

SUPPORTING INFORMATION

Title: Thermally Induced Oxidation of $[\text{Fe}^{\text{II}}(\text{tacn})_2](\text{OTf})_2$ ($\text{tacn} = 1,4,7\text{-triazacyclononane}$)

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Crystallographic Data for [Fe(tacn)₂](OTf)₃ (3)

A orange-red plate crystal with dimensions 0.53 x 0.35 x 0.15 mm was mounted on a Nylon loop using very small amount of paratone oil. Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 0.5° per frame for 30 s. The total number of images was based on results from the program COSMO¹ where redundancy was expected to be 4.0 and completeness to 0.83 Å to 100%. Cell parameters were retrieved using APEX II software² and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software³ which corrects for Lp. Scaling and absorption corrections were applied using SADABS⁴ multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F², SHELXL-97⁵, which are incorporated in OLEX2.⁶

The structure was solved in the space group P2₁/n (# 14). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. Although there is disorder in one of the anions, (SO₃CF₃)⁻, modeling of this disordered failed to yield chemical and crystallographic correct models and therefore no disorder model is provided here, although there is a large electron density peak within the anion. All drawings are done at 50% ellipsoids.

Acknowledgement. The CCD based x-ray diffractometer at Michigan State University were upgraded and/or replaced by departmental funds.

References

1. COSMO V1.61, *Software for the CCD Detector Systems for Determining Data Collection Parameters*. Bruker Analytical X-ray Systems, Madison, WI (2009).
2. APEX2 V2010.11-3. *Software for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2010).
3. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).
4. SADABS V2008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. *Acta Cryst.* A51, 1995, 33-38.
5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst.* A64, 2008, 112-122.
6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* (2009). 42, 339-341.

^a Obtained with graphite monochromated Cu K α ($\lambda = 0.71073$) radiation.

^b $R_1 = \sum |F_o| - |F_c| / |F_o|$ ^c $wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum w(F_o^2)^2 \}^{1/2}$.

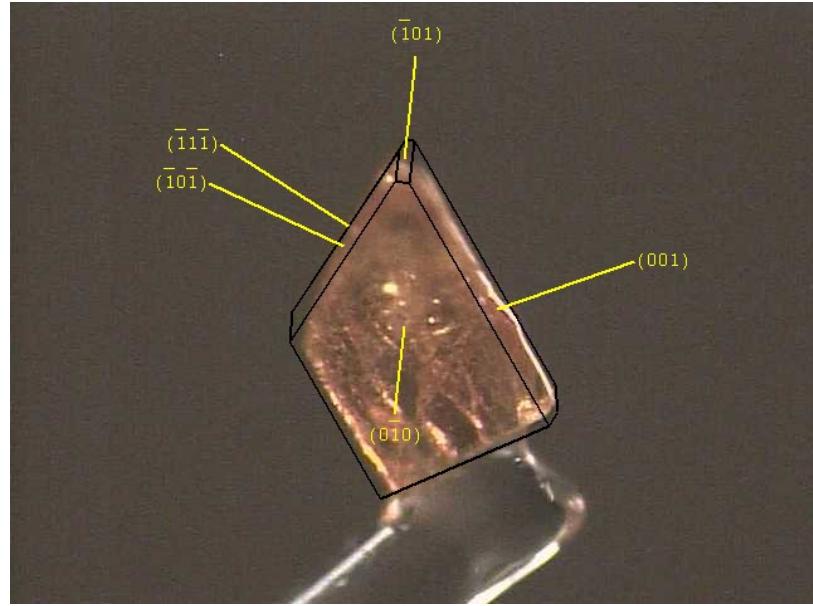


Figure S1. Image of $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**) mounted crystal.

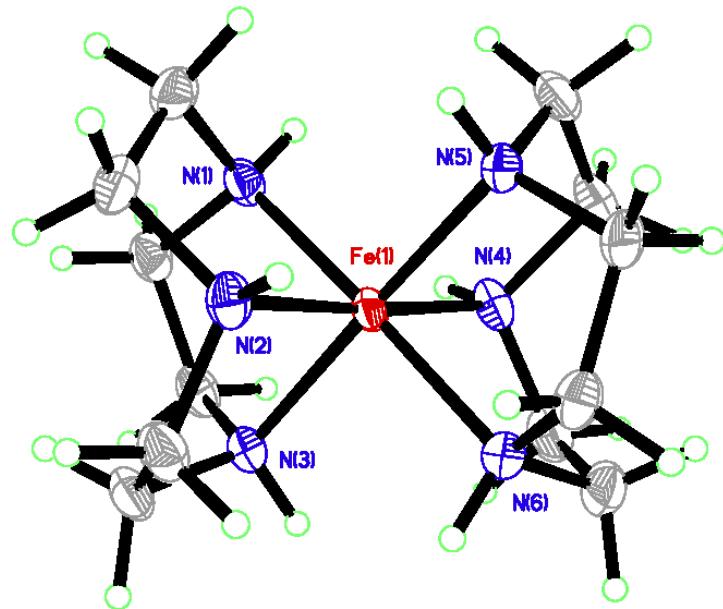


Figure S2. 50% thermal ellipsoidal drawings of $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**).

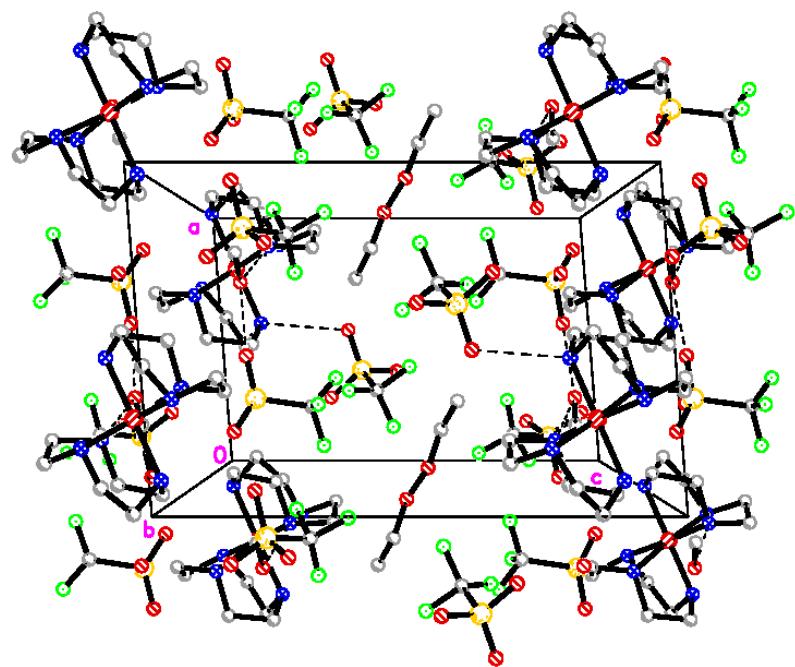


Figure S3. Packing diagram for $[Fe(tacn)_2](OTf)_3$ (**3**) along the b -axis where the dotted lines represent potential hydrogen bonding.

Table S1. Crystal data and structure refinement for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**).

Identification code	fc313b
Empirical formula	$\text{C}_{19}\text{H}_{43}\text{F}_9\text{FeN}_6\text{O}_{12}\text{S}_3$
Formula weight	870.62
Temperature/K	173.15
Crystal system	monoclinic
Space group	$\text{P}2_1/\text{n}$
a/Å	9.0622(6)
b/Å	28.8446(19)
c/Å	13.6738(9)
$\alpha/^\circ$	90.00
$\beta/^\circ$	94.5010(10)
$\gamma/^\circ$	90.00
Volume/Å ³	3563.2(4)
Z	4
ρ_{calc} mg/mm ³	1.623
m/mm ⁻¹	0.707
F(000)	1800.0
Crystal size/mm ³	0.53 × 0.353 × 0.152
2θ range for data collection	4.12 to 50.72°
Index ranges	-10 ≤ h ≤ 10, -34 ≤ k ≤ 34, -16 ≤ l ≤ 16
Reflections collected	58036
exptl absorpt T max, min	0.7452, 0.6193
Independent reflections	6527[R(int) = 0.0317]
Data/restraints/parameters	6527/6/455
2θ 25.36 fraction collected	0.999

Goodness-of-fit on F^2 1.054
Final R indexes [$|I| \geq 2\sigma(I)$] $R_1 = 0.0611$, $wR_2 = 0.1505$
Final R indexes [all data] $R_1 = 0.0669$, $wR_2 = 0.1553$
Largest diff. peak/hole / e Å⁻³ 1.75/-0.99

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Fe1	2601(5)	1600.2(18)	6008(4)	17.0(16)
N1	1600(30)	1172(11)	5020(20)	22(7)
N2	1910(30)	2097(11)	5060(20)	22(7)
N3	600(30)	1666(11)	6500(20)	21(7)
N4	3360(30)	1084(12)	6890(20)	24(7)
N5	4620(30)	1590(11)	5530(20)	22(7)
N6	3510(30)	2004(12)	7080(20)	23(7)
C1	1690(40)	1389(15)	4040(30)	27(9)
C2	1250(40)	1893(14)	4110(30)	26(9)
C3	40(40)	1078(14)	5250(30)	25(8)
C4	-170(40)	1216(14)	6300(30)	25(9)
C5	840(40)	2386(14)	5550(30)	27(9)
C6	-230(40)	2069(14)	6020(30)	27(9)
C7	4880(40)	935(15)	6640(30)	31(10)
C8	5160(40)	1104(15)	5630(30)	28(9)
C9	3350(50)	1250(16)	7910(30)	30(9)
C10	4730(40)	2264(14)	6660(30)	26(9)
C11	5630(40)	1928(15)	6100(30)	26(9)
C12	4030(50)	1728(16)	7970(30)	31(9)
S1	8866(11)	1854(4)	8860(7)	26(2)
F1	8160(70)	995(15)	8550(40)	120(20)
F2	6830(40)	1336(19)	9530(30)	100(17)
F3	9020(50)	1140(13)	10030(30)	78(12)

O1	7840(40)	1971(14)	8050(30)	48(9)
O2	8820(40)	2142(12)	9710(30)	47(9)
O3	10340(30)	1752(13)	8610(20)	40(8)
S2	6403(11)	1877(4)	3309(8)	28(2)
C1A	8150(80)	1290(20)	9200(50)	62(16)
F4	1330(60)	11(17)	1680(30)	107(17)
F5	2190(70)	679(15)	2080(30)	101(16)
F6	3660(60)	96(19)	2060(30)	101(16)
O4	4880(40)	1890(16)	3470(30)	57(11)
O5	7300(40)	1710(20)	4140(30)	69(14)
O6	6930(70)	2265(17)	2830(30)	100(20)
S3	2040(12)	110(4)	3539(9)	32(3)
C2A	6540(100)	1440(20)	2420(50)	80(20)
F7	5660(80)	1041(15)	2710(50)	130(20)
F8	7790(70)	1290(30)	2320(50)	190(40)
F9	5840(60)	1539(15)	1550(30)	87(13)
O7	2250(40)	-379(12)	3610(30)	49(9)
O8	3150(40)	393(12)	4050(30)	43(8)
O9	560(40)	265(13)	3660(30)	54(10)
C3A	2300(80)	230(20)	2260(50)	65(17)
O1S	2490(50)	2113(16)	230(30)	66(12)
C1S	2320(80)	1770(30)	950(60)	90(20)
O2S	8000(40)	-238(11)	3730(30)	46(9)
C2S	7020(60)	148(18)	3750(50)	57(16)
C4S	3100(200)	-160(60)	9360(110)	200(100)
C5S	2100(400)	180(140)	8900(300)	500(400)
O3S	4430(130)	130(40)	9730(80)	170(40)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hkaxbU_{12}]$

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Fe1	11(3)	20(3)	20(3)	-1(2)	-0.1(19)	0.3(19)
N1	15(15)	21(16)	29(18)	-3(13)	0(13)	0(12)
N2	18(15)	20(16)	27(17)	1(13)	-2(13)	-3(13)
N3	15(15)	25(17)	23(16)	-1(13)	0(12)	3(13)
N4	15(15)	27(18)	30(18)	6(14)	2(13)	3(13)
N5	16(15)	27(17)	22(16)	-3(13)	-1(12)	-2(13)
N6	19(16)	27(17)	21(16)	-4(13)	-1(13)	2(13)
C1	20(20)	30(20)	20(20)	-5(17)	-2(16)	-5(17)
C2	30(20)	30(20)	21(19)	2(16)	-5(16)	-2(17)
C3	15(18)	30(20)	30(20)	-3(17)	0(16)	-2(15)
C4	15(18)	30(20)	40(20)	3(17)	4(16)	-2(15)
C5	20(20)	21(19)	40(20)	0(17)	-1(17)	5(16)
C6	17(19)	30(20)	30(20)	-1(17)	1(16)	6(16)
C7	17(19)	30(20)	40(30)	4(19)	2(17)	8(17)
C8	16(19)	30(20)	40(20)	-6(18)	4(16)	4(16)
C9	20(20)	40(20)	30(20)	8(18)	3(17)	6(18)
C10	20(20)	30(20)	30(20)	-5(17)	-3(16)	-6(16)
C11	16(18)	30(20)	30(20)	-5(17)	-2(15)	-7(16)
C12	20(20)	50(30)	20(20)	0(18)	-3(16)	2(19)
S1	21(5)	33(6)	23(5)	-2(4)	-1(4)	3(4)
F1	210(60)	50(20)	100(30)	-20(20)	0(40)	-60(30)
F2	50(20)	160(50)	90(30)	50(30)	0(20)	-40(30)
F3	90(30)	60(20)	80(30)	30(20)	-20(20)	-10(20)

O1	29(17)	70(30)	39(19)	12(18)	-10(14)	-7(17)
O2	60(20)	40(20)	40(19)	-13(16)	-2(16)	20(17)
O3	28(16)	60(20)	37(18)	-1(16)	7(13)	10(15)
S2	25(5)	33(6)	27(5)	-1(4)	2(4)	-5(4)
C1A	70(40)	60(40)	60(40)	20(30)	0(30)	-20(30)
F4	150(50)	100(30)	70(30)	-30(30)	-30(30)	10(30)
F5	180(50)	70(30)	60(30)	20(20)	10(30)	10(30)
F6	110(40)	130(40)	70(30)	0(30)	50(30)	20(30)
O4	28(18)	100(30)	40(20)	10(20)	3(15)	1(19)
O5	30(20)	140(40)	40(20)	-10(20)	-6(16)	20(20)
O6	180(60)	70(30)	60(30)	-10(20)	50(30)	-80(40)
S3	28(5)	24(5)	47(7)	-6(5)	9(5)	-1(4)
C2A	130(70)	50(40)	60(40)	-10(30)	0(40)	40(40)
F7	210(70)	40(20)	140(50)	-10(30)	-20(40)	0(30)
F8	130(50)	300(100)	140(50)	-120(60)	-30(40)	150(60)
F9	130(40)	80(30)	39(19)	-18(19)	-10(20)	-10(30)
O7	40(20)	28(17)	80(30)	-5(17)	12(18)	2(15)
O8	38(19)	39(19)	50(20)	-10(16)	5(15)	-6(15)
O9	29(18)	40(20)	90(30)	-20(20)	11(18)	2(15)
C3A	90(50)	50(40)	50(40)	-10(30)	0(30)	0(30)
O1S	40(20)	70(30)	80(30)	-10(20)	-20(20)	-10(20)
C1S	60(40)	90(60)	100(60)	20(50)	-20(40)	0(40)
O2S	35(18)	28(17)	70(30)	4(17)	4(18)	0(14)
C2S	50(30)	30(30)	90(40)	0(30)	-10(30)	10(20)
C4S	300(200)	170(140)	140(120)	-70(110)	110(140)	-150(160)
C5S	600(800)	400(600)	500(700)	200(500)	-100(600)	100(500)
O3S	220(140)	150(100)	140(100)	-10(70)	80(90)	-10(80)

Table S4. Bond Lengths for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	N1	2.00(3)	S1	O2	1.43(3)
Fe1	N2	2.00(3)	S1	O3	1.44(3)
Fe1	N3	1.99(3)	S1	C1A	1.84(6)
Fe1	N4	2.00(3)	F1	C1A	1.22(8)
Fe1	N5	1.99(3)	F2	C1A	1.32(8)
Fe1	N6	2.00(3)	F3	C1A	1.39(7)
N1	C1	1.48(5)	S2	O4	1.41(4)
N1	C3	1.50(5)	S2	O5	1.43(4)
N2	C2	1.50(5)	S2	O6	1.40(4)
N2	C5	1.48(5)	S2	C2A	1.77(7)
N3	C4	1.49(5)	F4	C3A	1.30(8)
N3	C6	1.51(5)	F5	C3A	1.32(7)
N4	C7	1.51(5)	F6	C3A	1.34(8)
N4	C9	1.48(5)	S3	O7	1.43(4)
N5	C8	1.49(5)	S3	O8	1.43(3)
N5	C11	1.51(5)	S3	O9	1.43(3)
N6	C10	1.49(5)	S3	C3A	1.81(7)
N6	C12	1.50(5)	C2A	F7	1.46(10)
C1	C2	1.51(6)	C2A	F8	1.23(9)
C3	C4	1.51(6)	C2A	F9	1.34(8)
C5	C6	1.51(6)	O1S	C1S	1.41(9)
C7	C8	1.51(6)	O2S	C2S	1.43(6)

C9	C12	1.51(6)	C4S	C5S	1.4(3)
C10	C11	1.51(6)	C4S	O3S	1.49(18)
S1	O1	1.43(3)	O3S	O3S ¹	1.4(2)

¹1-X,-Y,2-Z

Table S5. Bond Angles for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**).

Atom	Atom	Atom	Angle/ $^{\circ}$	Atom	Atom	Atom	Angle/ $^{\circ}$
N1	Fe1	N2	84.3(13)	N6	C10	C11	109(3)
N1	Fe1	N4	93.6(14)	N5	C11	C10	110(3)
N3	Fe1	N1	84.9(13)	N6	C12	C9	110(3)
N3	Fe1	N2	84.4(13)	O1	S1	O3	115(2)
N3	Fe1	N4	98.5(13)	O1	S1	C1A	101(3)
N3	Fe1	N6	91.8(13)	O2	S1	O1	116(2)
N4	Fe1	N2	176.2(14)	O2	S1	O3	113(2)
N5	Fe1	N1	98.3(13)	O2	S1	C1A	106(3)
N5	Fe1	N2	92.5(13)	O3	S1	C1A	103(3)
N5	Fe1	N3	175.3(13)	O4	S2	O5	113(2)
N5	Fe1	N4	84.7(13)	O4	S2	C2A	104(4)
N5	Fe1	N6	85.2(13)	O5	S2	C2A	104(3)
N6	Fe1	N1	175.4(14)	O6	S2	O4	115(4)
N6	Fe1	N2	98.5(14)	O6	S2	O5	117(3)
N6	Fe1	N4	83.8(14)	O6	S2	C2A	102(3)
C1	N1	Fe1	107(2)	F1	C1A	S1	114(5)
C1	N1	C3	112(3)	F1	C1A	F2	113(6)
C3	N1	Fe1	111(2)	F1	C1A	F3	110(6)
C2	N2	Fe1	111(2)	F2	C1A	S1	110(5)
C5	N2	Fe1	107(2)	F2	C1A	F3	103(5)
C5	N2	C2	113(3)	F3	C1A	S1	107(4)
C4	N3	Fe1	106(2)	O7	S3	O8	116(2)
C4	N3	C6	113(3)	O7	S3	O9	115(2)
C6	N3	Fe1	112(2)	O7	S3	C3A	103(3)

C7	N4	Fe1	111(2)	O8	S3	O9	113(2)
C9	N4	Fe1	107(2)	O8	S3	C3A	103(3)
C9	N4	C7	112(3)	O9	S3	C3A	104(3)
C8	N5	Fe1	107(2)	F7	C2A	S2	108(5)
C8	N5	C11	112(3)	F8	C2A	S2	117(7)
C11	N5	Fe1	111(2)	F8	C2A	F7	106(7)
C10	N6	Fe1	107(2)	F8	C2A	F9	111(7)
C10	N6	C12	113(3)	F9	C2A	S2	113(4)
C12	N6	Fe1	112(3)	F9	C2A	F7	100(6)
N1	C1	C2	109(3)	F4	C3A	F5	109(6)
N2	C2	C1	110(3)	F4	C3A	F6	109(6)
N1	C3	C4	110(3)	F4	C3A	S3	111(5)
N3	C4	C3	108(3)	F5	C3A	F6	107(6)
N2	C5	C6	109(3)	F5	C3A	S3	111(4)
N3	C6	C5	109(3)	F6	C3A	S3	109(5)
C8	C7	N4	109(3)	C5S	C4S	O3S	102(10)
N5	C8	C7	108(3)	O3S ¹	O3S	C4S	113(10)
N4	C9	C12	108(3)				

¹1-X,-Y,2-Z

Table S6. Hydrogen Bonds for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (**3**).

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2	H2	O2 ¹	0.93	1.98	2.86(5)	157.2
N4	H4	O2S ²	0.93	1.95	2.83(5)	156.4
N6	H6	O6 ³	0.93	1.90	2.79(5)	160.8

¹-1/2+X,1/2-Y,-1/2+Z; ²1-X,-Y,1-Z; ³-1/2+X,1/2-Y,1/2+Z

Table S7. Torsion Angles for [Fe(tacn)₂](OTf)₃ (**3**).

A B C D	Angle/°	A B C D	Angle/°
Fe1 N1 C1 C2	-46(3)	N5 Fe1 N2 C2	90(3)
Fe1 N1 C3 C4	-17(4)	N5 Fe1 N2 C5	-146(2)
Fe1 N2 C2 C1	-16(4)	N5 Fe1 N3 C4	165(15)
Fe1 N2 C5 C6	-47(3)	N5 Fe1 N3 C6	42(17)
Fe1 N3 C4 C3	-48(3)	N5 Fe1 N4 C7	-7(3)
Fe1 N3 C6 C5	-17(4)	N5 Fe1 N4 C9	116(3)
Fe1 N4 C7 C8	-18(4)	N5 Fe1 N6 C10	30(2)
Fe1 N4 C9 C12	-47(4)	N5 Fe1 N6 C12	-93(3)
Fe1 N5 C8 C7	-48(3)	N6 Fe1 N1 C1	158(16)
Fe1 N5 C11 C10	-16(4)	N6 Fe1 N1 C3	35(18)
Fe1 N6 C10 C11	-46(3)	N6 Fe1 N2 C2	176(2)
Fe1 N6 C12 C9	-15(4)	N6 Fe1 N2 C5	-61(2)
N1 Fe1 N2 C2	-8(3)	N6 Fe1 N3 C4	-146(2)
N1 Fe1 N2 C5	115(2)	N6 Fe1 N3 C6	91(3)
N1 Fe1 N3 C4	31(2)	N6 Fe1 N4 C7	-92(3)
N1 Fe1 N3 C6	-92(3)	N6 Fe1 N4 C9	31(2)
N1 Fe1 N4 C7	91(3)	N6 Fe1 N5 C8	114(3)
N1 Fe1 N4 C9	-146(3)	N6 Fe1 N5 C11	-8(3)
N1 Fe1 N5 C8	-63(3)	N6 C10 C11 N5	41(4)
N1 Fe1 N5 C11	175(3)	C1 N1 C3 C4	-137(3)
N1 Fe1 N6 C10	170(16)	C2 N2 C5 C6	75(4)
N1 Fe1 N6 C12	47(18)	C3 N1 C1 C2	76(4)
N1 C1 C2 N2	41(4)	C4 N3 C6 C5	-136(3)
N1 C3 C4 N3	42(4)	C5 N2 C2 C1	-136(3)

N2 Fe1 N1 C1	30(2) C6 N3 C4 C3	75(4)
N2 Fe1 N1 C3	-93(3) C7 N4 C9 C12	75(4)
N2 Fe1 N3 C4	116(3) C8 N5 C11 C10	-135(4)
N2 Fe1 N3 C6	-7(3) C9 N4 C7 C8	-138(4)
N2 Fe1 N4 C7	35(21) C10 N6 C12 C9	-135(3)
N2 Fe1 N4 C9	158(19) C11 N5 C8 C7	74(4)
N2 Fe1 N5 C8	-147(2) C12 N6 C10 C11	77(4)
N2 Fe1 N5 C11	90(3) O1 S1 C1A F1	61(6)
N2 Fe1 N6 C10	-62(3) O1 S1 C1A F2	-66(5)
N2 Fe1 N6 C12	175(3) O1 S1 C1A F3	-177(4)
N2 C5 C6 N3	42(4) O2 S1 C1A F1	-178(5)
N3 Fe1 N1 C1	115(2) O2 S1 C1A F2	55(5)
N3 Fe1 N1 C3	-8(3) O2 S1 C1A F3	-56(5)
N3 Fe1 N2 C2	-93(3) O3 S1 C1A F1	-58(6)
N3 Fe1 N2 C5	30(2) O3 S1 C1A F2	175(4)
N3 Fe1 N4 C7	177(3) O3 S1 C1A F3	64(5)
N3 Fe1 N4 C9	-60(3) O4 S2 C2A F7	-44(5)
N3 Fe1 N5 C8	164(15) O4 S2 C2A F8	-164(7)
N3 Fe1 N5 C11	41(17) O4 S2 C2A F9	66(7)
N3 Fe1 N6 C10	-146(2) O5 S2 C2A F7	74(6)
N3 Fe1 N6 C12	90(3) O5 S2 C2A F8	-46(8)
N4 Fe1 N1 C1	-147(2) O5 S2 C2A F9	-176(6)
N4 Fe1 N1 C3	90(3) O6 S2 C2A F7	-165(5)
N4 Fe1 N2 C2	49(21) O6 S2 C2A F8	76(8)
N4 Fe1 N2 C5	172(19) O6 S2 C2A F9	-54(7)
N4 Fe1 N3 C4	-62(3) O7 S3 C3A F4	61(5)
N4 Fe1 N3 C6	175(3) O7 S3 C3A F5	-178(5)

N4 Fe1 N5 C8	30(3) O7 S3 C3A F6	-59(5)
N4 Fe1 N5 C11	-92(3) O8 S3 C3A F4	-178(5)
N4 Fe1 N6 C10	115(3) O8 S3 C3A F5	-56(6)
N4 Fe1 N6 C12	-8(3) O8 S3 C3A F6	62(5)
N4 C7 C8 N5	43(4) O9 S3 C3A F4	-59(5)
N4 C9 C12 N6	40(4) O9 S3 C3A F5	62(6)
N5 Fe1 N1 C1	-62(3) O9 S3 C3A F6	-180(4)
N5 Fe1 N1 C3	175(3) C5S C4S O3S O3S ¹	174(21)

¹1-X,-Y,2-Z

Table S8. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}(\text{tacn})_2](\text{OTf})_3$ (3).

Atom	x	y	z	U(eq)
H1	2119	892	5032	26
H2	2716	2280	4927	26
H3	705	1714	7172	26
H4	2720	833	6801	29
H5	4549	1673	4866	26
H6	2798	2216	7252	27
H1A	1013	1228	3549	32
H1B	2709	1364	3836	32
H2A	1606	2067	3551	32
H2B	159	1919	4078	32
H3A	-190	745	5157	30
H3B	-654	1257	4798	30
H4A	-1233	1247	6394	31
H4B	259	975	6753	31
H5A	294	2592	5072	32
H5B	1369	2582	6063	32
H6A	-749	2242	6519	32
H6B	-987	1954	5515	32
H7A	5639	1065	7125	37
H7B	4958	592	6664	37
H8A	6226	1091	5530	34
H8B	4622	906	5125	34
H9A	3927	1037	8361	36

H9B	2321	1262	8108	36
H10A	5366	2411	7190	32
H10B	4313	2510	6213	32
H11A	6216	2101	5637	31
H11B	6320	1756	6558	31
H12A	3736	1888	8569	37
H12B	5119	1703	8018	37
H1S	1908	2058	-266	98
H1SA	2821	1870	1575	128
H1SB	2748	1477	745	128
H1SC	1261	1726	1030	128
H2S	8866	-142	3695	68
H2SA	7569	421	4006	86
H2SB	6230	77	4184	86
H2SC	6579	211	3090	86
H4SA	3431	-383	8858	244
H4SB	2730	-330	9902	244
H5SA	1221	22	8678	788
H5SB	2573	344	8417	788
H5SC	1883	398	9453	788