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Supporting Information

A Structural Model for the Iron–Nitrosyl Adduct of Gentisate Dioxygenase

Atanu Banerjee, Jia Li, Amy L. Speelman, Corey J. White, Piotr L. Pawlak, William W. Brennessel, Nicolai Lehnert, and Ferman A. Chavez*

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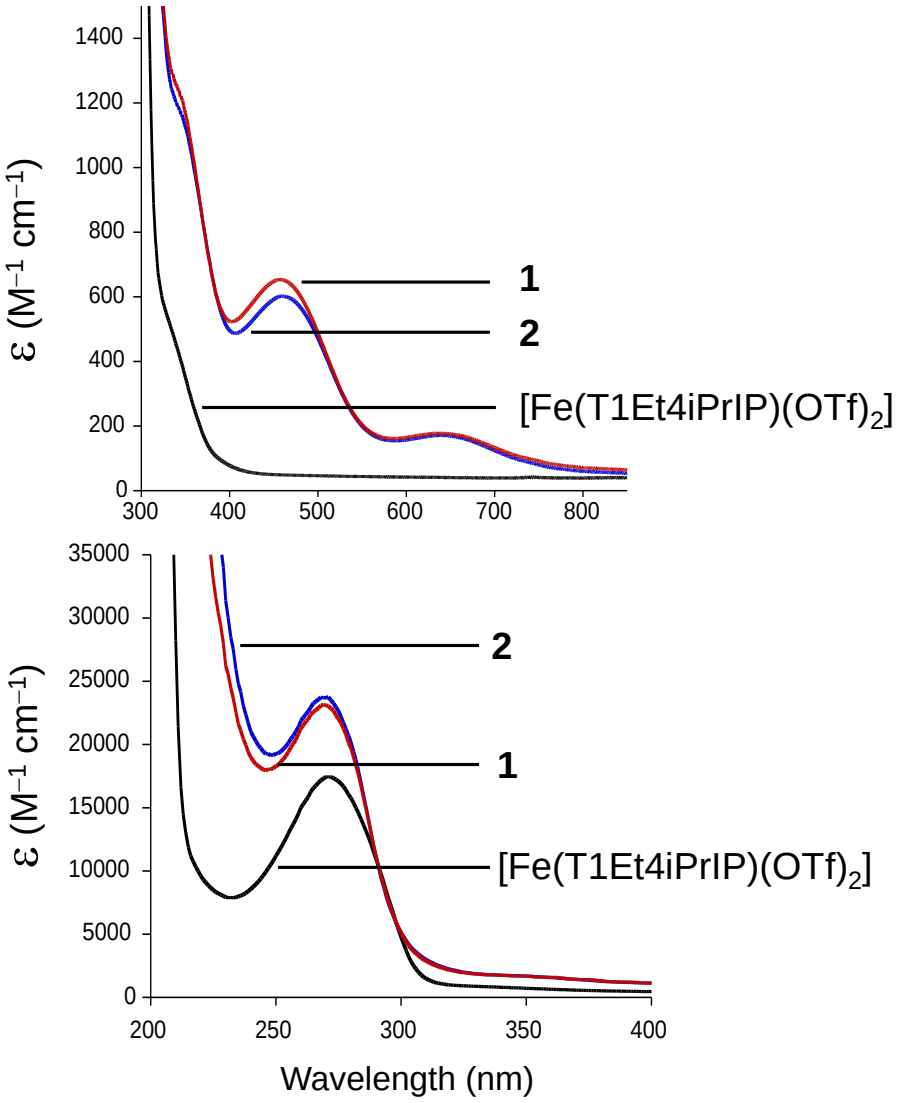

Figure S1. UV-vis spectrum of [Fe(T1Et4iPrIP)($OTf)_2$] in THF solution (black), after addition of excess NO gas (**2**, blue), and after addition of NO and 2.2 equiv H_2O (**1**, red).

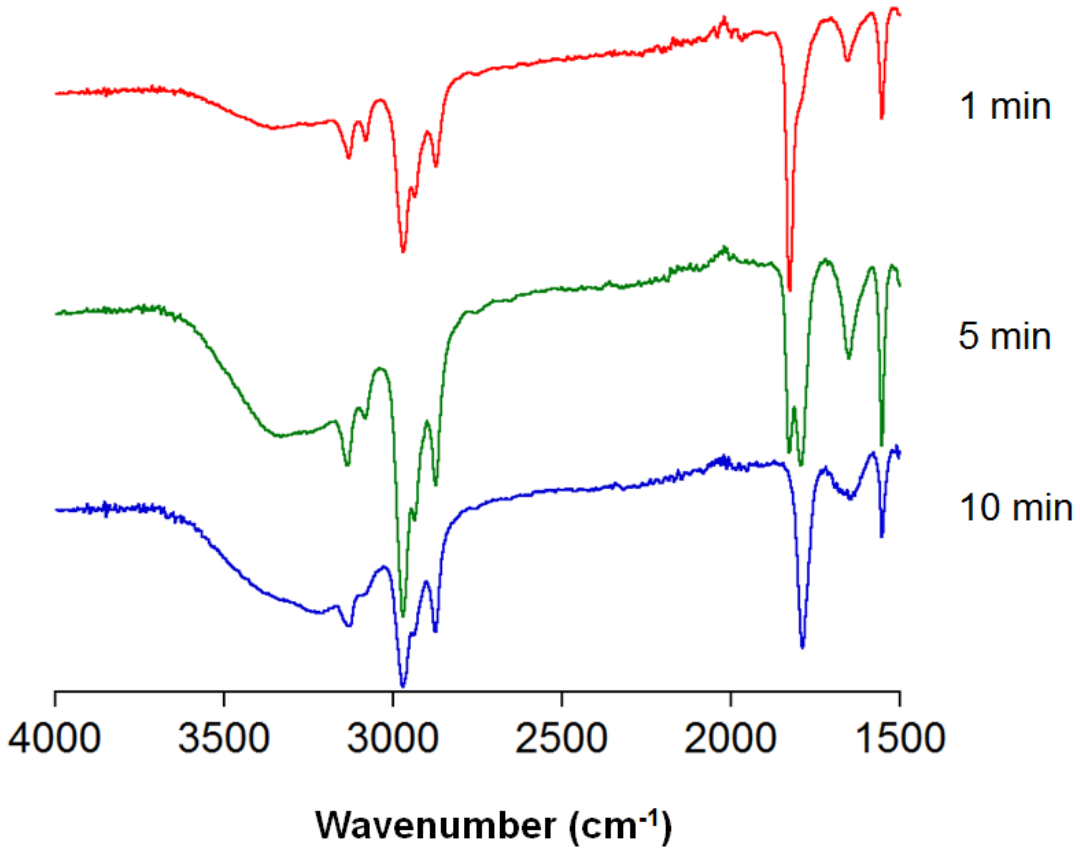

Figure S2. Changes in the ATR-IR spectrum for [Fe(T1Et4iPrIP)(NO)(THF)(OTf)](OTf) (**2**) during exposure to moist air (red, t = 1 min; green, t = 5 min; blue, t = 10 min).

Table S1. Crystallographic parameters for [Fe(T1Et4iPrIP)(H_2O)$_2$(NO)](OTf)$_2$·3THF (**1**·3THF).

	1·3THF
chemical formula	C_{38} H_{67} F_6 Fe N_7 O_{12} P S_2
fw / g mol^{-1}	1078.93
Temperature / K	100.0(5)
λ / Å	0.71073
cryst. system	Triclinic
space group	$P\bar{1}$
a / Å	9.5655(7)
b / Å	13.2592(10)
c / Å	22.3910(17)
α / °	102.546(2)
β / °	95.887(2)
γ / °	110.627(2)
Volume / Å^3	2544.0(3)
Z	2
μ / mm^{-1}	0.494
D_{calcd} / Mg m^{-3}	1.408
GOF on F^2	1.009
Final *R* indices[$I>2\sigma(I)$]	*R*1= 0.0503, *wR*2= 0.1051
R indices (all data)	*R*1= 0.0946, *wR*2= 0.1248

Table S2. Selected Angles (º) and bond distances (Å) For [Fe(T1Et4iPrIP)(H_2O)$_2$(NO)]-(OTf)$_2$·3THF (**1**·3THF). Calculated data shown in brackets.

Bond Lengths			
Fe(1)-N(1)	2.2432(2) [2.214]	Fe(1)-O(2)	2.079(2) [2.253]
Fe(1)-N(2)	2.165(2) [2.136]	Fe(1)-O(3)	2.095(2) [2.236]
Fe(1)-N(3)	2.158(2) [2.125]	N(7)-O(1)	1.127(5) [1.116]
Fe(1)-N(7)	1.789(4) [1.793]	N(7)′-O(1)′	1.114(16) [1.116]
Fe(1)-N(7)′	1.770(14) [1.793]		
Bond Angles			
N(1)-Fe(1)-N(2)	87.68(8) [90.552]	N(1)-Fe(1)-O(2)	82.06(9) [80.505]
N(1)-Fe(1)-N(3)	86.61(8) [90.264]	N(2)-Fe(1)-O(2)	88.78(8) [89.677]
N(2)-Fe(1)-N(3)	87.19(8) [89.367]	N(3)-Fe(1)-O(2)	168.12(9) [170.710]
N(1)-Fe(1)-N(7)	170.76(19) [161.780]	N(1)-Fe(1)-O(3)	84.31(9) [82.231]
N(1)-Fe(1)-N(7)′	177.3(12) [161.780]	N(2)-Fe(1)-O(3)	171.87(9) [172.619]
N(2)-Fe(1)-N(7)	98.2(3) [102.242]	N(3)-Fe(1)-O(3)	90.89(8) [89.120]
N(2)-Fe(1)-N(7)′	93.8(12) [102.242]	O(2)-Fe(1)-O(3)	91.53(9) [90.651]
N(3)-Fe(1)-N(7)	100.7(2) [102.652]	Fe(1)-N(7)-O(1)	164.5(5) [159.304]
N(3)-Fe(1)-N(7)′	91.2(9) [102.652]		

Crystallographic Information for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (1)

Data collection

A crystal (0.30 x 0.20 x 0.06 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD Platform diffractometer for a data collection at 100.0(5) K.[1] A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 60 seconds and a detector distance of 3.98 cm. A randomly oriented region of reciprocal space was surveyed: six major sections of frames were collected with 0.50º steps in ω at six different ϕ settings and a detector position of -38º in 2θ. The intensity data were corrected for absorption.[2] Final cell constants were calculated from the xyz centroids of 4008 strong reflections from the actual data collection after integration.[3] See Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97[4] and refined using SHELXL-97.[5] The space group *P*-1 was determined based on intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms on the aqua ligands were found from the difference Fourier map. Their positional and isotropic displacement parameters were refined independently from those of their bonded oxygen atoms. All other hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0503$ (F^2, $I > 2\sigma(I)$) and $wR2 = 0.1248$ (F^2, all data).

Structure description

The structure is the one suggested with all atoms in general positions. The nitrosyl ligand is modeled as disordered over two positions (77:23). The aqua ligands participate in hydrogen bonding (see diagram and Table 7).

Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B51 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.

[1] *APEX2*, version 2011.4-1; Bruker AXS: Madison, WI, 2011.

[2] Sheldrick, G. M. *SADABS*, version 2008/1; University of Göttingen: Göttingen, Germany, 2008.

[3] *SAINT*, version 7.68A; Bruker AXS: Madison, WI, 2009.

[4] Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *SIR97: A new program for solving and refining crystal structures*; Istituto di Cristallografia, CNR: Bari, Italy, 1999.

[5] Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112-122.

Some equations of interest:

$$R_{int} = \Sigma\, |F_o^2 - < F_o^2 >| \,/\, \Sigma |F_o^2|$$

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

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

where $w = 1 \,/\, [\sigma^2 (F_o^2) + (aP)^2 + bP]$ and

$$P = 1/3 \max (0, F_o^2) + 2/3\, F_c^2$$

$$\text{GOF} = S = [\Sigma [w(F_o^2 - F_c^2)^2] \,/\, (m-n)]^{1/2}$$

where m = number of reflections and n = number of parameters

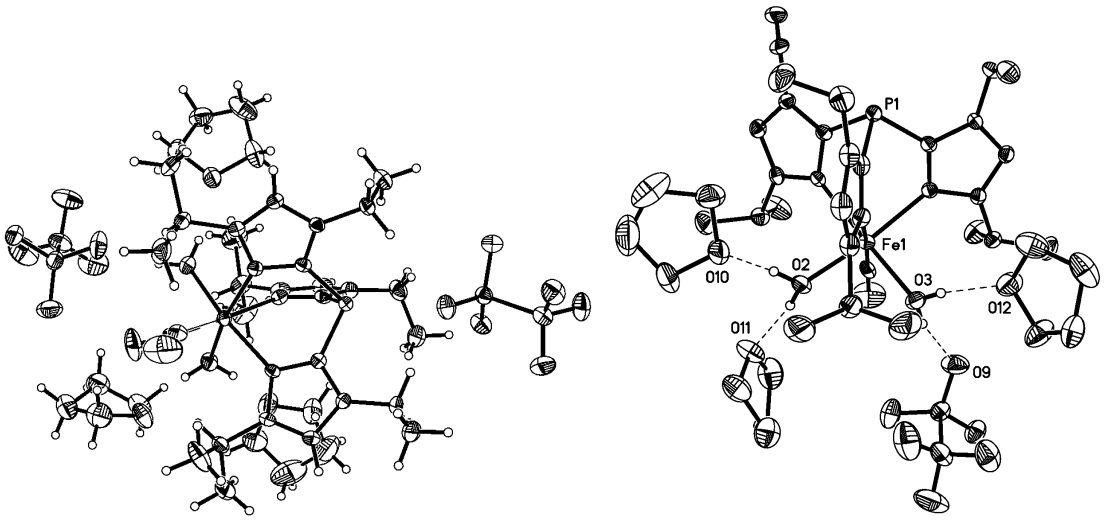

Figure S3. ORTEP plots for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**).

Table S3. Crystal data and structure refinement for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**).

Identification code	oakfc28	
Empirical formula	C38 H67 F6 Fe N7 O12 P S2	
Formula weight	1078.93	
Temperature	100.0(5) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 9.5655(7) Å	α = 102.546(2)°
	b = 13.2592(10) Å	β = 95.887(2)°
	c = 22.3910(17) Å	γ = 110.627(2)°
Volume	2544.0(3) Å^3	
Z	2	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	0.494 mm^{-1}	
F(000)	1134	
Crystal color, morphology	pale yellow-orange, needle	
Crystal size	0.30 x 0.20 x 0.06 mm^3	
Theta range for data collection	1.71 to 28.28°	
Index ranges	$-12 \le h \le 12$, $-17 \le k \le 17$, $-29 \le l \le 29$	
Reflections collected	54456	
Independent reflections	12611 [R(int) = 0.0835]	
Observed reflections	8111	
Completeness to theta = 28.28°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9710 and 0.8660	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12611 / 9 / 642	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0503, wR2 = 0.1051	
R indices (all data)	R1 = 0.0946, wR2 = 0.1248	
Largest diff. peak and hole	0.656 and -0.444 e.Å^{-3}	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Fe1	5081(1)	804(1)	2864(1)	19(1)
N7	4247(6)	359(8)	3489(3)	23(1)
O1	3982(5)	-3(3)	3895(2)	59(2)
N7'	3940(30)	330(30)	3400(12)	23(1)
O1'	3010(20)	319(13)	3663(9)	93(9)
P1	4138(1)	1930(1)	1657(1)	18(1)
O2	7164(2)	1754(2)	3467(1)	28(1)
O3	5655(2)	-602(2)	2660(1)	27(1)
N1	6456(2)	1326(2)	2151(1)	22(1)
N2	4621(2)	2312(2)	2962(1)	17(1)
N3	3133(2)	4(2)	2106(1)	18(1)
N4	7040(3)	2214(2)	1423(1)	26(1)
N5	4177(2)	3650(2)	2642(1)	20(1)
N6	1887(2)	-198(2)	1177(1)	19(1)
C1	5968(3)	1810(2)	1756(1)	21(1)
C2	4296(3)	2649(2)	2463(1)	18(1)
C3	2997(3)	512(2)	1660(1)	18(1)
C4	8822(3)	907(3)	2371(2)	33(1)
C5	10484(4)	1726(3)	2608(2)	60(1)
C6	8744(5)	-158(3)	1913(2)	56(1)
C7	7907(3)	1427(2)	2062(1)	26(1)
C8	8267(3)	1978(2)	1615(1)	30(1)
C9	6956(4)	2857(3)	974(1)	36(1)
C10	7507(5)	4093(3)	1285(2)	50(1)
C11	1760(3)	-1908(2)	2271(1)	24(1)
C12	1064(4)	-3100(2)	1854(2)	42(1)
C13	743(4)	-1721(3)	2731(2)	42(1)
C14	2046(3)	-1079(2)	1890(1)	19(1)
C15	1286(3)	-1198(2)	1314(1)	20(1)
C16	1452(3)	23(2)	584(1)	24(1)
C17	2484(4)	-125(3)	133(1)	36(1)

C18	4955(3)	3049(2)	4134(1)	25(1)
C19	6128(4)	4146(3)	4566(2)	45(1)
C20	3461(4)	2711(4)	4367(2)	50(1)
C21	4696(3)	3133(2)	3478(1)	20(1)
C22	4423(3)	3958(2)	3278(1)	22(1)
C23	3871(3)	4311(2)	2231(1)	26(1)
C24	2555(4)	4646(3)	2360(2)	34(1)
S1	1912(1)	3071(1)	462(1)	23(1)
O4	1685(2)	2234(2)	-109(1)	29(1)
O5	3451(2)	3857(2)	705(1)	31(1)
O6	1093(2)	2653(2)	921(1)	32(1)
C25	941(4)	3916(3)	220(1)	31(1)
F1	1044(2)	4760(2)	692(1)	48(1)
F2	-539(2)	3311(2)	-11(1)	39(1)
F3	1527(2)	4355(2)	-223(1)	46(1)
S2	5262(1)	-2442(1)	3795(1)	30(1)
O7	4387(3)	-3503(2)	3882(1)	37(1)
O8	5824(3)	-1514(2)	4342(1)	50(1)
O9	4643(3)	-2230(2)	3245(1)	45(1)
C26	6979(4)	-2593(3)	3609(2)	40(1)
F4	7962(2)	-1661(2)	3528(1)	66(1)
F5	6701(2)	-3399(2)	3084(1)	58(1)
F6	7678(3)	-2866(2)	4053(1)	72(1)
O10	9149(3)	3727(2)	3407(1)	56(1)
C27	8699(5)	4371(3)	3052(2)	51(1)
C28	9775(7)	5542(4)	3346(3)	88(2)
C29	10382(6)	5598(4)	3962(3)	90(2)
C30	10319(5)	4468(3)	3929(2)	60(1)
O11	8142(3)	2066(2)	4656(1)	43(1)
C31	9643(4)	2078(4)	4647(2)	51(1)
C32	9562(5)	1048(3)	4808(2)	54(1)
C33	8534(4)	941(4)	5282(2)	51(1)
C34	7355(5)	1361(3)	5010(2)	57(1)
O12	4856(3)	-2072(2)	1541(1)	44(1)
C35	5219(5)	-3028(3)	1571(2)	49(1)
C36	5732(4)	-3357(3)	976(2)	45(1)

C37	4783(4)	-3040(4)	527(2)	54(1)
C38	4719(5)	-1998(3)	909(2)	51(1)

Table S5. Bond lengths [Å] and angles [°] for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**).

Fe(1)-N(7')	1.770(14)	C(4)-H(4)	1.0000
Fe(1)-N(7)	1.789(4)	C(5)-H(5A)	0.9800
Fe(1)-O(2)	2.079(2)	C(5)-H(5B)	0.9800
Fe(1)-O(3)	2.095(2)	C(5)-H(5C)	0.9800
Fe(1)-N(3)	2.158(2)	C(6)-H(6A)	0.9800
Fe(1)-N(2)	2.165(2)	C(6)-H(6B)	0.9800
Fe(1)-N(1)	2.243(2)	C(6)-H(6C)	0.9800
N(7)-O(1)	1.127(5)	C(7)-C(8)	1.366(4)
N(7')-O(1')	1.114(16)	C(8)-H(8)	0.9500
P(1)-C(1)	1.808(3)	C(9)-C(10)	1.505(5)
P(1)-C(2)	1.812(3)	C(9)-H(9A)	0.9900
P(1)-C(3)	1.814(3)	C(9)-H(9B)	0.9900
O(2)-H(2A)	0.99(5)	C(10)-H(10A)	0.9800
O(2)-H(2B)	0.85(4)	C(10)-H(10B)	0.9800
O(3)-H(3A)	0.85(4)	C(10)-H(10C)	0.9800
O(3)-H(3B)	0.81(4)	C(11)-C(14)	1.502(4)
N(1)-C(1)	1.336(3)	C(11)-C(12)	1.518(4)
N(1)-C(7)	1.387(3)	C(11)-C(13)	1.526(4)
N(2)-C(2)	1.337(3)	C(11)-H(11)	1.0000
N(2)-C(21)	1.381(3)	C(12)-H(12A)	0.9800
N(3)-C(3)	1.338(3)	C(12)-H(12B)	0.9800
N(3)-C(14)	1.386(3)	C(12)-H(12C)	0.9800
N(4)-C(1)	1.356(3)	C(13)-H(13A)	0.9800
N(4)-C(8)	1.369(4)	C(13)-H(13B)	0.9800
N(4)-C(9)	1.466(4)	C(13)-H(13C)	0.9800
N(5)-C(2)	1.349(3)	C(14)-C(15)	1.363(4)
N(5)-C(22)	1.365(3)	C(15)-H(15)	0.9500
N(5)-C(23)	1.476(3)	C(16)-C(17)	1.512(4)
N(6)-C(3)	1.342(3)	C(16)-H(16A)	0.9900
N(6)-C(15)	1.363(3)	C(16)-H(16B)	0.9900
N(6)-C(16)	1.470(3)	C(17)-H(17A)	0.9800
C(4)-C(7)	1.492(4)	C(17)-H(17B)	0.9800
C(4)-C(6)	1.527(5)	C(17)-H(17C)	0.9800
C(4)-C(5)	1.533(4)	C(18)-C(21)	1.499(4)

C(18)-C(20)	1.522(4)	C(28)-C(29)	1.415(7)
C(18)-C(19)	1.526(4)	C(28)-H(28A)	0.9900
C(18)-H(18)	1.0000	C(28)-H(28B)	0.9900
C(19)-H(19A)	0.9800	C(29)-C(30)	1.464(6)
C(19)-H(19B)	0.9800	C(29)-H(29A)	0.9900
C(19)-H(19C)	0.9800	C(29)-H(29B)	0.9900
C(20)-H(20A)	0.9800	C(30)-H(30A)	0.9900
C(20)-H(20B)	0.9800	C(30)-H(30B)	0.9900
C(20)-H(20C)	0.9800	O(11)-C(34)	1.422(4)
C(21)-C(22)	1.363(4)	O(11)-C(31)	1.433(4)
C(22)-H(22)	0.9500	C(31)-C(32)	1.465(5)
C(23)-C(24)	1.510(4)	C(31)-H(31A)	0.9900
C(23)-H(23A)	0.9900	C(31)-H(31B)	0.9900
C(23)-H(23B)	0.9900	C(32)-C(33)	1.517(5)
C(24)-H(24A)	0.9800	C(32)-H(32A)	0.9900
C(24)-H(24B)	0.9800	C(32)-H(32B)	0.9900
C(24)-H(24C)	0.9800	C(33)-C(34)	1.550(5)
S(1)-O(5)	1.434(2)	C(33)-H(33A)	0.9900
S(1)-O(4)	1.440(2)	C(33)-H(33B)	0.9900
S(1)-O(6)	1.442(2)	C(34)-H(34A)	0.9900
S(1)-C(25)	1.818(3)	C(34)-H(34B)	0.9900
C(25)-F(1)	1.329(3)	O(12)-C(38)	1.436(4)
C(25)-F(3)	1.332(3)	O(12)-C(35)	1.439(4)
C(25)-F(2)	1.336(4)	C(35)-C(36)	1.496(5)
S(2)-O(7)	1.428(2)	C(35)-H(35A)	0.9900
S(2)-O(8)	1.432(2)	C(35)-H(35B)	0.9900
S(2)-O(9)	1.436(2)	C(36)-C(37)	1.510(5)
S(2)-C(26)	1.802(3)	C(36)-H(36A)	0.9900
C(26)-F(6)	1.325(4)	C(36)-H(36B)	0.9900
C(26)-F(4)	1.326(4)	C(37)-C(38)	1.484(5)
C(26)-F(5)	1.336(4)	C(37)-H(37A)	0.9900
O(10)-C(27)	1.425(4)	C(37)-H(37B)	0.9900
O(10)-C(30)	1.429(4)	C(38)-H(38A)	0.9900
C(27)-C(28)	1.482(6)	C(38)-H(38B)	0.9900
C(27)-H(27A)	0.9900	N(7')-Fe(1)-O(2)	100.2(10)
C(27)-H(27B)	0.9900	N(7)-Fe(1)-O(2)	90.9(2)

N(7')-Fe(1)-O(3)	94.1(12)	C(3)-N(3)-Fe(1)	119.49(17)
N(7)-Fe(1)-O(3)	89.9(3)	C(14)-N(3)-Fe(1)	132.88(17)
O(2)-Fe(1)-O(3)	91.53(9)	C(1)-N(4)-C(8)	107.2(2)
N(7')-Fe(1)-N(3)	91.2(9)	C(1)-N(4)-C(9)	126.7(2)
N(7)-Fe(1)-N(3)	100.7(2)	C(8)-N(4)-C(9)	126.0(2)
O(2)-Fe(1)-N(3)	168.12(9)	C(2)-N(5)-C(22)	107.5(2)
O(3)-Fe(1)-N(3)	90.89(8)	C(2)-N(5)-C(23)	126.7(2)
N(7')-Fe(1)-N(2)	93.8(12)	C(22)-N(5)-C(23)	125.8(2)
N(7)-Fe(1)-N(2)	98.2(3)	C(3)-N(6)-C(15)	107.8(2)
O(2)-Fe(1)-N(2)	88.78(8)	C(3)-N(6)-C(16)	126.8(2)
O(3)-Fe(1)-N(2)	171.87(9)	C(15)-N(6)-C(16)	125.3(2)
N(3)-Fe(1)-N(2)	87.19(8)	N(1)-C(1)-N(4)	110.9(2)
N(7')-Fe(1)-N(1)	177.3(12)	N(1)-C(1)-P(1)	126.26(19)
N(7)-Fe(1)-N(1)	170.76(19)	N(4)-C(1)-P(1)	122.9(2)
O(2)-Fe(1)-N(1)	82.06(9)	N(2)-C(2)-N(5)	110.3(2)
O(3)-Fe(1)-N(1)	84.31(9)	N(2)-C(2)-P(1)	126.03(19)
N(3)-Fe(1)-N(1)	86.61(8)	N(5)-C(2)-P(1)	123.60(19)
N(2)-Fe(1)-N(1)	87.68(8)	N(3)-C(3)-N(6)	110.4(2)
O(1)-N(7)-Fe(1)	164.5(5)	N(3)-C(3)-P(1)	127.5(2)
O(1')-N(7')-Fe(1)	152(3)	N(6)-C(3)-P(1)	122.09(19)
C(1)-P(1)-C(2)	96.63(12)	C(7)-C(4)-C(6)	109.8(3)
C(1)-P(1)-C(3)	96.98(12)	C(7)-C(4)-C(5)	110.9(3)
C(2)-P(1)-C(3)	99.47(12)	C(6)-C(4)-C(5)	110.0(3)
Fe(1)-O(2)-H(2A)	122(3)	C(7)-C(4)-H(4)	108.7
Fe(1)-O(2)-H(2B)	120(3)	C(6)-C(4)-H(4)	108.7
H(2A)-O(2)-H(2B)	112(4)	C(5)-C(4)-H(4)	108.7
Fe(1)-O(3)-H(3A)	117(3)	C(4)-C(5)-H(5A)	109.5
Fe(1)-O(3)-H(3B)	119(3)	C(4)-C(5)-H(5B)	109.5
H(3A)-O(3)-H(3B)	112(4)	H(5A)-C(5)-H(5B)	109.5
C(1)-N(1)-C(7)	105.9(2)	C(4)-C(5)-H(5C)	109.5
C(1)-N(1)-Fe(1)	119.11(17)	H(5A)-C(5)-H(5C)	109.5
C(7)-N(1)-Fe(1)	134.17(19)	H(5B)-C(5)-H(5C)	109.5
C(2)-N(2)-C(21)	106.5(2)	C(4)-C(6)-H(6A)	109.5
C(2)-N(2)-Fe(1)	121.07(16)	C(4)-C(6)-H(6B)	109.5
C(21)-N(2)-Fe(1)	132.24(17)	H(6A)-C(6)-H(6B)	109.5
C(3)-N(3)-C(14)	106.4(2)	C(4)-C(6)-H(6C)	109.5

H(6A)-C(6)-H(6C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(6B)-C(6)-H(6C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(8)-C(7)-N(1)	108.8(3)	C(15)-C(14)-N(3)	108.1(2)
C(8)-C(7)-C(4)	127.2(3)	C(15)-C(14)-C(11)	128.6(2)
N(1)-C(7)-C(4)	123.7(3)	N(3)-C(14)-C(11)	123.2(2)
C(7)-C(8)-N(4)	107.1(2)	N(6)-C(15)-C(14)	107.4(2)
C(7)-C(8)-H(8)	126.4	N(6)-C(15)-H(15)	126.3
N(4)-C(8)-H(8)	126.4	C(14)-C(15)-H(15)	126.3
N(4)-C(9)-C(10)	112.1(3)	N(6)-C(16)-C(17)	112.2(2)
N(4)-C(9)-H(9A)	109.2	N(6)-C(16)-H(16A)	109.2
C(10)-C(9)-H(9A)	109.2	C(17)-C(16)-H(16A)	109.2
N(4)-C(9)-H(9B)	109.2	N(6)-C(16)-H(16B)	109.2
C(10)-C(9)-H(9B)	109.2	C(17)-C(16)-H(16B)	109.2
H(9A)-C(9)-H(9B)	107.9	H(16A)-C(16)-H(16B)	107.9
C(9)-C(10)-H(10A)	109.5	C(16)-C(17)-H(17A)	109.5
C(9)-C(10)-H(10B)	109.5	C(16)-C(17)-H(17B)	109.5
H(10A)-C(10)-H(10B)	109.5	H(17A)-C(17)-H(17B)	109.5
C(9)-C(10)-H(10C)	109.5	C(16)-C(17)-H(17C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(17A)-C(17)-H(17C)	109.5
H(10B)-C(10)-H(10C)	109.5	H(17B)-C(17)-H(17C)	109.5
C(14)-C(11)-C(12)	110.9(2)	C(21)-C(18)-C(20)	110.6(2)
C(14)-C(11)-C(13)	111.3(2)	C(21)-C(18)-C(19)	111.0(2)
C(12)-C(11)-C(13)	110.4(3)	C(20)-C(18)-C(19)	110.9(3)
C(14)-C(11)-H(11)	108.0	C(21)-C(18)-H(18)	108.0
C(12)-C(11)-H(11)	108.0	C(20)-C(18)-H(18)	108.0
C(13)-C(11)-H(11)	108.0	C(19)-C(18)-H(18)	108.0
C(11)-C(12)-H(12A)	109.5	C(18)-C(19)-H(19A)	109.5
C(11)-C(12)-H(12B)	109.5	C(18)-C(19)-H(19B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(11)-C(12)-H(12C)	109.5	C(18)-C(19)-H(19C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(11)-C(13)-H(13A)	109.5	C(18)-C(20)-H(20A)	109.5
C(11)-C(13)-H(13B)	109.5	C(18)-C(20)-H(20B)	109.5
H(13A)-C(13)-H(13B)	109.5	H(20A)-C(20)-H(20B)	109.5
C(11)-C(13)-H(13C)	109.5	C(18)-C(20)-H(20C)	109.5

H(20A)-C(20)-H(20C)	109.5	O(8)-S(2)-C(26)	102.67(15)
H(20B)-C(20)-H(20C)	109.5	O(9)-S(2)-C(26)	102.65(15)
C(22)-C(21)-N(2)	108.3(2)	F(6)-C(26)-F(4)	107.7(3)
C(22)-C(21)-C(18)	128.0(2)	F(6)-C(26)-F(5)	106.3(3)
N(2)-C(21)-C(18)	123.6(2)	F(4)-C(26)-F(5)	106.6(3)
C(21)-C(22)-N(5)	107.4(2)	F(6)-C(26)-S(2)	111.7(2)
C(21)-C(22)-H(22)	126.3	F(4)-C(26)-S(2)	112.1(2)
N(5)-C(22)-H(22)	126.3	F(5)-C(26)-S(2)	112.1(2)
N(5)-C(23)-C(24)	112.4(2)	C(27)-O(10)-C(30)	109.1(3)
N(5)-C(23)-H(23A)	109.1	O(10)-C(27)-C(28)	104.9(3)
C(24)-C(23)-H(23A)	109.1	O(10)-C(27)-H(27A)	110.8
N(5)-C(23)-H(23B)	109.1	C(28)-C(27)-H(27A)	110.8
C(24)-C(23)-H(23B)	109.1	O(10)-C(27)-H(27B)	110.8
H(23A)-C(23)-H(23B)	107.9	C(28)-C(27)-H(27B)	110.8
C(23)-C(24)-H(24A)	109.5	H(27A)-C(27)-H(27B)	108.8
C(23)-C(24)-H(24B)	109.5	C(29)-C(28)-C(27)	107.1(4)
H(24A)-C(24)-H(24B)	109.5	C(29)-C(28)-H(28A)	110.3
C(23)-C(24)-H(24C)	109.5	C(27)-C(28)-H(28A)	110.3
H(24A)-C(24)-H(24C)	109.5	C(29)-C(28)-H(28B)	110.3
H(24B)-C(24)-H(24C)	109.5	C(27)-C(28)-H(28B)	110.3
O(5)-S(1)-O(4)	115.54(12)	H(28A)-C(28)-H(28B)	108.6
O(5)-S(1)-O(6)	115.11(13)	C(28)-C(29)-C(30)	104.7(4)
O(4)-S(1)-O(6)	114.58(13)	C(28)-C(29)-H(29A)	110.8
O(5)-S(1)-C(25)	103.49(14)	C(30)-C(29)-H(29A)	110.8
O(4)-S(1)-C(25)	102.75(13)	C(28)-C(29)-H(29B)	110.8
O(6)-S(1)-C(25)	102.82(13)	C(30)-C(29)-H(29B)	110.8
F(1)-C(25)-F(3)	107.3(2)	H(29A)-C(29)-H(29B)	108.9
F(1)-C(25)-F(2)	107.3(2)	O(10)-C(30)-C(29)	106.7(4)
F(3)-C(25)-F(2)	107.0(2)	O(10)-C(30)-H(30A)	110.4
F(1)-C(25)-S(1)	111.8(2)	C(29)-C(30)-H(30A)	110.4
F(3)-C(25)-S(1)	111.5(2)	O(10)-C(30)-H(30B)	110.4
F(2)-C(25)-S(1)	111.7(2)	C(29)-C(30)-H(30B)	110.4
O(7)-S(2)-O(8)	115.94(14)	H(30A)-C(30)-H(30B)	108.6
O(7)-S(2)-O(9)	113.95(14)	C(34)-O(11)-C(31)	111.9(3)
O(8)-S(2)-O(9)	115.41(16)	O(11)-C(31)-C(32)	103.6(3)
O(7)-S(2)-C(26)	103.64(15)	O(11)-C(31)-H(31A)	111.0

C(32)-C(31)-H(31A)	111.0	C(38)-C(37)-H(37A)	111.0
O(11)-C(31)-H(31B)	111.0	C(36)-C(37)-H(37A)	111.0
C(32)-C(31)-H(31B)	111.0	C(38)-C(37)-H(37B)	111.0
H(31A)-C(31)-H(31B)	109.0	C(36)-C(37)-H(37B)	111.0
C(31)-C(32)-C(33)	104.2(3)	H(37A)-C(37)-H(37B)	109.0
C(31)-C(32)-H(32A)	110.9	O(12)-C(38)-C(37)	106.1(3)
C(33)-C(32)-H(32A)	110.9	O(12)-C(38)-H(38A)	110.5
C(31)-C(32)-H(32B)	110.9	C(37)-C(38)-H(38A)	110.5
C(33)-C(32)-H(32B)	110.9	O(12)-C(38)-H(38B)	110.5
H(32A)-C(32)-H(32B)	108.9	C(37)-C(38)-H(38B)	110.5
C(32)-C(33)-C(34)	100.6(3)	H(38A)-C(38)-H(38B)	108.7
C(32)-C(33)-H(33A)	111.6		
C(34)-C(33)-H(33A)	111.6		
C(32)-C(33)-H(33B)	111.6		
C(34)-C(33)-H(33B)	111.6		
H(33A)-C(33)-H(33B)	109.4		
O(11)-C(34)-C(33)	104.6(3)		
O(11)-C(34)-H(34A)	110.8		
C(33)-C(34)-H(34A)	110.8		
O(11)-C(34)-H(34B)	110.8		
C(33)-C(34)-H(34B)	110.8		
H(34A)-C(34)-H(34B)	108.9		
C(38)-O(12)-C(35)	109.1(3)		
O(12)-C(35)-C(36)	106.0(3)		
O(12)-C(35)-H(35A)	110.5		
C(36)-C(35)-H(35A)	110.5		
O(12)-C(35)-H(35B)	110.5		
C(36)-C(35)-H(35B)	110.5		
H(35A)-C(35)-H(35B)	108.7		
C(35)-C(36)-C(37)	101.5(3)		
C(35)-C(36)-H(36A)	111.5		
C(37)-C(36)-H(36A)	111.5		
C(35)-C(36)-H(36B)	111.5		
C(37)-C(36)-H(36B)	111.5		
H(36A)-C(36)-H(36B)	109.3		
C(38)-C(37)-C(36)	103.6(3)		

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**). 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}
Fe1	18(1)	20(1)	19(1)	6(1)	3(1)	8(1)
N7	16(3)	25(1)	23(2)	3(2)	-2(2)	4(3)
O1	70(3)	79(3)	49(2)	47(2)	33(2)	31(2)
N7'	16(3)	25(1)	23(2)	3(2)	-2(2)	4(3)
O1'	93(14)	67(10)	92(13)	4(8)	70(11)	-5(9)
P1	21(1)	18(1)	16(1)	5(1)	3(1)	7(1)
O2	24(1)	30(1)	27(1)	8(1)	-2(1)	9(1)
O3	29(1)	24(1)	30(1)	10(1)	6(1)	13(1)
N1	19(1)	20(1)	26(1)	5(1)	6(1)	7(1)
N2	16(1)	20(1)	14(1)	2(1)	2(1)	7(1)
N3	17(1)	19(1)	19(1)	4(1)	3(1)	8(1)
N4	25(1)	26(1)	24(1)	7(1)	11(1)	6(1)
N5	20(1)	19(1)	21(1)	6(1)	4(1)	9(1)
N6	18(1)	19(1)	17(1)	2(1)	0(1)	7(1)
C1	21(1)	21(1)	18(1)	2(1)	8(1)	7(1)
C2	14(1)	20(1)	20(1)	5(1)	3(1)	7(1)
C3	17(1)	21(1)	17(1)	2(1)	2(1)	10(1)
C4	20(2)	30(2)	50(2)	9(1)	8(1)	11(1)
C5	22(2)	55(2)	99(3)	27(2)	-1(2)	12(2)
C6	54(2)	56(2)	71(3)	13(2)	19(2)	38(2)
C7	16(1)	26(2)	32(2)	3(1)	7(1)	8(1)
C8	22(2)	31(2)	34(2)	4(1)	13(1)	5(1)
C9	39(2)	40(2)	27(2)	15(1)	10(1)	7(2)
C10	71(3)	33(2)	42(2)	19(2)	12(2)	11(2)
C11	23(1)	19(1)	28(2)	8(1)	3(1)	7(1)
C12	61(2)	17(2)	40(2)	10(1)	3(2)	6(2)
C13	51(2)	39(2)	45(2)	23(2)	24(2)	18(2)
C14	16(1)	18(1)	22(1)	4(1)	4(1)	7(1)
C15	20(1)	17(1)	23(1)	4(1)	3(1)	6(1)
C16	26(2)	25(1)	19(1)	6(1)	-4(1)	8(1)
C17	49(2)	41(2)	21(2)	9(1)	6(1)	19(2)

C18	30(2)	29(2)	18(1)	6(1)	6(1)	14(1)
C19	60(2)	38(2)	24(2)	3(1)	-7(2)	10(2)
C20	40(2)	86(3)	29(2)	26(2)	15(2)	23(2)
C21	21(1)	21(1)	15(1)	1(1)	3(1)	7(1)
C22	25(1)	22(1)	20(1)	2(1)	5(1)	10(1)
C23	36(2)	21(1)	24(2)	10(1)	2(1)	13(1)
C24	41(2)	35(2)	34(2)	9(1)	-1(1)	24(2)
S1	24(1)	24(1)	22(1)	8(1)	7(1)	7(1)
O4	28(1)	27(1)	29(1)	2(1)	5(1)	9(1)
O5	23(1)	35(1)	27(1)	7(1)	3(1)	2(1)
O6	32(1)	39(1)	32(1)	19(1)	13(1)	12(1)
C25	37(2)	32(2)	23(2)	6(1)	5(1)	14(1)
F1	66(1)	38(1)	40(1)	-2(1)	5(1)	31(1)
F2	31(1)	50(1)	40(1)	12(1)	4(1)	20(1)
F3	56(1)	50(1)	43(1)	31(1)	16(1)	22(1)
S2	33(1)	26(1)	32(1)	11(1)	8(1)	12(1)
O7	48(1)	28(1)	37(1)	14(1)	14(1)	13(1)
O8	60(2)	35(1)	47(2)	-3(1)	16(1)	16(1)
O9	39(1)	48(1)	55(2)	33(1)	4(1)	14(1)
C26	31(2)	48(2)	32(2)	2(2)	-2(2)	13(2)
F4	38(1)	68(2)	69(2)	4(1)	19(1)	-2(1)
F5	48(1)	70(2)	43(1)	-11(1)	9(1)	26(1)
F6	60(2)	111(2)	55(2)	16(1)	-5(1)	54(2)
O10	56(2)	32(1)	58(2)	16(1)	-19(1)	-2(1)
C27	53(2)	52(2)	54(2)	27(2)	7(2)	20(2)
C28	122(5)	57(3)	110(5)	41(3)	44(4)	48(3)
C29	62(3)	49(3)	122(5)	-9(3)	-7(3)	4(2)
C30	52(2)	50(2)	53(3)	4(2)	-17(2)	2(2)
O11	31(1)	69(2)	31(1)	19(1)	4(1)	20(1)
C31	43(2)	70(3)	38(2)	15(2)	8(2)	21(2)
C32	60(3)	50(2)	49(2)	11(2)	15(2)	17(2)
C33	48(2)	60(2)	43(2)	19(2)	6(2)	16(2)
C34	48(2)	55(2)	58(3)	14(2)	19(2)	6(2)
O12	72(2)	43(1)	30(1)	13(1)	14(1)	32(1)
C35	78(3)	41(2)	46(2)	22(2)	29(2)	33(2)
C36	50(2)	33(2)	47(2)	4(2)	20(2)	11(2)

C37	33(2)	82(3)	32(2)	3(2)	8(2)	14(2)
C38	54(2)	71(3)	36(2)	29(2)	13(2)	25(2)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**).

	x	y	z	U(eq)
H2A	7880(50)	2450(40)	3410(20)	80(14)
H2B	7270(50)	1750(30)	3850(20)	62(13)
H3A	5480(40)	-1020(30)	2902(19)	60(13)
H3B	5480(40)	-960(30)	2300(19)	50(12)
H4	8379	703	2734	40
H5A	10524	2406	2902	89
H5B	10937	1921	2255	89
H5C	11055	1375	2820	89
H6A	7680	-683	1770	84
H6B	9328	-505	2120	84
H6C	9174	31	1554	84
H8	9195	2163	1466	37
H9A	5889	2584	750	43
H9B	7582	2732	662	43
H10A	7458	4492	968	74
H10B	8561	4365	1509	74
H10C	6859	4224	1580	74
H11	2762	-1796	2517	28
H12A	1746	-3215	1572	64
H12B	77	-3231	1609	64
H12C	921	-3625	2112	64
H13A	1110	-922	2947	63
H13B	771	-2145	3037	63
H13C	-306	-1977	2504	63
H15	485	-1856	1055	25
H16A	1493	799	668	29
H16B	390	-493	390	29
H17A	2159	34	-253	55
H17B	2426	-898	40	55
H17C	3535	391	322	55

H18	5364	2451	4135	30
H19A	7113	4300	4437	68
H19B	6231	4086	4996	68
H19C	5793	4758	4544	68
H20A	2716	2019	4075	75
H20B	3072	3308	4396	75
H20C	3634	2588	4779	75
H22	4406	4625	3534	27
H23A	3642	3865	1791	31
H23B	4796	4994	2289	31
H24A	2373	5061	2068	52
H24B	2798	5122	2789	52
H24C	1639	3974	2308	52
H27A	7637	4293	3069	61
H27B	8777	4129	2610	61
H28A	10601	5756	3110	105
H28B	9237	6059	3354	105
H29A	9764	5806	4257	108
H29B	11444	6153	4097	108
H30A	11310	4423	3872	72
H30B	10079	4267	4318	72
H31A	10416	2746	4957	61
H31B	9894	2070	4228	61
H32A	10586	1108	4990	65
H32B	9123	395	4435	65
H33A	9094	1421	5705	61
H33B	8047	156	5298	61
H34A	6450	726	4742	68
H34B	7023	1785	5349	68
H35A	4311	-3649	1607	59
H35B	6039	-2830	1935	59
H36A	5509	-4170	850	54
H36B	6835	-2935	1012	54
H37A	5272	-2903	167	64
H37B	3750	-3634	371	64
H38A	5563	-1332	872	61

H38B	3741	-1939	769	61

Table S8. Torsion angles [°] for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**).

O2-Fe1-N7-O1	-57(3)
O3-Fe1-N7-O1	35(3)
N3-Fe1-N7-O1	126(3)
N2-Fe1-N7-O1	-146(3)
N1-Fe1-N7-O1	-16(5)
O2-Fe1-N7'-O1'	111(6)
O3-Fe1-N7'-O1'	-157(6)
N3-Fe1-N7'-O1'	-66(6)
N2-Fe1-N7'-O1'	22(6)
N1-Fe1-N7'-O1'	-101(22)
N7'-Fe1-N1-C1	85(20)
N7-Fe1-N1-C1	-168(2)
O2-Fe1-N1-C1	-127.1(2)
O3-Fe1-N1-C1	140.6(2)
N3-Fe1-N1-C1	49.3(2)
N2-Fe1-N1-C1	-38.0(2)
N7'-Fe1-N1-C7	-107(20)
N7-Fe1-N1-C7	0(2)
O2-Fe1-N1-C7	41.1(2)
O3-Fe1-N1-C7	-51.2(2)
N3-Fe1-N1-C7	-142.5(2)
N2-Fe1-N1-C7	130.2(2)
N7'-Fe1-N2-C2	-136.0(10)
N7-Fe1-N2-C2	-145.4(3)
O2-Fe1-N2-C2	123.9(2)
O3-Fe1-N2-C2	31.6(7)
N3-Fe1-N2-C2	-44.96(19)
N1-Fe1-N2-C2	41.76(19)
N7'-Fe1-N2-C21	49.8(10)
N7-Fe1-N2-C21	40.4(3)
O2-Fe1-N2-C21	-50.4(2)
O3-Fe1-N2-C21	-142.6(6)
N3-Fe1-N2-C21	140.8(2)
N1-Fe1-N2-C21	-132.5(2)

N7'-Fe1-N3-C3	142.2(12)
N7-Fe1-N3-C3	146.3(4)
O2-Fe1-N3-C3	-21.8(5)
O3-Fe1-N3-C3	-123.63(19)
N2-Fe1-N3-C3	48.47(18)
N1-Fe1-N3-C3	-39.38(18)
N7'-Fe1-N3-C14	-52.7(12)
N7-Fe1-N3-C14	-48.6(4)
O2-Fe1-N3-C14	143.3(4)
O3-Fe1-N3-C14	41.5(2)
N2-Fe1-N3-C14	-146.4(2)
N1-Fe1-N3-C14	125.7(2)
C7-N1-C1-N4	-0.2(3)
Fe1-N1-C1-N4	171.05(17)
C7-N1-C1-P1	179.7(2)
Fe1-N1-C1-P1	-9.1(3)
C8-N4-C1-N1	-0.1(3)
C9-N4-C1-N1	-175.9(3)
C8-N4-C1-P1	-179.9(2)
C9-N4-C1-P1	4.3(4)
C2-P1-C1-N1	56.7(3)
C3-P1-C1-N1	-43.8(3)
C2-P1-C1-N4	-123.5(2)
C3-P1-C1-N4	136.0(2)
C21-N2-C2-N5	0.6(3)
Fe1-N2-C2-N5	-174.98(16)
C21-N2-C2-P1	177.24(19)
Fe1-N2-C2-P1	1.7(3)
C22-N5-C2-N2	-0.5(3)
C23-N5-C2-N2	178.3(2)
C22-N5-C2-P1	-177.28(19)
C23-N5-C2-P1	1.5(4)
C1-P1-C2-N2	-52.9(2)
C3-P1-C2-N2	45.3(2)
C1-P1-C2-N5	123.3(2)
C3-P1-C2-N5	-138.4(2)

C14-N3-C3-N6	-0.3(3)
Fe1-N3-C3-N6	168.44(15)
C14-N3-C3-P1	-178.13(19)
Fe1-N3-C3-P1	-9.4(3)
C15-N6-C3-N3	-0.1(3)
C16-N6-C3-N3	-176.1(2)
C15-N6-C3-P1	177.94(18)
C16-N6-C3-P1	1.9(4)
C1-P1-C3-N3	56.8(2)
C2-P1-C3-N3	-41.1(2)
C1-P1-C3-N6	-120.8(2)
C2-P1-C3-N6	141.2(2)
C1-N1-C7-C8	0.4(3)
Fe1-N1-C7-C8	-168.9(2)
C1-N1-C7-C4	-174.3(3)
Fe1-N1-C7-C4	16.4(4)
C6-C4-C7-C8	-72.5(4)
C5-C4-C7-C8	49.3(4)
C6-C4-C7-N1	101.2(3)
C5-C4-C7-N1	-137.0(3)
N1-C7-C8-N4	-0.4(3)
C4-C7-C8-N4	174.0(3)
C1-N4-C8-C7	0.3(3)
C9-N4-C8-C7	176.2(3)
C1-N4-C9-C10	86.2(4)
C8-N4-C9-C10	-88.9(4)
C3-N3-C14-C15	0.5(3)
Fe1-N3-C14-C15	-166.05(18)
C3-N3-C14-C11	-176.1(2)
Fe1-N3-C14-C11	17.3(4)
C12-C11-C14-C15	28.6(4)
C13-C11-C14-C15	-94.8(3)
C12-C11-C14-N3	-155.5(3)
C13-C11-C14-N3	81.1(3)
C3-N6-C15-C14	0.4(3)
C16-N6-C15-C14	176.5(2)

N3-C14-C15-N6	-0.5(3)
C11-C14-C15-N6	175.9(2)
C3-N6-C16-C17	81.2(3)
C15-N6-C16-C17	-94.1(3)
C2-N2-C21-C22	-0.4(3)
Fe1-N2-C21-C22	174.43(18)
C2-N2-C21-C18	176.6(2)
Fe1-N2-C21-C18	-8.6(4)
C20-C18-C21-C22	75.2(4)
C19-C18-C21-C22	-48.4(4)
C20-C18-C21-N2	-101.2(3)
C19-C18-C21-N2	135.2(3)
N2-C21-C22-N5	0.1(3)
C18-C21-C22-N5	-176.7(3)
C2-N5-C22-C21	0.2(3)
C23-N5-C22-C21	-178.6(2)
C2-N5-C23-C24	127.8(3)
C22-N5-C23-C24	-53.6(4)
O5-S1-C25-F1	-58.6(2)
O4-S1-C25-F1	-179.2(2)
O6-S1-C25-F1	61.6(2)
O5-S1-C25-F3	61.5(2)
O4-S1-C25-F3	-59.1(2)
O6-S1-C25-F3	-178.3(2)
O5-S1-C25-F2	-178.82(19)
O4-S1-C25-F2	60.6(2)
O6-S1-C25-F2	-58.7(2)
O7-S2-C26-F6	-57.2(3)
O8-S2-C26-F6	63.8(3)
O9-S2-C26-F6	-176.1(2)
O7-S2-C26-F4	-178.2(2)
O8-S2-C26-F4	-57.2(3)
O9-S2-C26-F4	62.9(3)
O7-S2-C26-F5	62.0(3)
O8-S2-C26-F5	-177.0(3)
O9-S2-C26-F5	-56.9(3)

C30-O10-C27-C28	5.9(5)
O10-C27-C28-C29	-21.4(6)
C27-C28-C29-C30	28.0(6)
C27-O10-C30-C29	11.0(5)
C28-C29-C30-O10	-24.2(6)
C34-O11-C31-C32	20.6(4)
O11-C31-C32-C33	-36.4(4)
C31-C32-C33-C34	37.7(4)
C31-O11-C34-C33	3.5(4)
C32-C33-C34-O11	-25.0(4)
C38-O12-C35-C36	15.6(4)
O12-C35-C36-C37	-32.2(4)
C35-C36-C37-C38	36.7(4)
C35-O12-C38-C37	8.2(4)
C36-C37-C38-O12	-28.3(4)

Table S9. Hydrogen bonds and close contacts for [Fe(T1Et4iPrIP)(NO)(H_2O)$_2$](OTf) (**1**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O2-H2A...O10	0.99(5)	1.70(5)	2.678(3)	172(4)
O2-H2B...O11	0.85(4)	1.81(4)	2.620(3)	160(4)
O3-H3A...O9	0.85(4)	1.88(4)	2.707(3)	164(4)
O3-H3B...O12	0.81(4)	1.87(4)	2.664(3)	167(4)

Symmetry transformations used to generate equivalent atoms: