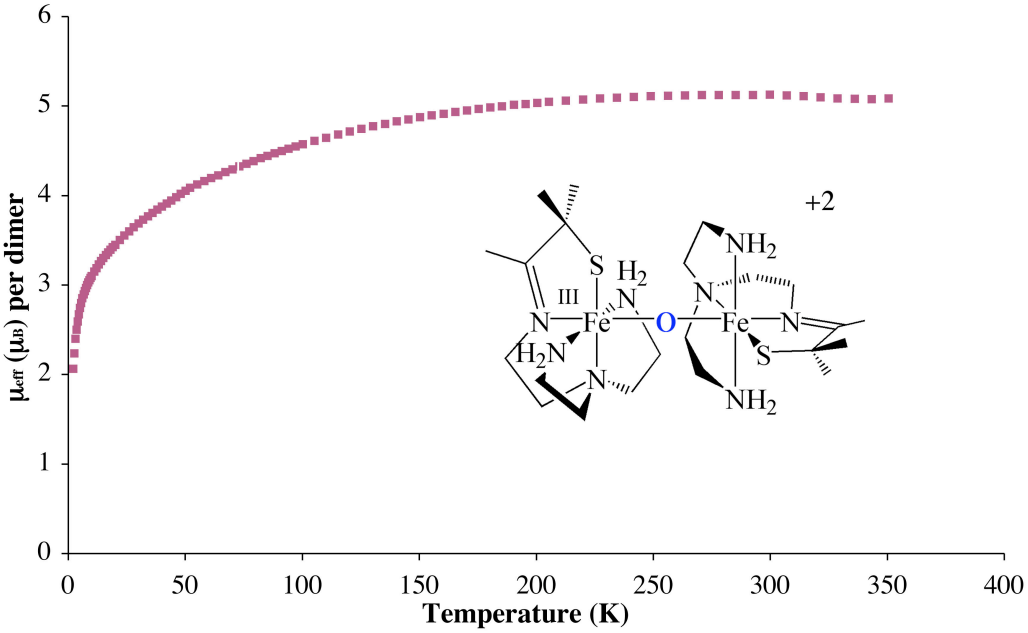

Figure S–8.

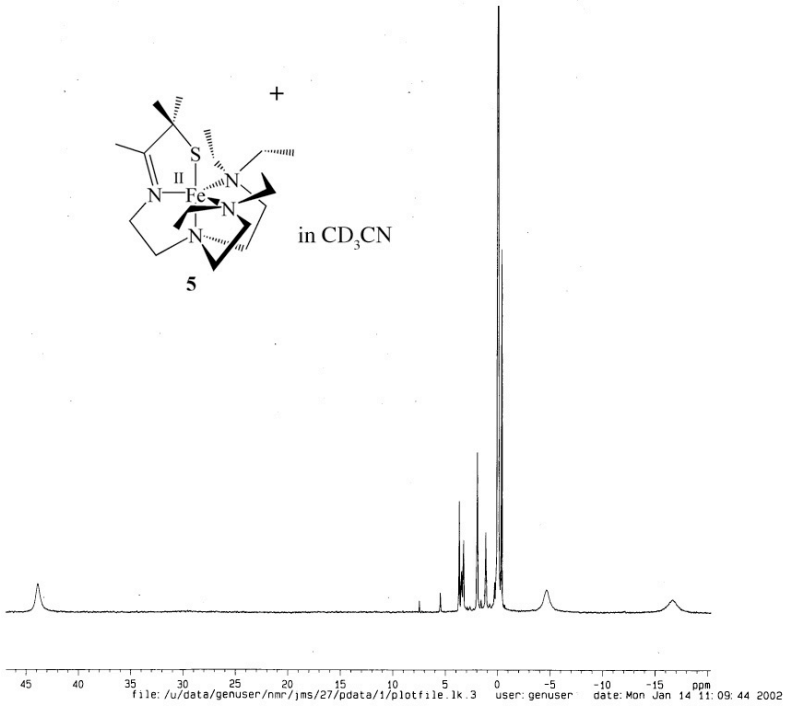
+
S
II
N
N
Fe
N
N
in CD3CN
5
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
ppm
file: /u/data/genuser/nmr/jms/27/pdata/1/plotfile.1k.3
user: genuser
date: Mon Jan 14 11:09:44 2002

Figure S–9.

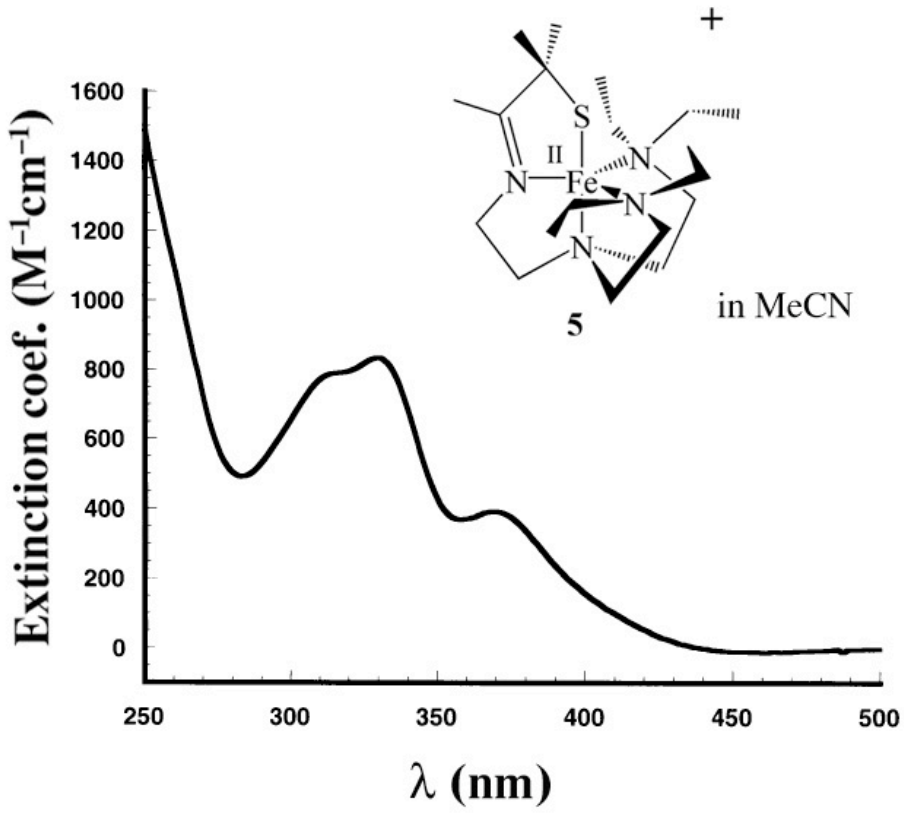
Extinction coef. (M⁻¹cm⁻¹)
1600
1400
1200
1000
800
600
400
200
0
250
300
350
400
450
500
λ (nm)
S
II
Fe
N
N
N
N
+
5
in MeCN

Figure S-10.

Table S-1. Crystal data and structure refinement for $[Fe^{II}(S^{Me2}N_4(tren\text{-}Et_4))](PF_6)$ (**5**).

Empirical formula	C19 H41 F6 Fe N4 P S
Formula weight	558.44
Temperature	130(2) K
Wavelength	0.71070 A
Crystal description/color	prism / yellowish clear
Crystal system, space group	Monoclinic, P c (No.7)
Unit cell dimensions	a = 8.4540(2)A alpha = 90 deg.
	b = 10.8940(3)A beta = 106.1270(19) deg.
	c = 14.4500(4)A gamma = 90 deg.
Volume	1278.44(6) A^3
Z, Calculated density	2, 1.451 Mg/m^3
Absorption coefficient	0.792 mm^-1
F(000)	588
Crystal size	0.43 x 0.29 x 0.22 mm
Reflections for indexing	627
Theta range for data collection	3.48 to 28.28 deg.
Index ranges	-11<=h<=10, -13<=k<=14, -18<=l<=18
Reflections collected / unique	5300 / 5300 [R(int) = 0.013]
Completeness to theta = 28.28	96.3%
Absorption correction	HKL-Scalepack
Max. and min. transmission	0.8450 and 0.7270
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5300 / 0 / 295
Goodness-of-fit on F^2	S = 1.091; S = root(sum(w*D*D)/(n-p)),
	where D = (Fo*Fo - Fc*Fc)
Final R indices [I>2sigma(I)]	*R1 = 0.0406, wR2 = 0.1074
R indices (all data)	R1 = 0.0448, *wR2 = 0.1112
	R1 = sum||Fo|-|Fc||/sum|Fo|, wR2=
	root(sum(w*D*D)/sum(w*Fo*Fo)),
	where D = (Fo*Fo - Fc*Fc)
Weighting scheme	calc
	w=1/[\s^2^(Fo^2^)+(0.0663P)^2^+0.6198P]
	where P=(Fo^2^+2Fc^2^)/3
Absolute structure parameter	0.5(3)
Largest diff. peak and hole	0.873 and -0.507 e.A^-3

Table S-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $[Fe^{II}(S^{Me2}N_4(tren\text{–}Et_4))](PF_6)$ (**5**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-1541(5)	-1079(3)	5862(3)	28(1)
C(2)	-3968(4)	-217(3)	4601(2)	28(1)
C(3)	-2116(4)	-69(3)	5102(2)	20(1)
C(4)	-1186(4)	-177(3)	4348(2)	20(1)
C(5)	-1239(4)	-1409(3)	3848(3)	26(1)
C(6)	587(4)	625(3)	3464(2)	24(1)
C(7)	866(4)	1917(3)	3135(2)	24(1)
C(8)	3193(4)	2541(3)	4468(2)	22(1)
C(9)	3589(4)	2974(3)	5500(2)	22(1)
C(10)	1149(4)	4050(3)	3658(2)	20(1)
C(11)	-649(4)	4383(3)	3526(2)	22(1)
C(12)	2925(4)	1077(3)	6252(2)	21(1)
C(13)	4632(4)	828(3)	6923(2)	28(1)
C(14)	2692(4)	3132(3)	6930(2)	23(1)
C(15)	1826(5)	2610(3)	7636(2)	27(1)
C(16)	-3003(4)	4008(3)	4136(2)	25(1)
C(17)	-3954(5)	5192(4)	3768(3)	34(1)
C(18)	-553(4)	5094(3)	5122(2)	23(1)
C(19)	-1146(5)	4975(3)	6022(3)	28(1)
N(3)	1440(3)	2755(2)	3965(2)	20(1)
N(2)	-1178(3)	4113(2)	4398(2)	19(1)
N(1)	-362(3)	734(2)	4171(2)	19(1)
N(4)	2498(4)	2405(2)	6029(2)	19(1)
F(1)	2879(7)	1854(3)	782(3)	112(2)
F(2)	4575(5)	2342(3)	2190(2)	66(1)
F(3)	4943(6)	4213(3)	1565(3)	93(1)
F(4)	3128(4)	3713(2)	180(2)	51(1)
F(5)	5294(7)	2535(5)	785(4)	114(2)
F(6)	2513(5)	3605(4)	1592(3)	96(2)
P(1)	3872(1)	3014(1)	1178(1)	31(1)
S(1)	-1820(1)	1428(1)	5725(1)	27(1)
Fe(1)	0	2350(1)	5000	17(1)

Table S-3. Bond lengths [A] and angles [deg] for $[Fe^{II}(S^{Me2}N_4(tren\text{-}Et_4))](PF_6)$ (**5**)

N(3)-Fe(1)	2.219(3)
N(2)-Fe(1)	2.227(3)
N(1)-Fe(1)	2.104(3)
N(4)-Fe(1)	2.220(3)
S(1)-Fe(1)	2.3171(9)
C(1)-C(3)	1.535(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.540(4)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-C(4)	1.516(4)
C(3)-S(1)	1.845(3)
C(4)-N(3)	1.278(4)
C(4)-C(5)	1.519(4)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-N(3)	1.468(4)
C(6)-C(7)	1.525(5)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-N(1)	1.478(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(10)-N(3)	1.477(4)
C(8)-C(9)	1.509(5)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-N(4)	1.488(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(8)-N(3)	1.479(4)
C(10)-C(11)	1.522(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-N(2)	1.479(4)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(4)	1.504(4)
C(12)-C(13)	1.523(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(4)	1.492(4)
C(14)-C(15)	1.521(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9800

Table S-3. (cont.)

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-N(2)	1.487(4)
C(16)-C(17)	1.534(5)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-N(2)	1.486(4)
C(18)-C(19)	1.523(5)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
F(1)-P(1)	1.537(3)
F(2)-P(1)	1.595(3)
F(3)-P(1)	1.598(4)
F(4)-P(1)	1.597(3)
F(5)-P(1)	1.556(4)
F(6)-P(1)	1.573(3)
C(3)-C(1)-H(1A)	109.5
C(3)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(3)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-C(1)	109.5(3)
C(4)-C(3)-C(2)	108.5(3)
C(1)-C(3)-C(2)	109.9(3)
C(4)-C(3)-S(1)	113.1(2)
C(1)-C(3)-S(1)	108.1(2)
C(2)-C(3)-S(1)	107.8(2)
N(3)-C(4)-C(3)	120.3(3)
N(3)-C(4)-C(5)	122.4(3)
C(3)-C(4)-C(5)	117.3(3)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(3)-C(6)-C(7)	107.7(3)
N(3)-C(6)-H(6A)	110.2
C(7)-C(6)-H(6A)	110.2
N(3)-C(6)-H(6B)	110.2
C(7)-C(6)-H(6B)	110.2

Table S-3. (cont.)

H(6A)-C(6)-H(6B)	108.5
N(1)-C(7)-C(6)	111.2(3)
N(1)-C(7)-H(7A)	109.4
C(6)-C(7)-H(7A)	109.4
N(1)-C(7)-H(7B)	109.4
C(6)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
N(1)-C(8)-C(9)	110.7(3)
N(1)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8A)	109.5
N(1)-C(8)-H(8B)	109.5
C(9)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
N(4)-C(9)-C(8)	112.3(3)
N(4)-C(9)-H(9A)	109.1
C(8)-C(9)-H(9A)	109.1
N(4)-C(9)-H(9B)	109.1
C(8)-C(9)-H(9B)	109.1
H(9A)-C(9)-H(9B)	107.9
N(1)-C(10)-C(11)	110.0(2)
N(1)-C(10)-H(10A)	109.7
C(11)-C(10)-H(10A)	109.7
N(1)-C(10)-H(10B)	109.7
C(11)-C(10)-H(10B)	109.7
H(10A)-C(10)-H(10B)	108.2
N(2)-C(11)-C(10)	111.9(2)
N(2)-C(11)-H(11A)	109.2
C(10)-C(11)-H(11A)	109.2
N(2)-C(11)-H(11B)	109.2
C(10)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
N(4)-C(12)-C(13)	115.9(3)
N(4)-C(12)-H(12A)	108.3
C(13)-C(12)-H(12A)	108.3
N(4)-C(12)-H(12B)	108.3
C(13)-C(12)-H(12B)	108.3
H(12A)-C(12)-H(12B)	107.4
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(4)-C(14)-C(15)	115.4(3)
N(4)-C(14)-H(14A)	108.4
C(15)-C(14)-H(14A)	108.4
N(4)-C(14)-H(14B)	108.4
C(15)-C(14)-H(14B)	108.4
H(14A)-C(14)-H(14B)	107.5
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

Table S-3. (cont.)

N(2)-C(16)-C(17)	115.5(3)
N(2)-C(16)-H(16A)	108.4
C(17)-C(16)-H(16A)	108.4
N(2)-C(16)-H(16B)	108.4
C(17)-C(16)-H(16B)	108.4
H(16A)-C(16)-H(16B)	107.5
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(2)-C(18)-C(19)	113.8(3)
N(2)-C(18)-H(18A)	108.8
C(19)-C(18)-H(18A)	108.8
N(2)-C(18)-H(18B)	108.8
C(19)-C(18)-H(18B)	108.8
H(18A)-C(18)-H(18B)	107.7
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(7)-N(3)-C(10)	110.9(2)
C(7)-N(3)-C(8)	111.1(3)
C(10)-N(3)-C(8)	111.0(2)
C(7)-N(3)-Fe(1)	107.82(19)
C(10)-N(3)-Fe(1)	108.38(19)
C(8)-N(3)-Fe(1)	107.48(18)
C(11)-N(2)-C(18)	108.9(2)
C(11)-N(2)-C(16)	109.7(2)
C(18)-N(2)-C(16)	112.1(3)
C(11)-N(2)-Fe(1)	107.22(18)
C(18)-N(2)-Fe(1)	108.20(18)
C(16)-N(2)-Fe(1)	110.64(19)
C(4)-N(1)-C(6)	120.7(3)
C(4)-N(1)-Fe(1)	122.4(2)
C(6)-N(1)-Fe(1)	116.27(19)
C(9)-N(4)-C(14)	107.1(2)
C(9)-N(4)-C(12)	111.4(3)
C(14)-N(4)-C(12)	111.2(2)
C(9)-N(4)-Fe(1)	106.06(18)
C(14)-N(4)-Fe(1)	116.9(2)
C(12)-N(4)-Fe(1)	104.14(18)
F(1)-P(1)-F(5)	89.2(3)
F(1)-P(1)-F(6)	95.6(3)
F(5)-P(1)-F(6)	175.2(3)
F(1)-P(1)-F(2)	89.4(2)
F(5)-P(1)-F(2)	93.0(2)
F(6)-P(1)-F(2)	88.00(19)
F(1)-P(1)-F(4)	91.04(19)
F(5)-P(1)-F(4)	88.8(2)
F(6)-P(1)-F(4)	90.12(16)
F(2)-P(1)-F(4)	178.10(18)
F(1)-P(1)-F(3)	178.0(3)

Table S-3. (cont.)

F(5)-P(1)-F(3)	89.0(3)
F(6)-P(1)-F(3)	86.3(3)
F(2)-P(1)-F(3)	91.3(2)
F(4)-P(1)-F(3)	88.27(19)
C(3)-S(1)-Fe(1)	100.34(10)
N(3)-Fe(1)-N(1)	78.63(10)
N(1)-Fe(1)-N(4)	111.43(10)
N(3)-Fe(1)-N(4)	81.28(10)
N(1)-Fe(1)-N(2)	121.40(10)
N(3)-Fe(1)-N(2)	80.48(10)
N(4)-Fe(1)-N(2)	118.49(9)
N(1)-Fe(1)-S(1)	83.41(7)
N(3)-Fe(1)-S(1)	161.53(7)
N(4)-Fe(1)-S(1)	109.64(7)
N(2)-Fe(1)-S(1)	105.63(8)

Table S-4. Anisotropic displacement parameters (A^2 x 10^3) for $[Fe^{II}(S^{Me2}N_4(tren\text{-}Et_4))](PF_6)$ (**5**). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	36(2)	22(2)	27(2)	7(1)	9(1)	1(1)
C(2)	21(2)	37(2)	26(2)	-5(1)	6(1)	-3(1)
C(3)	21(2)	18(1)	20(1)	1(1)	5(1)	-1(1)
C(4)	21(2)	19(1)	19(1)	1(1)	4(1)	-2(1)
C(5)	31(2)	16(2)	34(2)	-4(1)	13(1)	-5(1)
C(6)	30(2)	21(2)	27(2)	-6(1)	16(1)	-3(1)
C(7)	28(2)	26(2)	20(2)	-6(1)	12(1)	-6(1)
C(8)	16(2)	27(2)	26(2)	4(1)	10(1)	-1(1)
C(9)	17(2)	24(2)	26(2)	5(1)	7(1)	-3(1)
C(10)	26(2)	17(1)	19(1)	2(1)	9(1)	-2(1)
C(11)	27(2)	20(1)	19(1)	4(1)	6(1)	-1(1)
C(12)	22(2)	21(1)	19(1)	2(1)	5(1)	-3(1)
C(13)	30(2)	26(2)	26(2)	3(1)	2(1)	3(1)
C(14)	26(2)	20(2)	22(2)	-1(1)	4(1)	-3(1)
C(15)	35(2)	26(2)	19(2)	-3(1)	8(1)	-2(1)
C(16)	19(2)	26(2)	28(2)	2(1)	4(1)	-2(1)
C(17)	24(2)	33(2)	43(2)	12(2)	6(1)	6(1)
C(18)	27(2)	19(2)	24(2)	-1(1)	6(1)	-2(1)
C(19)	29(2)	32(2)	26(2)	-4(1)	10(1)	2(1)
N(3)	24(2)	17(1)	19(1)	0(1)	4(1)	-1(1)
N(2)	20(1)	19(1)	19(1)	0(1)	5(1)	-1(1)
N(1)	23(1)	17(1)	19(1)	-2(1)	9(1)	-1(1)
N(4)	21(1)	17(1)	18(1)	1(1)	4(1)	-3(1)
F(1)	152(4)	51(2)	85(3)	18(2)	-44(3)	-48(2)
F(2)	93(3)	39(2)	50(2)	7(1)	-8(2)	23(1)
F(3)	120(4)	64(2)	85(3)	0(2)	10(2)	-38(2)
F(4)	71(2)	45(2)	46(2)	17(1)	28(1)	24(1)
F(5)	114(4)	138(4)	101(3)	12(3)	50(3)	91(3)
F(6)	108(3)	119(3)	87(3)	61(2)	72(2)	77(3)
P(1)	34(1)	23(1)	39(1)	3(1)	12(1)	10(1)
S(1)	34(1)	22(1)	30(1)	-5(1)	19(1)	-9(1)
Fe(1)	19(1)	16(1)	16(1)	0(1)	6(1)	-2(1)

Table S-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $[Fe^{II}(S^{Me2}N_4(tren\text{-}Et_4))](PF_6)$ (**5**).

	x	y	z	U(eq)
H(1A)	-1905	-1880	5572	43
H(1B)	-2013	-934	6399	43
H(1C)	-336	-1067	6099	43
H(2A)	-4320	415	4104	42
H(2B)	-4590	-130	5077	42
H(2C)	-4171	-1031	4303	42
H(5A)	-1563	-1286	3148	40
H(5B)	-2041	-1944	4024	40
H(5C)	-147	-1791	4048	40
H(6A)	-28	126	2908	29
H(6B)	1656	220	3761	29
H(7A)	1696	1888	2769	28
H(7B)	-174	2234	2701	28
H(8A)	3891	2987	4131	27
H(8B)	3442	1654	4455	27
H(9A)	4748	2770	5833	26
H(9B)	3470	3878	5508	26
H(10A)	1431	4173	3044	24
H(10B)	1863	4592	4150	24
H(11A)	-808	5269	3373	26
H(11B)	-1347	3916	2975	26
H(12A)	2828	642	5637	25
H(12B)	2099	719	6543	25
H(13A)	5468	1161	6640	43
H(13B)	4792	-59	7016	43
H(13C)	4733	1223	7547	43
H(14A)	2269	3971	6749	27
H(14B)	3882	3202	7263	27
H(15A)	660	2475	7303	40
H(15B)	1921	3191	8166	40
H(15C)	2338	1829	7892	40
H(16A)	-3322	3723	4710	30
H(16B)	-3350	3369	3633	30
H(17A)	-3765	5790	4293	51
H(17B)	-5133	5009	3534	51
H(17C)	-3571	5532	3240	51
H(18A)	-906	5900	4819	28
H(18B)	665	5076	5314	28
H(19A)	-2337	5114	5853	43
H(19B)	-585	5585	6499	43
H(19C)	-896	4150	6293	43

Table S-6. Crystal data and structure refinement for $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)](PF_6)_2 \cdot MeCN$ (**3**).

Empirical formula	C24 H53 F12 Fe2 N9 O P2 S2
Formula weight	949.51
Temperature	130(2) K
Wavelength	0.71070 A
Crystal description/color	plate / dark-red
Crystal system, space group	Monoclinic, P 21/c (No.14)
Unit cell dimensions	a = 12.6470(9)A alpha = 90.000(10) deg. b = 17.004(2)A beta = 91.455(7) deg. c = 36.359(5)A gamma = 90.000(10) deg.
Volume	7816.5(16) A^3
Z, Calculated density	8, 1.614 Mg/m^3
Absorption coefficient	1.023 mm^-1
F(000)	3920
Crystal size	0.41 x 0.24 x 0.05 mm
Reflections for indexing	373
Theta range for data collection	5.14 to 26.37 deg.
Index ranges	-11<=h<=11, -21<=k<=20, -45<=l<=45
Reflections collected/unique	19377 / 12010 [R(int) = 0.1519]
Completeness to theta	26.37 72.6%
Absorption correction	HKL-SCALEPACK
Max. and min. transmission	0.9506 and 0.6790
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	12010 / 0 / 947
Goodness-of-fit on F^2	S = 0.949 S = root(sum(w*D*D)/(n-p)), where D = (Fo*Fo - Fc*Fc)
Final R indices [I>2sigma(I)]	*R1 = 0.1108, wR2 = 0.2369
R indices (all data)	R1 = 0.2320, *wR2 = 0.2882 R1 = sum||Fo|-|Fc||/sum|Fo|, wR2=root(sum(w*D*D)/sum(w*Fo*Fo)), where D = (Fo*Fo - Fc*Fc)
Weighting scheme	calc w=1/[\s^2^(Fo^2^)+(0.1369P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3
Extinction coefficient	0.0051(7)
Largest diff. peak and hole	1.301 and -0.675 e.A^-3

Table S-7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)](PF_6)_2 \cdot MeCN$ (**3**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	1572(11)	1205(8)	5090(3)	43(4)
C(2)	248(11)	721(7)	4585(4)	42(4)
C(3)	929(9)	1451(7)	4749(3)	26(3)
C(4)	128(10)	2095(8)	4842(3)	36(3)
C(5)	-678(10)	1919(8)	5133(4)	44(4)
C(6)	-694(10)	3340(8)	4737(4)	40(4)
C(7)	-385(12)	4129(8)	4592(4)	47(4)
C(8)	-874(13)	3414(9)	3788(5)	61(5)
C(9)	-406(13)	4133(10)	3910(5)	63(5)
C(10)	1909(12)	4603(8)	4549(5)	63(5)
C(11)	1031(11)	4709(7)	4247(4)	48(4)
C(12)	6128(10)	4360(9)	3984(3)	43(4)
C(13)	5232(12)	5221(9)	3511(4)	61(5)
C(14)	5285(9)	4433(8)	3683(3)	29(3)
C(15)	5459(11)	3729(9)	3406(3)	38(4)
C(16)	6502(11)	3763(9)	3222(4)	52(4)
C(17)	4952(11)	2596(8)	3077(4)	47(4)
C(18)	3910(10)	2316(8)	2873(3)	34(3)
C(19)	2102(10)	2682(8)	2892(4)	36(3)
C(20)	2304(11)	3557(8)	2793(3)	39(4)
C(21)	3550(13)	1395(8)	3578(4)	54(4)
C(22)	2678(13)	1602(7)	3287(4)	55(4)
C(23)	10894(10)	4262(7)	1051(4)	36(3)

Table S-7 (cont.).

C(24)	10133(12)	5101(8)	1553(4)	56(4)
C(25)	10100(9)	4300(7)	1351(4)	30(3)
C(26)	10344(12)	3653(9)	1633(3)	44(4)
C(27)	11447(10)	3554(11)	1790(4)	60(5)
C(28)	9819(11)	2437(9)	1945(4)	49(4)
C(29)	8786(11)	2167(8)	2112(4)	38(3)
C(30)	7109(12)	3326(9)	2224(3)	52(4)
C(31)	6923(11)	2474(9)	2082(4)	51(4)
C(32)	8422(13)	1370(7)	1372(4)	50(4)
C(33)	7575(12)	1509(7)	1664(4)	45(4)
C(34)	4762(11)	900(8)	313(5)	58(4)
C(35)	6413(10)	1270(7)	-37(3)	36(3)
C(36)	5601(9)	1550(7)	247(3)	27(3)
C(37)	5032(9)	2282(7)	111(3)	28(3)
C(38)	4545(11)	2260(8)	-274(4)	47(4)
C(39)	4571(10)	3630(7)	172(3)	34(3)
C(40)	4341(10)	4216(7)	471(3)	30(3)
C(41)	6655(12)	4563(7)	462(4)	49(4)
C(42)	5964(9)	4749(7)	768(3)	29(3)
C(43)	3940(13)	3519(9)	1228(4)	54(4)
C(44)	4572(10)	4238(7)	1155(3)	31(3)
C(45)	2642(11)	1262(8)	1984(4)	49(4)
C(46)	3500(11)	1797(9)	1957(4)	41(4)
C(47)	2190(13)	6263(9)	2015(4)	58(5)
C(48)	1249(15)	6725(8)	1964(4)	49(4)
N(3)	2152(8)	3754(6)	4567(3)	34(3)
N(2)	239(8)	4102(6)	4248(3)	34(3)
N(1))	147(8)	2757(6)	4671(2)	26(2)

Table S-7 (cont.).

N(4)	-196(7)	2746(6)	3850(3)	35(3)
N(5)	3792(8)	2102(6)	3819(3)	33(3)
N(6)	2571(8)	3982(6)	3131(3)	35(3)
N(7)	4745(8)	3250(6)	3327(3)	28(2)
N(8)	3002(9)	2386(6)	3118(3)	40(3)
N(9)	8566(9)	2110(6)	1161(3)	45(3)
N(10)	7475(8)	3819(6)	1926(3)	39(3)
N(11)	9610(8)	3141(6)	1701(3)	31(3)
N(12)	7853(9)	2233(6)	1877(3)	32(3)
N(13)	6999(7)	3737(5)	482(3)	29(2)
N(14)	5107(8)	4161(5)	791(3)	27(2)
N(15)	5054(7)	2903(6)	307(3)	25(2)
N(16)	4540(8)	2783(6)	1146(3)	35(3)
N(17)	4244(11)	2188(8)	1923(4)	63(4)
N(18)	472(14)	7049(10)	1925(4)	94(6)
O(1)	1990(6)	3165(4)	3816(2)	35(2)
O(2)	6733(6)	3131(4)	1231(2)	32(2)
F(1)	8879(10)	5198(9)	2432(3)	132(6)
F(2)	10630(8)	5088(5)	2550(3)	96(4)
F(3)	10261(9)	4444(9)	3039(3)	140(6)
F(4)	8541(7)	4606(6)	2929(4)	104(4)
F(5)	9549(7)	5616(7)	2957(4)	137(6)
F(6)	9616(8)	4087(6)	2495(3)	109(4)
F(7)	2632(8)	5745(6)	563(4)	120(5)
F(8)	4195(6)	6214(6)	767(4)	107(4)
F(9)	3418(8)	7269(7)	911(4)	132(5)
F(10)	1807(7)	6768(6)	746(3)	89(3)
F(11)	3111(8)	6847(9)	370(3)	126(5)

Table S-7 (cont.).

F(12)	2808(9)	6079(11)	1118(4)	186(9)
F(13)	994(10)	1160(8)	1060(3)	132(5)
F(14)	2613(14)	1674(12)	993(4)	210(10)
F(15)	2235(10)	1896(7)	422(4)	125(5)
F(16)	655(11)	1333(10)	495(4)	162(6)
F(17)	2091(9)	729(6)	629(5)	147(6)
F(18)	1070(12)	2331(6)	821(6)	191(9)
F(19)	5329(7)	4673(6)	2002(2)	77(3)
F(20)	5579(7)	5281(6)	2533(3)	82(3)
F(21)	3830(8)	5276(6)	2610(2)	86(3)
F(22)	3588(6)	4657(5)	2072(2)	64(3)
F(23)	4500(6)	5783(5)	2109(3)	65(3)
F(24)	4702(6)	4136(5)	2517(3)	70(3)
P(1)	9589(3)	4835(2)	2742(1)	40(1)
P(2)	2996(3)	6490(2)	762(1)	39(1)
P(3)	1645(3)	1541(2)	752(1)	42(1)
P(4)	4594(3)	4957(2)	2304(1)	36(1)
S(1)	1809(3)	1764(2)	4385(1)	36(1)
S(2)	4017(3)	4224(2)	3929(1)	35(1)
S(3)	8772(3)	4207(2)	1142(1)	37(1)
S(4)	6327(3)	1723(2)	677(1)	43(1)
Fe(1)	1169(1)	2987(1)	4207(1)	25(1)
Fe(2)	3224(1)	3231(1)	3577(1)	26(1)
Fe(3)	8036(1)	3173(1)	1453(1)	28(1)
Fe(4)	5926(1)	3007(1)	823(1)	26(1)

Table S-8. Bond lengths [A] and angles [deg] for $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)](PF_6)_2 \cdot MeCN$ (**3**)

S(1)-Fe(1)	2.317(4)
S(2)-Fe(2)	2.330(4)
S(3)-Fe(3)	2.300(4)
S(4)-Fe(4)	2.307(4)
N(3)-Fe(1)	2.208(10)
N(3)-H(1D)	0.9200
N(3)-H(1E)	0.9200
N(2)-Fe(1)	2.239(10)
N(1)-Fe(1)	2.186(10)
N(4)-Fe(1)	2.173(10)
N(4)-H(4A)	0.9200
N(4)-H(4B)	0.9200
N(5)-Fe(2)	2.223(10)
N(5)-H(5D)	0.9200
N(5)-H(5E)	0.9200
N(6)-Fe(2)	2.208(10)
N(6)-H(6C)	0.9200
N(6)-H(6D)	0.9200
N(7)-Fe(2)	2.150(10)
N(8)-Fe(2)	2.216(10)
N(9)-Fe(3)	2.211(11)
N(9)-H(9C)	0.9200
N(9)-H(9D)	0.9200
N(10)-Fe(3)	2.172(10)
N(10)-H(10C)	0.9200
N(10)-H(10D)	0.9200

Table S-8 (cont.).

N(11)-Fe(3)	2.165(10)
N(12)-Fe(3)	2.237(9)
N(13)-Fe(4)	2.238(9)
N(13)-H(13D)	0.9200
N(13)-H(13E)	0.9200
N(14)-Fe(4)	2.221(9)
N(15)-Fe(4)	2.157(9)
N(16)-Fe(4)	2.168(10)
N(16)-H(16D)	0.9200
N(16)-H(16E)	0.9200
O(1)-Fe(1)	1.807(8)
O(1)-Fe(2)	1.809(8)
O(2)-Fe(4)	1.792(8)
O(2)-Fe(3)	1.819(8)
C(1)-C(3)	1.522(16)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.615(16)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-C(4)	1.535(17)
C(3)-S(1)	1.831(11)
C(4)-N(3)	1.285(15)
C(4)-C(5)	1.517(16)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800

Table S-8 (cont.).

C(5)-H(5C)	0.9800
C(6)-N(3)	1.478(15)
C(6)-C(7)	1.498(17)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-N(2)	1.494(16)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.42(2)
C(8)-N(4)	1.437(16)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-N(2)	1.461(17)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-N(1)	1.477(16)
C(10)-C(11)	1.55(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-N(2)	1.437(15)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(14)	1.512(16)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.480(18)
C(13)-H(13A)	0.9800

Table S-8 (cont.).

C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.585(18)
C(14)-S(2)	1.890(11)
C(15)-N(7)	1.244(16)
C(15)-C(16)	1.495(18)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-N(7)	1.463(15)
C(17)-C(18)	1.568(18)
C(17)-H(17A)	0.9900
C(9)-N(2)	1.461(17)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-N(1)	1.477(16)
C(10)-C(11)	1.55(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-N(2)	1.437(15)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(14)	1.512(16)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.480(18)
C(13)-H(13A)	0.9800

Table S-8 (cont.).

C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.585(18)
C(14)-S(2)	1.890(11)
C(15)-N(7)	1.244(16)
C(15)-C(16)	1.495(18)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-N(7)	1.463(15)
C(17)-C(18)	1.568(18)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-N(8)	1.475(15)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-N(8)	1.476(16)
C(19)-C(20)	1.553(17)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-N(6)	1.460(15)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-N(5)	1.514(16)
C(21)-C(22)	1.55(2)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-N(8)	1.528(16)

Table S-8 (cont.).

C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(25)	1.502(16)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.549(16)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.529(18)
C(25)-S(3)	1.832(13)
C(26)-N(11)	1.302(16)
C(26)-C(27)	1.504(18)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-N(11)	1.507(15)
C(28)-C(29)	1.526(18)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-N(12)	1.443(16)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-N(10)	1.455(16)
C(30)-C(31)	1.553(19)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900

Table S-8 (cont.).

C(31)-N(12)	1.466(17)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-N(9)	1.487(15)
C(32)-C(33)	1.544(19)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-N(12)	1.491(15)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(36)	1.554(17)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.550(15)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.514(17)
C(36)-S(4)	1.818(12)
C(37)-N(15)	1.276(14)
C(37)-C(38)	1.516(17)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-N(15)	1.460(14)
C(39)-C(40)	1.509(15)
C(39)-H(39A)	0.9900

Table S-8 (cont.).

C(39)-H(39B)	0.9900
C(40)-N(14)	1.498(14)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.466(16)
C(41)-N(13)	1.471(14)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-N(14)	1.479(14)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.487(18)
C(43)-N(16)	1.498(17)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-N(14)	1.507(15)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(46)	1.422(19)
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-N(17)	1.161(16)
C(47)-C(48)	1.43(2)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-N(18)	1.133(19)

Table S-8 (cont.).

F(1)-P(1)	1.550(10)
F(2)-P(1)	1.566(10)
F(3)-P(1)	1.511(11)
F(4)-P(1)	1.555(9)
F(5)-P(1)	1.542(9)
F(6)-P(1)	1.559(10)
F(7)-P(2)	1.524(11)
F(8)-P(2)	1.586(9)
F(9)-P(2)	1.522(10)
F(10)-P(2)	1.577(9)
F(11)-P(2)	1.559(12)
F(12)-P(2)	1.497(12)
F(13)-P(3)	1.550(10)
F(14)-P(3)	1.506(12)
F(15)-P(3)	1.550(10)
F(16)-P(3)	1.583(13)
F(17)-P(3)	1.560(11)
F(18)-P(3)	1.552(10)
F(19)-P(4)	1.534(8)
F(20)-P(4)	1.579(9)
F(21)-P(4)	1.587(9)
F(22)-P(4)	1.594(9)
F(23)-P(4)	1.576(8)
F(24)-P(4)	1.602(8)
C(3)-S(1)-Fe(1)	104.4(4)
C(14)-S(2)-Fe(2)	103.6(4)
C(25)-S(3)-Fe(3)	103.9(4)
C(36)-S(4)-Fe(4)	104.0(4)

Table S-8 (cont.).

O(1)-Fe(1)-N(4)	91.4(4)
O(1)-Fe(1)-N(1)	178.6(4)
N(4)-Fe(1)-N(1)	87.2(4)
O(1)-Fe(1)-N(3)	92.3(4)
N(4)-Fe(1)-N(3)	153.2(4)
N(3)-Fe(1)-N(1)	89.1(4)
O(1)-Fe(1)-N(2)	102.9(4)
N(4)-Fe(1)-N(2)	77.8(4)
N(1)-Fe(1)-N(2)	77.2(4)
N(3)-Fe(1)-N(2)	75.4(4)
O(1)-Fe(1)-S(1)	99.6(3)
N(4)-Fe(1)-S(1)	105.3(3)
N(1)-Fe(1)-S(1)	80.4(3)
N(3)-Fe(1)-S(1)	100.2(3)
N(2)-Fe(1)-S(1)	157.2(3)
O(1)-Fe(2)-N(7)	175.4(4)
O(1)-Fe(2)-N(6)	94.4(4)
N(7)-Fe(2)-N(6)	90.1(4)
O(1)-Fe(2)-N(8)	103.2(4)
N(7)-Fe(2)-N(8)	77.7(4)
N(6)-Fe(2)-N(8)	77.5(4)
O(1)-Fe(2)-N(5)	91.7(4)
N(7)-Fe(2)-N(5)	84.1(4)
N(6)-Fe(2)-N(5)	154.3(4)
N(8)-Fe(2)-N(5)	76.8(4)
O(1)-Fe(2)-S(2)	98.4(3)
N(7)-Fe(2)-S(2)	81.1(3)
N(6)-Fe(2)-S(2)	97.6(3)

Table S-8 (cont.).

N(8)-Fe(2)-S(2)	158.2(3)
N(5)-Fe(2)-S(2)	106.1(3)
O(2)-Fe(3)-N(11)	175.8(4)
O(2)-Fe(3)-N(10)	93.5(4)
N(11)-Fe(3)-N(10)	90.0(4)
O(2)-Fe(3)-N(9)	92.0(4)
N(11)-Fe(3)-N(9)	83.8(4)
N(10)-Fe(3)-N(9)	154.5(4)
O(2)-Fe(3)-N(12)	99.8(4)
N(11)-Fe(3)-N(12)	78.8(4)
N(10)-Fe(3)-N(12)	77.0(4)
N(9)-Fe(3)-N(12)	77.5(4)
O(2)-Fe(3)-S(3)	100.6(3)
N(11)-Fe(3)-S(3)	81.1(3)
N(10)-Fe(3)-S(3)	98.4(3)
N(9)-Fe(3)-S(3)	104.9(3)
N(12)-Fe(3)-S(3)	159.4(3)
O(2)-Fe(4)-N(15)	175.4(4)
O(2)-Fe(4)-N(16)	91.3(4)
N(15)-Fe(4)-N(16)	93.1(4)
O(2)-Fe(4)-N(14)	101.2(3)
N(15)-Fe(4)-N(14)	78.5(4)
N(16)-Fe(4)-N(14)	78.5(4)
O(2)-Fe(4)-N(13)	93.0(4)
N(15)-Fe(4)-N(13)	82.4(4)
N(16)-Fe(4)-N(13)	155.2(4)
N(14)-Fe(4)-N(13)	76.7(4)
O(2)-Fe(4)-S(4)	100.2(3)

Table S-8 (cont.).

N(15)-Fe(4)-S(4)	80.4(3)
N(16)-Fe(4)-S(4)	98.3(3)
N(14)-Fe(4)-S(4)	158.4(3)
N(13)-Fe(4)-S(4)	105.0(3)
C(10)-N(3)-Fe(1)	116.0(9)
C(10)-N(3)-H(1D)	108.3
Fe(1)-N(3)-H(1D)	108.3
C(10)-N(3)-H(1E)	108.3
Fe(1)-N(3)-H(1E)	108.3
H(1D)-N(3)-H(1E)	107.4
C(11)-N(2)-C(9)	110.3(12)
C(11)-N(2)-C(7)	111.4(10)
C(9)-N(2)-C(7)	114.0(12)
C(11)-N(2)-Fe(1)	103.9(8)
C(9)-N(2)-Fe(1)	104.9(8)
C(7)-N(2)-Fe(1)	111.8(8)
C(4)-N(1)-C(6)	119.1(10)
C(4)-N(1)-Fe(1)	123.2(8)
C(6)-N(1)-Fe(1)	116.6(7)
C(8)-N(4)-Fe(1)	114.0(9)
C(8)-N(4)-H(4A)	108.8
Fe(1)-N(4)-H(4A)	108.8
C(8)-N(4)-H(4B)	108.8
Fe(1)-N(4)-H(4B)	108.8
H(4A)-N(4)-H(4B)	107.7
C(21)-N(5)-Fe(2)	113.4(7)
C(21)-N(5)-H(5D)	108.9
Fe(2)-N(5)-H(5D)	108.9

Table S-8 (cont.).

C(21)-N(5)-H(5E)	108.9
Fe(2)-N(5)-H(5E)	108.9
H(5D)-N(5)-H(5E)	107.7
C(20)-N(6)-Fe(2)	114.0(7)
C(20)-N(6)-H(6C)	108.7
Fe(2)-N(6)-H(6C)	108.7
C(20)-N(6)-H(6D)	108.7
Fe(2)-N(6)-H(6D)	108.7
H(6C)-N(6)-H(6D)	107.6
C(15)-N(7)-C(17)	120.1(11)
C(15)-N(7)-Fe(2)	124.3(9)
C(17)-N(7)-Fe(2)	115.3(8)
C(18)-N(8)-C(19)	107.1(10)
C(18)-N(8)-C(22)	113.1(10)
C(19)-N(8)-C(22)	108.1(10)
C(18)-N(8)-Fe(2)	114.9(8)
C(19)-N(8)-Fe(2)	106.2(7)
C(22)-N(8)-Fe(2)	107.0(8)
C(32)-N(9)-Fe(3)	113.7(8)
C(32)-N(9)-H(9C)	108.8
Fe(3)-N(9)-H(9C)	108.8
C(32)-N(9)-H(9D)	108.8
Fe(3)-N(9)-H(9D)	108.8
H(9C)-N(9)-H(9D)	107.7
C(30)-N(10)-Fe(3)	114.4(8)
C(30)-N(10)-H(10C)	108.6
Fe(3)-N(10)-H(10C)	108.6
C(30)-N(10)-H(10D)	108.6

Table S-8 (cont.).

Fe(3)-N(10)-H(10D)	108.6
H(10C)-N(10)-H(10D)	107.6
C(26)-N(11)-C(28)	121.9(12)
C(26)-N(11)-Fe(3)	123.7(9)
C(28)-N(11)-Fe(3)	114.3(8)
C(29)-N(12)-C(31)	112.1(10)
C(29)-N(12)-C(33)	115.0(10)
C(31)-N(12)-C(33)	108.3(11)
C(29)-N(12)-Fe(3)	111.4(7)
C(31)-N(12)-Fe(3)	104.3(7)
C(33)-N(12)-Fe(3)	105.0(7)
C(41)-N(13)-Fe(4)	111.9(8)
C(41)-N(13)-H(13D)	109.2
Fe(4)-N(13)-H(13D)	109.2
C(41)-N(13)-H(13E)	109.2
Fe(4)-N(13)-H(13E)	109.2
H(13D)-N(13)-H(13E)	107.9
C(42)-N(14)-C(40)	112.0(10)
C(42)-N(14)-C(44)	109.7(9)
C(40)-N(14)-C(44)	112.4(9)
C(42)-N(14)-Fe(4)	105.0(7)
C(40)-N(14)-Fe(4)	112.8(6)
C(44)-N(14)-Fe(4)	104.5(6)
C(37)-N(15)-C(39)	120.6(10)
C(37)-N(15)-Fe(4)	123.9(8)
C(39)-N(15)-Fe(4)	115.1(7)
C(43)-N(16)-Fe(4)	112.4(8)
C(43)-N(16)-H(16D)	109.1

Table S-8 (cont.).

Fe(4)-N(16)-H(16D)	109.1
C(43)-N(16)-H(16E)	109.1
Fe(4)-N(16)-H(16E)	109.1
H(16D)-N(16)-H(16E)	107.9
Fe(1)-O(1)-Fe(2)	155.3(5)
Fe(4)-O(2)-Fe(3)	149.8(5)
C(3)-C(1)-H(1A)	109.5
C(3)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(3)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-C(4)	111.1(10)
C(1)-C(3)-C(2)	111.0(10)
C(4)-C(3)-C(2)	106.3(10)
C(1)-C(3)-S(1)	110.2(9)
C(4)-C(3)-S(1)	111.5(8)
C(2)-C(3)-S(1)	106.6(8)
N(3)-C(4)-C(5)	122.0(12)
N(3)-C(4)-C(3)	119.9(10)
C(5)-C(4)-C(3)	118.1(11)
C(4)-C(5)-H(5A)	109.5

Table S-8 (cont.).

C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(3)-C(6)-C(7)	110.3(10)
N(3)-C(6)-H(6A)	109.6
C(7)-C(6)-H(6A)	109.6
N(3)-C(6)-H(6B)	109.6
C(7)-C(6)-H(6B)	109.6
H(6A)-C(6)-H(6B)	108.1
N(2)-C(7)-C(6)	114.6(10)
N(2)-C(7)-H(7A)	108.6
C(6)-C(7)-H(7A)	108.6
N(2)-C(7)-H(7B)	108.6
C(6)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.6
C(9)-C(8)-N(4)	112.9(13)
C(9)-C(8)-H(8A)	109.0
N(4)-C(8)-H(8A)	109.0
C(9)-C(8)-H(8B)	109.0
N(4)-C(8)-H(8B)	109.0
H(8A)-C(8)-H(8B)	107.8
C(8)-C(9)-N(2)	116.8(14)
C(8)-C(9)-H(9A)	108.1
N(2)-C(9)-H(9A)	108.1
C(8)-C(9)-H(9B)	108.1
N(2)-C(9)-H(9B)	108.1

Table S-8 (cont.).

H(9A)-C(9)-H(9B)	107.3
N(1)-C(10)-C(11)	106.8(11)
N(1)-C(10)-H(10A)	110.4
C(11)-C(10)-H(10A)	110.4
N(1)-C(10)-H(10B)	110.4
C(11)-C(10)-H(10B)	110.4
H(10A)-C(10)-H(10B)	108.6
N(2)-C(11)-C(10)	113.6(12)
N(2)-C(11)-H(11A)	108.8
C(10)-C(11)-H(11A)	108.8
N(2)-C(11)-H(11B)	108.8
C(10)-C(11)-H(11B)	108.8
H(11A)-C(11)-H(11B)	107.7
C(14)-C(12)-H(12A)	109.5
C(14)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(14)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(13)-C(14)-C(12)	113.8(12)
C(13)-C(14)-C(15)	114.8(10)
C(12)-C(14)-C(15)	106.9(10)

Table S-8 (cont.).

C(13)-C(14)-S(2)	110.0(8)
C(12)-C(14)-S(2)	103.6(8)
C(15)-C(14)-S(2)	107.0(9)
N(7)-C(15)-C(16)	124.4(12)
N(7)-C(15)-C(14)	122.1(11)
C(16)-C(15)-C(14)	113.1(12)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(7)-C(17)-C(18)	111.3(10)
N(7)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
N(7)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
N(8)-C(18)-C(17)	110.4(10)
N(8)-C(18)-H(18A)	109.6
C(17)-C(18)-H(18A)	109.6
N(8)-C(18)-H(18B)	109.6
C(17)-C(18)-H(18B)	109.6
H(18A)-C(18)-H(18B)	108.1
N(8)-C(19)-C(20)	109.1(10)
N(8)-C(19)-H(19A)	109.9
C(20)-C(19)-H(19A)	109.9
N(8)-C(19)-H(19B)	109.9

Table S-8 (cont.).

C(20)-C(19)-H(19B)	109.9
H(19A)-C(19)-H(19B)	108.3
N(6)-C(20)-C(19)	108.3(9)
N(6)-C(20)-H(20A)	110.0
C(19)-C(20)-H(20A)	110.0
N(6)-C(20)-H(20B)	110.0
C(19)-C(20)-H(20B)	110.0
H(20A)-C(20)-H(20B)	108.4
N(5)-C(21)-C(22)	110.2(10)
N(5)-C(21)-H(21A)	109.6
C(22)-C(21)-H(21A)	109.6
N(5)-C(21)-H(21B)	109.6
C(22)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1
N(8)-C(22)-C(21)	106.2(12)
N(8)-C(22)-H(22A)	110.5
C(21)-C(22)-H(22A)	110.5
N(8)-C(22)-H(22B)	110.5
C(21)-C(22)-H(22B)	110.5
H(22A)-C(22)-H(22B)	108.7
C(25)-C(23)-H(23A)	109.5
C(25)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(25)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-H(24A)	109.5
C(25)-C(24)-H(24B)	109.5

Table S-8 (cont.).

H(24A)-C(24)-H(24B)	109.5
C(25)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-C(26)	109.1(10)
C(23)-C(25)-C(24)	111.8(10)
C(26)-C(25)-C(24)	108.2(11)
C(23)-C(25)-S(3)	108.6(9)
C(26)-C(25)-S(3)	112.5(9)
C(24)-C(25)-S(3)	106.6(9)
N(11)-C(26)-C(27)	120.8(13)
N(11)-C(26)-C(25)	118.5(12)
C(27)-C(26)-C(25)	120.3(12)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(11)-C(28)-C(29)	109.5(10)
N(11)-C(28)-H(28A)	109.8
C(29)-C(28)-H(28A)	109.8
N(11)-C(28)-H(28B)	109.8
C(29)-C(28)-H(28B)	109.8
H(28A)-C(28)-H(28B)	108.2
N(12)-C(29)-C(28)	115.9(11)
N(12)-C(29)-H(29A)	108.3
C(28)-C(29)-H(29A)	108.3

Table S-8 (cont.).

N(12)-C(29)-H(29B)	108.3
C(28)-C(29)-H(29B)	108.3
H(29A)-C(29)-H(29B)	107.4
N(10)-C(30)-C(31)	109.7(10)
N(10)-C(30)-H(30A)	109.7
C(31)-C(30)-H(30A)	109.7
N(10)-C(30)-H(30B)	109.7
C(31)-C(30)-H(30B)	109.7
H(30A)-C(30)-H(30B)	108.2
N(12)-C(31)-C(30)	108.3(10)
N(12)-C(31)-H(31A)	110.0
C(30)-C(31)-H(31A)	110.0
N(12)-C(31)-H(31B)	110.0
C(30)-C(31)-H(31B)	110.0
H(31A)-C(31)-H(31B)	108.4
N(9)-C(32)-C(33)	108.7(10)
N(9)-C(32)-H(32A)	109.9
C(33)-C(32)-H(32A)	109.9
N(9)-C(32)-H(32B)	109.9
C(33)-C(32)-H(32B)	109.9
H(32A)-C(32)-H(32B)	108.3
N(12)-C(33)-C(32)	109.0(11)
N(12)-C(33)-H(33A)	109.9
C(32)-C(33)-H(33A)	109.9
N(12)-C(33)-H(33B)	109.9
C(32)-C(33)-H(33B)	109.9
H(33A)-C(33)-H(33B)	108.3
C(36)-C(34)-H(34A)	109.5

Table S-8 (cont.).

C(36)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(36)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-H(35A)	109.5
C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(36)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(37)-C(36)-C(35)	110.7(10)
C(37)-C(36)-C(34)	108.3(10)
C(35)-C(36)-C(34)	110.5(11)
C(37)-C(36)-S(4)	111.9(8)
C(35)-C(36)-S(4)	107.1(8)
C(34)-C(36)-S(4)	108.3(9)
N(15)-C(37)-C(36)	119.7(10)
N(15)-C(37)-C(38)	122.7(11)
C(36)-C(37)-C(38)	117.4(10)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
N(15)-C(39)-C(40)	113.7(10)
N(15)-C(39)-H(39A)	108.8

Table S-8 (cont.).

C(40)-C(39)-H(39A)	108.8
N(15)-C(39)-H(39B)	108.8
C(40)-C(39)-H(39B)	108.8
H(39A)-C(39)-H(39B)	107.7
N(14)-C(40)-C(39)	112.7(9)
N(14)-C(40)-H(40A)	109.0
C(39)-C(40)-H(40A)	109.0
N(14)-C(40)-H(40B)	109.0
C(39)-C(40)-H(40B)	109.0
H(40A)-C(40)-H(40B)	107.8
C(42)-C(41)-N(13)	110.6(10)
C(42)-C(41)-H(41A)	109.5
N(13)-C(41)-H(41A)	109.5
C(42)-C(41)-H(41B)	109.5
N(13)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	108.1
C(41)-C(42)-N(14)	110.4(10)
C(41)-C(42)-H(42A)	109.6
N(14)-C(42)-H(42A)	109.6
C(41)-C(42)-H(42B)	109.6
N(14)-C(42)-H(42B)	109.6
H(42A)-C(42)-H(42B)	108.1
C(44)-C(43)-N(16)	112.0(11)
C(44)-C(43)-H(43A)	109.2
N(16)-C(43)-H(43A)	109.2
C(44)-C(43)-H(43B)	109.2
N(16)-C(43)-H(43B)	109.2
H(43A)-C(43)-H(43B)	107.9

Table S-8 (cont.).

C(43)-C(44)-N(14)	109.9(10)
C(43)-C(44)-H(44A)	109.7
N(14)-C(44)-H(44A)	109.7
C(43)-C(44)-H(44B)	109.7
N(14)-C(44)-H(44B)	109.7
H(44A)-C(44)-H(44B)	108.2
C(46)-C(45)-H(45A)	109.5
C(46)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(46)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
N(17)-C(46)-C(45)	174.8(15)
C(48)-C(47)-H(47A)	109.5
C(48)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(48)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
N(18)-C(48)-C(47)	175.9(19)
F(3)-P(1)-F(5)	92.4(8)
F(3)-P(1)-F(1)	177.3(9)
F(5)-P(1)-F(1)	90.0(8)
F(3)-P(1)-F(4)	92.7(7)
F(5)-P(1)-F(4)	87.4(6)
F(1)-P(1)-F(4)	86.1(7)
F(3)-P(1)-F(6)	91.9(7)
F(5)-P(1)-F(6)	175.2(8)

Table S-8 (cont.).

F(1)-P(1)-F(6)	85.8(7)
F(4)-P(1)-F(6)	94.5(6)
F(3)-P(1)-F(2)	88.6(7)
F(5)-P(1)-F(2)	91.6(6)
F(1)-P(1)-F(2)	92.6(7)
F(4)-P(1)-F(2)	178.4(6)
F(6)-P(1)-F(2)	86.4(6)
F(12)-P(2)-F(9)	99.2(10)
F(12)-P(2)-F(7)	88.3(9)
F(9)-P(2)-F(7)	172.3(9)
F(12)-P(2)-F(11)	173.5(8)
F(9)-P(2)-F(11)	87.0(8)
F(7)-P(2)-F(11)	85.6(8)
F(12)-P(2)-F(10)	89.9(7)
F(9)-P(2)-F(10)	94.4(6)
F(7)-P(2)-F(10)	87.5(6)
F(11)-P(2)-F(10)	87.8(6)
F(12)-P(2)-F(8)	91.4(7)
F(9)-P(2)-F(8)	85.8(6)
F(7)-P(2)-F(8)	92.1(6)
F(11)-P(2)-F(8)	90.9(7)
F(10)-P(2)-F(8)	178.6(7)
F(14)-P(3)-F(15)	89.7(8)
F(14)-P(3)-F(13)	94.6(8)
F(15)-P(3)-F(13)	175.6(8)
F(14)-P(3)-F(18)	98.8(11)
F(15)-P(3)-F(18)	91.5(7)
F(13)-P(3)-F(18)	89.1(8)

Table S-8 (cont.).

F(14)-P(3)-F(17)	90.3(11)
F(15)-P(3)-F(17)	86.6(7)
F(13)-P(3)-F(17)	92.2(8)
F(18)-P(3)-F(17)	170.8(11)
F(14)-P(3)-F(16)	175.6(11)
F(15)-P(3)-F(16)	91.2(8)
F(13)-P(3)-F(16)	84.5(8)
F(18)-P(3)-F(16)	85.5(10)
F(17)-P(3)-F(16)	85.5(9)
F(19)-P(4)-F(23)	89.9(5)
F(19)-P(4)-F(20)	90.2(6)
F(23)-P(4)-F(20)	88.7(5)
F(19)-P(4)-F(21)	178.3(6)
F(23)-P(4)-F(21)	88.4(5)
F(20)-P(4)-F(21)	89.8(6)
F(19)-P(4)-F(22)	90.6(5)
F(23)-P(4)-F(22)	89.8(5)
F(20)-P(4)-F(22)	178.4(5)
F(21)-P(4)-F(22)	89.4(5)
F(19)-P(4)-F(24)	91.5(5)
F(23)-P(4)-F(24)	177.8(6)
F(20)-P(4)-F(24)	89.6(5)
F(21)-P(4)-F(24)	90.2(5)
F(22)-P(4)-F(24)	91.9(5)

Table S-9. Anisotropic displacement parameters (A^2 x 10^3) for [(Fe^{III}(S^{Me2}N$_4$(tren))$_2$(μ-O)](PF$_6$)$_2$ •MeCN (**3**). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	43(2)	24(2)	44(2)	7(2)	15(2)	3(2)
S(2)	43(2)	30(2)	33(2)	-6(2)	6(2)	-10(2)
S(3)	39(2)	28(2)	45(2)	11(2)	-5(2)	-3(2)
S(4)	58(3)	26(2)	44(2)	-7(2)	-13(2)	9(2)
Fe(1)	30(1)	17(1)	29(1)	1(1)	3(1)	-1(1)
Fe(2)	29(1)	20(1)	30(1)	2(1)	2(1)	1(1)
Fe(3)	33(1)	23(1)	28(1)	-1(1)	-1(1)	2(1)
Fe(4)	31(1)	19(1)	28(1)	-1(1)	-1(1)	1(1)
N(3)	22(7)	49(7)	32(6)	-9(5)	1(5)	-5(5)
N(2)	37(7)	20(6)	45(7)	-5(5)	-6(5)	-11(5)
N(1)	29(7)	26(6)	21(5)	-7(4)	-5(4)	-8(5)
N(4)	5(7)	41(7)	58(7)	7(6)	-5(5)	-9(5)
N(5)	34(7)	35(6)	32(6)	6(5)	7(5)	7(5)
N(6)	33(7)	22(6)	52(7)	9(5)	6(5)	-7(5)
N(7)	20(7)	34(6)	32(6)	-5(5)	0(5)	-7(5)
N(8)	54(9)	36(7)	31(6)	-18(5)	9(6)	-1(6)
N(9)	47(9)	40(7)	47(7)	0(6)	-8(6)	7(6)
N(10)	30(7)	42(7)	46(7)	-9(6)	-6(5)	1(5)
N(11)	17(7)	27(6)	49(7)	0(5)	-3(5)	2(5)
N(12)	36(8)	24(6)	35(6)	13(5)	2(5)	1(5)
N(13)	18(7)	29(6)	40(6)	2(5)	0(5)	-2(4)
N(14)	30(7)	16(5)	35(6)	-3(5)	-10(5)	6(4)
N(15)	8(6)	36(6)	30(6)	2(5)	-10(4)	7(4)
N(16)	39(8)	40(7)	27(6)	-2(5)	3(5)	-14(5)

N(17)	57(11)	70(9)	63(9)	-3(7)	25(7)	-31(8)
N(18)	131(16)	112(14)	37(8)	-9(9)	-11(9)	74(12)
O(1)	34(6)	11(4)	58(6)	5(4)	0(4)	-9(4)
O(2)	36(6)	15(4)	44(5)	5(4)	-5(4)	6(4)
C(1)	63(11)	37(8)	27(7)	6(6)	1(7)	13(7)
C(2)	56(10)	23(7)	48(9)	13(6)	-1(7)	-28(7)
C(3)	27(8)	23(6)	26(7)	13(5)	-4(5)	2(5)
C(4)	31(9)	45(9)	33(7)	4(7)	9(6)	-3(6)
C(5)	31(10)	51(9)	52(9)	1(7)	23(7)	-15(7)
C(6)	31(10)	46(9)	43(8)	24(7)	12(6)	6(7)
C(7)	60(11)	33(8)	50(9)	-8(7)	25(8)	6(7)
C(8)	65(13)	44(10)	72(12)	5(8)	-20(9)	12(8)
C(9)	51(12)	77(13)	61(11)	-11(10)	-14(8)	12(9)
C(10)	35(11)	28(8)	126(16)	-26(9)	7(10)	-3(7)
C(11)	36(10)	14(7)	96(12)	-10(7)	33(9)	7(6)
C(12)	39(10)	72(11)	19(7)	-1(7)	16(6)	10(8)
C(13)	41(11)	78(12)	64(11)	44(9)	17(8)	32(9)
C(14)	1(8)	70(10)	16(6)	7(6)	4(5)	3(6)
C(15)	35(10)	60(10)	20(7)	6(7)	10(6)	16(8)
C(16)	32(10)	77(12)	48(9)	-26(8)	-15(7)	-11(8)
C(17)	51(11)	45(9)	46(9)	-2(7)	14(7)	13(7)
C(19)	12(9)	46(9)	49(9)	-5(7)	11(6)	17(6)
C(20)	52(10)	45(8)	21(7)	15(6)	4(6)	16(7)
C(21)	92(13)	26(8)	45(9)	3(7)	8(8)	37(8)
C(22)	93(14)	14(7)	57(10)	1(7)	-8(9)	-9(7)
C(23)	21(9)	34(8)	55(9)	7(7)	5(6)	0(6)
C(24)	42(11)	38(9)	87(12)	-24(9)	-3(8)	-7(7)
C(25)	22(8)	20(7)	50(8)	-6(6)	5(6)	-5(5)
C(26)	44(11)	79(11)	11(6)	-3(7)	13(6)	-9(8)

C(27)	10(10)	124(15)	45(9)	21(10)	-12(7)	-21(8)
C(28)	35(10)	74(11)	39(8)	22(8)	16(7)	25(8)
C(29)	39(10)	36(8)	38(8)	9(6)	2(7)	7(6)
C(30)	77(12)	70(11)	11(6)	-5(7)	10(7)	25(9)
C(31)	14(10)	65(11)	73(11)	21(9)	-5(7)	-20(7)
C(32)	100(13)	9(6)	40(8)	6(6)	-1(8)	12(7)
C(33)	71(11)	16(7)	45(9)	-2(6)	-22(8)	-3(7)
C(34)	56(12)	29(8)	88(12)	3(8)	12(9)	-5(7)
C(35)	51(10)	26(7)	32(7)	-13(6)	6(6)	17(6)
C(36)	11(8)	40(8)	30(7)	-10(6)	1(5)	1(5)
C(37)	18(8)	31(7)	35(7)	-15(6)	1(6)	-2(5)
C(38)	43(11)	51(9)	46(9)	-32(7)	-18(7)	-1(7)
C(39)	26(9)	32(7)	43(8)	-18(6)	-21(6)	5(6)
C(40)	24(8)	29(7)	35(7)	-6(6)	-10(6)	20(6)
C(41)	75(12)	6(6)	67(10)	8(6)	12(9)	1(6)
C(42)	20(8)	24(7)	44(8)	0(6)	17(6)	4(6)
C(43)	60(12)	62(11)	40(9)	9(8)	7(8)	8(9)
C(44)	37(9)	29(7)	26(7)	-8(6)	-12(6)	23(6)
C(45)	35(10)	51(10)	63(10)	11(8)	11(7)	-17(7)
C(46)	20(10)	51(10)	52(9)	-10(8)	5(7)	12(7)
C(47)	88(14)	59(11)	28(8)	-19(7)	0(8)	22(9)
C(48)	88(14)	29(8)	28(8)	-8(6)	-17(8)	4(8)
F(1)	110(10)	211(15)	75(7)	23(9)	6(7)	112(10)
F(2)	75(8)	40(6)	175(11)	6(6)	57(7)	2(5)
F(3)	101(10)	269(17)	49(6)	23(9)	19(6)	99(10)
F(4)	52(7)	76(7)	188(12)	25(8)	61(7)	12(5)
F(5)	50(7)	108(9)	251(16)	-141(10)	2(8)	1(6)
F(6)	100(9)	65(7)	161(12)	-55(7)	-10(8)	20(6)

F(7)	74(8)	67(7)	219(15)	-59(9)	5(8)	19(6)
F(8)	3(6)	102(9)	215(13)	25(8)	-20(6)	3(5)
F(9)	79(9)	82(8)	234(16)	-96(10)	-14(9)	-4(6)
F(10)	64(7)	70(7)	133(10)	-17(6)	18(6)	36(5)
F(11)	62(8)	234(16)	80(8)	14(9)	4(6)	-50(8)
F(12)	76(10)	340(20)	144(12)	153(14)	-14(8)	-75(11)
F(13)	141(11)	152(12)	104(9)	37(9)	40(8)	-69(9)
F(14)	212(17)	280(20)	130(12)	61(13)	-112(12)	-183(16)
F(15)	129(11)	126(11)	124(10)	67(9)	56(8)	1(8)
F(16)	114(12)	198(17)	172(15)	31(12)	-59(10)	-28(10)
F(17)	86(9)	53(7)	304(19)	-33(9)	70(10)	-5(6)
F(18)	171(14)	40(6)	370(20)	-30(10)	176(16)	16(7)
F(19)	55(7)	125(9)	52(6)	-3(6)	11(5)	48(6)
F(20)	75(8)	91(8)	77(7)	11(6)	-38(5)	-21(6)
F(21)	99(8)	98(8)	60(6)	-21(6)	10(5)	40(6)
F(22)	34(6)	68(6)	89(7)	-7(5)	-20(5)	1(4)
F(23)	38(6)	42(5)	115(8)	39(5)	7(5)	-1(4)
F(24)	50(6)	50(5)	109(8)	32(5)	10(5)	14(4)
P(1)	32(3)	42(2)	45(2)	-9(2)	1(2)	0(2)
P(2)	36(3)	30(2)	51(2)	6(2)	5(2)	1(2)
P(3)	44(3)	33(2)	49(2)	9(2)	5(2)	3(2)
P(4)	39(3)	31(2)	40(2)	5(2)	1(2)	-3(2)

Table S-10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $[(Fe^{III}(S^{Me2}N_4(tren))_2(\mu\text{-}O)](PF_6)_2 \cdot MeCN$ (**3**)

	x	y	z	U(eq)
H(1A)	2065	1627	5160	64
H(1B)	1970	726	5036	64
H(1C)	1094	1104	5293	64
H(2A)	709	378	4444	63
H(2B)	-324	921	4425	63
H(2C)	-52	423	4788	63
H(5A)	-582	2288	5338	66
H(5B)	-579	1380	5222	66
H(5C)	-1393	1976	5026	66
H(6A)	-815	3379	5005	47
H(6B)	-1362	3166	4615	47
H(7A)	-1036	4439	4542	57
H(7B)	35	4408	4784	57
H(8A)	-1049	3454	3522	73
H(8B)	-1542	3331	3918	73
H(9A)	-980	4519	3945	76
H(9B)	40	4335	3711	76
H(10A)	2548	4905	4486	76
H(10B)	1659	4790	4790	76
H(11A)	684	5224	4283	58
H(11B)	1363	4716	4004	58
H(12A)	6817	4503	3886	65
H(12B)	6153	3817	4073	65
H(12C)	5961	4714	4187	65

Table S-10 (cont.).

H(13A)	5095	5618	3699	91
H(13B)	4660	5230	3324	91
H(13C)	5906	5336	3395	91
H(16A)	6985	3377	3336	78
H(16B)	6803	4291	3251	78
H(16C)	6403	3643	2960	78
H(17A)	5263	2152	3218	56
H(17B)	5470	2764	2893	56
H(18A)	3783	2640	2650	41
H(18B)	3989	1762	2795	41
H(19A)	1441	2636	3030	43
H(19B)	2023	2366	2664	43
H(20A)	2892	3596	2619	47
H(20B)	1663	3787	2673	47
H(21A)	3310	953	3732	65
H(21B)	4199	1228	3453	65
H(22A)	2629	1188	3095	66
H(22B)	1983	1650	3403	66
H(23A)	11515	4577	1122	54
H(23B)	10577	4469	822	54
H(23C)	11109	3714	1014	54
H(24A)	10855	5203	1646	84
H(24B)	9651	5088	1760	84
H(24C)	9916	5519	1382	84
H(27A)	11421	3500	2058	90
H(27B)	11872	4016	1729	90
H(27C)	11768	3082	1685	90
H(28A)	10336	2578	2143	59

Table S-10 (cont.).

H(28B)	10123	2005	1799	59
H(29A)	8867	1610	2187	45
H(29B)	8672	2479	2338	45
H(30A)	6441	3541	2319	63
H(30B)	7643	3322	2428	63
H(31A)	6818	2114	2292	61
H(31B)	6283	2456	1919	61
H(32A)	9099	1214	1494	60
H(32B)	8194	941	1204	60
H(33A)	6871	1573	1542	54
H(33B)	7545	1051	1832	54
H(34A)	4260	1084	494	86
H(34B)	5116	423	404	86
H(34C)	4382	782	81	86
H(35A)	6038	1095	-262	54
H(35B)	6826	832	66	54
H(35C)	6888	1705	-96	54
H(38A)	3829	2480	-271	70
H(38B)	4513	1715	-361	70
H(38C)	4979	2572	-440	70
H(39A)	3901	3501	38	41
H(39B)	5049	3878	-6	41
H(40A)	4367	4754	367	36
H(40B)	3616	4126	559	36
H(41A)	7282	4912	472	59
H(41B)	6270	4657	226	59
H(42A)	5655	5279	731	35
H(42B)	6385	4754	1002	35

Table S-10 (cont.).

H(43A)	3282	3532	1075	64
H(43B)	3739	3515	1489	64
H(44A)	5111	4312	1354	37
H(44B)	4103	4704	1151	37
H(45A)	2304	1191	1740	74
H(45B)	2125	1472	2154	74
H(45C)	2906	755	2075	74
H(47A)	2725	6570	2152	87
H(47B)	2463	6119	1774	87
H(47C)	2026	5785	2153	87
H(1D)	2083	3589	4806	41
H(1E)	2849	3685	4507	41
H(4A)	36	2570	3627	42
H(4B)	-585	2348	3952	42
H(5D)	4511	2133	3860	40
H(5E)	3482	2031	4043	40
H(6C)	1972	4227	3213	42
H(6D)	3056	4366	3080	42
H(9C)	8195	2071	941	54
H(9D)	9270	2164	1109	54
H(10C)	8014	4135	2015	47
H(10D)	6929	4142	1849	47
H(13D)	7675	3715	581	35
H(13E)	7014	3533	248	35
H(16D)	4101	2440	1020	42
H(16E)	4747	2547	1364	42