Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and reactivity of a 4His enzyme model complex

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Structural Data

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Sample Reference Number: $Fe(Trlm)_4(OTf)_2$

X-ray Number: CF316a

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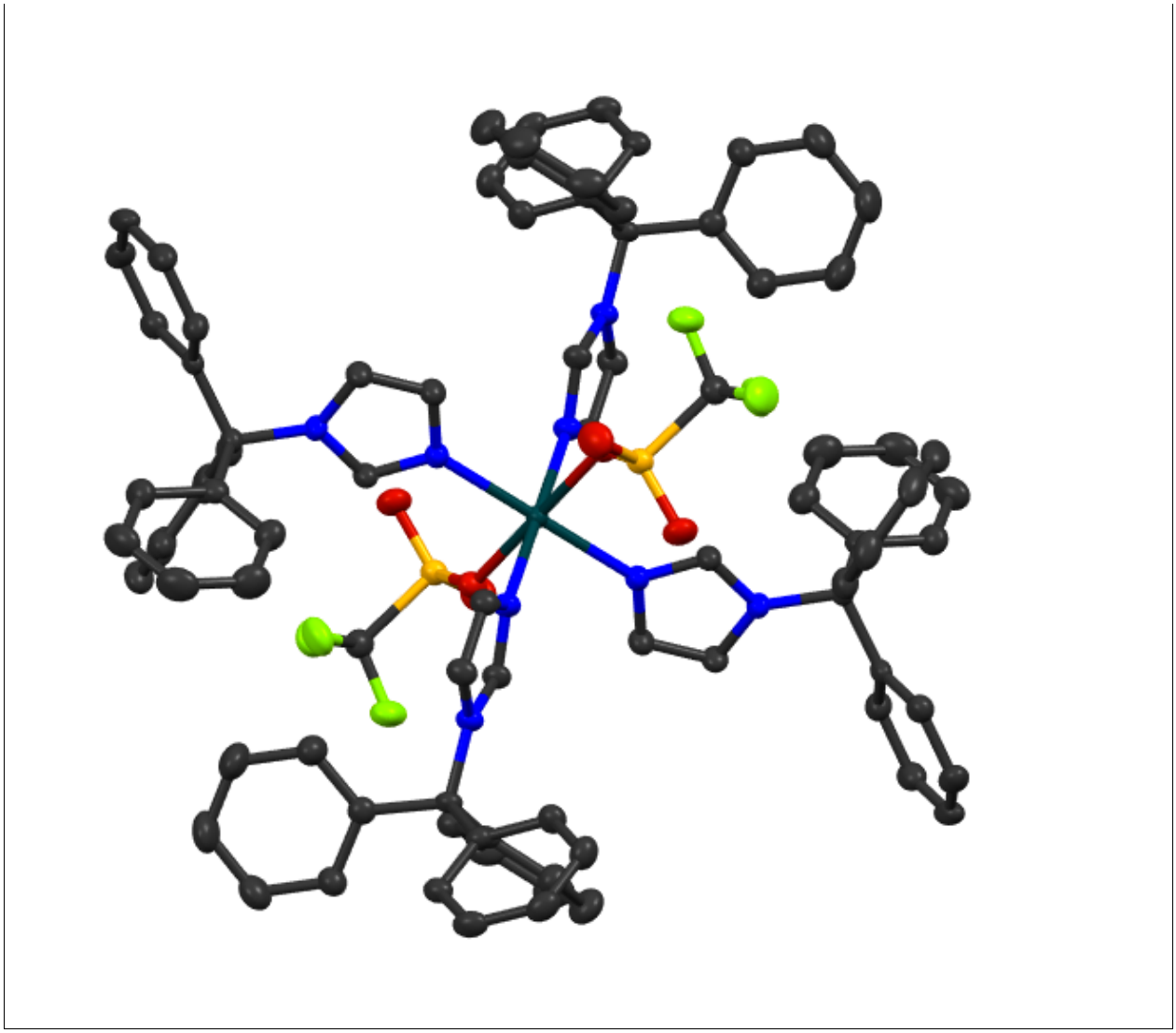
Introduction:

Single crystal study to confirm the identity of the sample submitted. One molecule of diethyl ether is also present in the asymmetric unit (not shown).



Experimental Section:

A colorless prism crystal with dimensions 0.224 x 0.185 x 0.064 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 10 s. The total number of images was based on results from the program COSMO[1] where redundancy was expected to be 4.0 and completeness of 100% out to 0.83 Å. Cell parameters were retrieved using APEX II software[2] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software,[3] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[4] 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 F^2, SHELXL-2014[5], which are incorporated in OLEX2.[6]

The structure was solved in the space group $P\bar{1}$ (# 2). All non-hydrogen atoms are refined anisotropically. Hydrogen atoms were calculated by geometrical methods and refined as a riding model. The crystal used for the diffraction study showed no decomposition during data collection. 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).

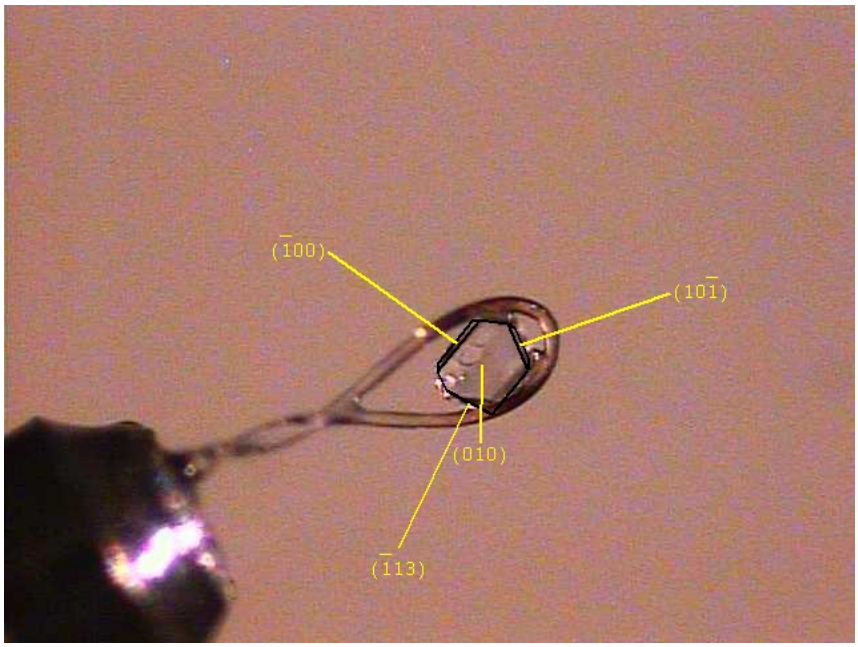
3. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).

4. SADABS V2.008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.

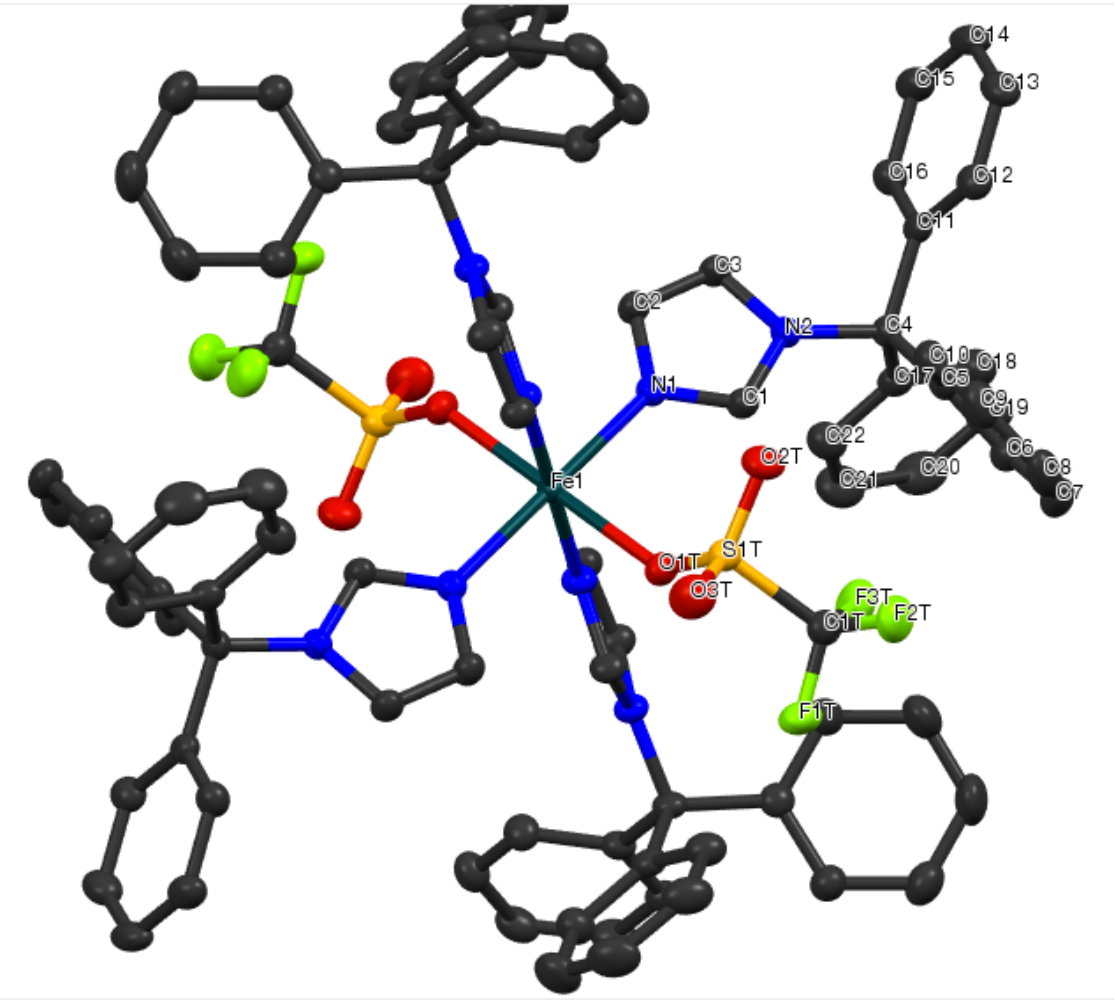
5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

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.

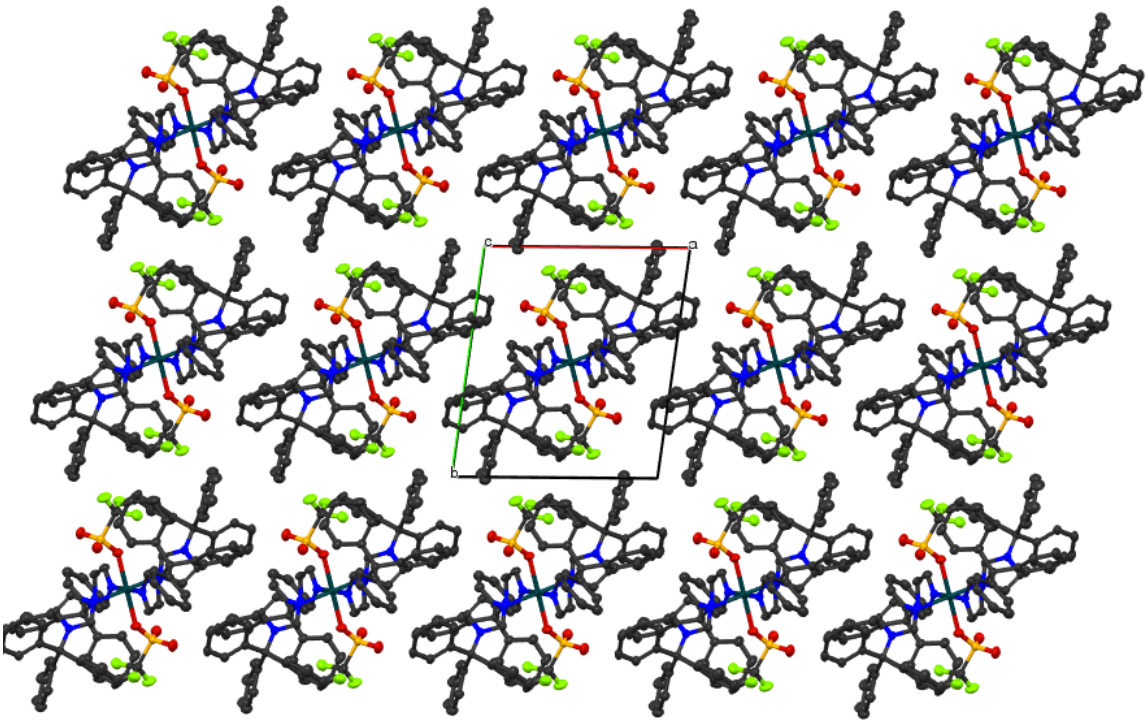
[a] Obtained with graphite monochromated Mo Kα (λ= 0.71073 Å) radiation.
[b] $R1 = \sum \big| |F_o| - |F_c| / |F_o| \big|$ [c] $wR_2 = \{ \big| [w(F_o^2 - F_c^2)^2 . \{\sum [w(F_o^2)^2]\}^{1/2}$.



The following are 50% thermal ellipsoidal drawings of the molecule in the asymmetric cell with various amount of labeling.



This figures shows the atom numbering scheme for the metal, one organic ligand and one triflate anion. The other crystallographically unique organic ligand follows the same numbering scheme as the one shown, but with an ‘a’ suffix.



This is a drawing of the packing along the c-axis. The solvent diethyl ether molecule is not shown.

Table S1. Crystal data and structure refinement for $[Fe(TrIm)_4(OTf)_2]$ (**1**).

Identification code	CF316a
Empirical formula	$C_{98}H_{92}F_6FeN_8O_8S_2$
Formula weight	1743.76
Temperature/K	173.15
Crystal system	triclinic
Space group	*P*1
a/Å	13.2342(7)
b/Å	13.5131(7)
c/Å	13.7025(7)
α/°	98.0060(10)
β/°	116.1990(10)
γ/°	93.3490(10)
Volume/Å^3	2157.39(19)
Z	1
ρ_{calc}g/cm^3	1.342
μ/mm^{-1}	0.300
F(000)	912.0
Crystal size/mm^3	0.224 × 0.185 × 0.064
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.072 to 50.786
Index ranges	$-15 \le h \le 15$, $-16 \le k \le 16$, $-16 \le l \le 16$
Reflections collected	29627
Independent reflections	7927 [R_{int} = 0.0346, R_{sigma} = 0.0345]
Data/restraints/parameters	7927/0/558
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.0948
Final R indexes [all data]	R_1 = 0.0508, wR_2 = 0.1032
Largest diff. peak/hole / e Å^{-3}	0.32/-0.35

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $[Fe(TrIm)_4(OTf)_2]$ (**1**). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe1	5000	5000	10000	18.66(10)
N1	5768.8(13)	5084.0(12)	8889.9(12)	21.3(3)
N2	6481.9(13)	4602.6(11)	7735.7(12)	21.4(3)
C1	5937.8(16)	4309.5(14)	8305.8(15)	23.0(4)
C2	6239.8(17)	5921.1(15)	8695.0(16)	26.2(4)

C3	6676.4(17)	5638.7(14)	7989.1(16)	26.1(4)
C4	6932.6(16)	3908.7(14)	7111.3(15)	22.2(4)
C5	6100.5(17)	2921.8(14)	6617.3(15)	24.1(4)
C6	6465.0(19)	1980.2(15)	6726.8(17)	30.0(5)
C7	5686(2)	1110.0(16)	6251.4(19)	40.4(6)
C8	4543(2)	1158.0(17)	5672.4(19)	41.4(6)
C9	4168.1(19)	2081.3(18)	5566.3(18)	37.5(5)
C10	4936.0(17)	2953.2(16)	6032.2(17)	29.9(5)
C11	7011.8(17)	4432.8(14)	6208.4(16)	23.2(4)
C12	6240.1(18)	4169.0(16)	5093.0(17)	29.1(5)
C13	6349.0(19)	4665.6(17)	4314.7(18)	34.8(5)
C14	7227.8(19)	5432.1(17)	4632.8(19)	36.1(5)
C15	8007.6(19)	5697.5(16)	5735.1(19)	33.7(5)
C16	7905.7(18)	5201.1(15)	6510.3(17)	28.4(4)
C17	8130.6(17)	3719.5(14)	7915.9(16)	25.2(4)
C18	8831.1(18)	3319.7(16)	7485.4(18)	32.7(5)
C19	9890.2(19)	3100.9(18)	8166(2)	40.2(6)
C20	10285.4(19)	3287.3(19)	9301(2)	44.1(6)
C21	9608(2)	3683.7(19)	9737(2)	43.1(6)
C22	8531.6(18)	3901.1(16)	9053.3(17)	32.6(5)
N1A	3470.8(13)	5577.7(12)	8920.8(13)	24.2(4)
N2A	2479.7(13)	6717.7(11)	8042.7(12)	21.8(3)
C1A	3519.0(16)	6447.2(14)	8597.8(15)	23.5(4)
C2A	2333.2(16)	5271.5(15)	8554.9(16)	25.5(4)
C3A	1713.3(16)	5958.8(15)	8014.8(16)	25.8(4)
C4A	2191.6(16)	7667.4(14)	7584.7(15)	22.4(4)
C5A	1161.4(16)	7349.1(14)	6431.5(15)	22.6(4)
C6A	1154.4(17)	6496.6(16)	5724.4(16)	28.2(4)
C7A	289.5(18)	6218.8(17)	4662.5(17)	31.8(5)
C8A	-603.6(17)	6775.4(17)	4276.9(17)	32.0(5)
C9A	-628.5(17)	7602.7(16)	4975.4(17)	30.9(5)
C10A	245.0(16)	7889.2(15)	6047.4(16)	25.8(4)
C11A	1936.7(16)	8418.4(15)	8375.8(15)	24.6(4)
C12A	1799(2)	8160.3(17)	9256.1(18)	36.2(5)
C13A	1579(2)	8875.7(19)	9946(2)	49.8(7)
C14A	1506(2)	9848.3(19)	9767(2)	50.2(7)
C15A	1653(2)	10121.0(17)	8900(2)	40.2(5)
C16A	1869.6(18)	9410.3(15)	8214.5(17)	30.1(5)
C17A	3250.5(16)	8138.0(14)	7519.0(16)	23.5(4)
C18A	4158.2(17)	8666.9(15)	8483.7(17)	30.0(5)
C19A	5147.3(19)	9061.3(17)	8480(2)	38.7(5)
C20A	5232(2)	8949.2(19)	7509(2)	43.6(6)

C21A	4337(2)	8447.5(19)	6542(2)	43.9(6)
C22A	3352.9(19)	8043.4(16)	6546.7(18)	32.7(5)
S1T	3404.7(4)	2831.7(4)	8301.4(4)	23.28(12)
F1T	4045.8(11)	1183.8(9)	9056.4(10)	39.9(3)
F2T	3286.1(12)	1011.6(9)	7284.9(10)	45.6(3)
F3T	4990.4(11)	1774.3(10)	8277.9(11)	42.9(3)
O1T	4311.4(12)	3411.4(10)	9320.7(11)	27.9(3)
O2T	3292.7(12)	3181.3(11)	7325.8(11)	34.1(3)
O3T	2379.3(12)	2572.0(12)	8370.4(13)	40.3(4)
C1T	3961.8(17)	1637.9(15)	8226.0(16)	28.4(4)
O1S	8456.0(16)	9357.5(12)	6519.9(14)	51.7(5)
C1S	8201(3)	8156(2)	7535(3)	74.8(10)
C2S	8401(3)	9226(2)	7483(2)	56.8(7)
C3S	8718(3)	10349.0(19)	6457(3)	55.4(7)
C4S	8768(4)	10451(3)	5444(3)	104.2(14)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $[Fe(TrIm)_4(OTf)_2]$ (**1**). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	19.6(2)	19.1(2)	20.3(2)	5.79(15)	10.67(16)	6.05(15)
N1	21.1(8)	22.5(8)	21.9(8)	4.6(7)	10.8(7)	4.5(7)
N2	22.7(8)	22.1(8)	23.7(8)	4.6(7)	14.2(7)	3.4(7)
C1	25.1(10)	21(1)	28.4(10)	6.4(8)	16.3(9)	3.7(8)
C2	31.6(11)	19.9(10)	31.0(11)	4.0(8)	17.9(9)	2.5(8)
C3	31.5(11)	20.1(10)	32.5(11)	5.5(8)	19.7(9)	1.5(8)
C4	24.7(10)	21.5(10)	25.3(10)	4.9(8)	15.3(9)	5.7(8)
C5	29.1(11)	24.5(10)	23.8(10)	2.8(8)	17.1(9)	3.4(8)
C6	36.7(12)	26.1(11)	34.3(11)	6.7(9)	21.8(10)	7.1(9)
C7	61.4(17)	22.4(11)	45.8(13)	1.6(10)	33.6(13)	2.2(11)
C8	52.1(16)	33.2(13)	39.7(13)	-10.8(10)	29.2(12)	-15.1(11)
C9	31.1(12)	45.1(14)	33.6(12)	-5.3(10)	17.4(10)	-5.4(10)
C10	29.5(12)	31.0(11)	32.1(11)	2.6(9)	17.6(10)	3.7(9)
C11	28.3(11)	21(1)	30(1)	7.9(8)	20.2(9)	9.6(8)
C12	29.2(11)	30.9(11)	31.6(11)	8.9(9)	16.2(9)	9.9(9)
C13	38.3(13)	43.7(13)	29.8(11)	16.3(10)	17.7(10)	18.2(11)
C14	45.6(14)	38.1(13)	46.0(13)	25.8(11)	32.5(12)	22.6(11)
C15	39.2(13)	31.5(12)	44.7(13)	14.2(10)	29.2(11)	10.2(10)
C16	30.8(11)	28.8(11)	30.0(11)	4.9(9)	18.0(9)	4.4(9)
C17	25(1)	22.8(10)	30.7(11)	8.3(8)	14.3(9)	3.0(8)
C18	30.5(12)	37.0(12)	38.4(12)	10.8(10)	21.1(10)	8.5(10)
C19	29.3(12)	42.8(14)	58.2(15)	18.3(12)	24.9(12)	12.7(10)

C20	24.0(12)	49.9(15)	54.7(15)	20.2(12)	11.0(11)	9.0(11)
C21	34.7(13)	51.3(15)	35.0(13)	11.3(11)	7.9(11)	3.2(11)
C22	29.6(12)	37.2(12)	32.3(11)	7.3(10)	15.4(10)	2.4(10)
N1A	22.5(9)	25.8(9)	25.7(8)	9.6(7)	10.4(7)	6.9(7)
N2A	19.1(8)	22.2(8)	23.6(8)	8.2(7)	7.9(7)	5.3(7)
C1A	18(1)	26.4(10)	25.6(10)	8.9(8)	7.9(8)	5.8(8)
C2A	24.7(11)	23.9(10)	27.9(10)	6.5(8)	11.6(9)	3.0(8)
C3A	17.8(10)	26.4(10)	31.3(11)	7.7(9)	8.8(9)	2.9(8)
C4A	22.1(10)	22.8(10)	24.4(10)	10.6(8)	10.0(8)	7.2(8)
C5A	21.4(10)	25.3(10)	22.6(10)	8.9(8)	9.9(8)	4.6(8)
C6A	23.8(11)	32.2(11)	28.9(11)	7.4(9)	11.2(9)	8.9(9)
C7A	30.7(12)	37.1(12)	26.3(11)	1.0(9)	13.4(9)	1.7(10)
C8A	23.2(11)	45.3(13)	24.7(10)	10.3(10)	7.7(9)	0.7(10)
C9A	20.4(10)	38.6(12)	35.6(12)	18.2(10)	10.8(9)	8.3(9)
C10A	23.1(10)	26.8(11)	31.2(11)	11.2(9)	13.6(9)	6.4(8)
C11A	19.5(10)	27.4(10)	24(1)	4.6(8)	7.4(8)	2.7(8)
C12A	46.5(14)	32.5(12)	32.2(12)	6.8(10)	20.0(11)	6.1(10)
C13A	72.7(19)	48.6(15)	40.4(14)	6.3(12)	37.4(14)	7.8(13)
C14A	68.7(18)	39.2(14)	49.1(15)	-6.5(12)	36.7(14)	7.1(13)
C15A	43.8(14)	28.3(12)	49.5(14)	3.3(10)	23.0(12)	6.3(10)
C16A	31.8(12)	27.3(11)	34.2(11)	6.6(9)	17.1(10)	5.8(9)
C17A	21.8(10)	21.7(10)	29.8(10)	10.8(8)	12.0(9)	7.2(8)
C18A	25.4(11)	31.3(11)	32.6(11)	11.1(9)	11.1(9)	3.8(9)
C19A	26.3(12)	39.3(13)	44.7(13)	16.0(11)	9.4(10)	-1.9(10)
C20A	31.0(13)	50.0(15)	60.1(16)	24.0(13)	25.9(12)	4.7(11)
C21A	46.0(15)	53.4(15)	46.2(14)	15.5(12)	31.7(13)	5.6(12)
C22A	34.3(12)	33.6(12)	32.3(11)	6.9(9)	16.9(10)	3(1)
S1T	20.7(3)	24.5(3)	24.6(2)	6.4(2)	9.7(2)	4.6(2)
F1T	52.8(8)	30.5(7)	38.3(7)	14.5(6)	19.7(6)	8.8(6)
F2T	59.2(9)	30.9(7)	36.3(7)	-8.1(6)	17.7(7)	-5.8(6)
F3T	38.1(7)	38.3(7)	62.0(9)	7.2(6)	30.9(7)	13.5(6)
O1T	33.5(8)	21.4(7)	25.7(7)	3.2(6)	11.2(6)	3.3(6)
O2T	33.7(8)	39.6(9)	27.7(8)	14.3(7)	10.1(7)	8.4(7)
O3T	26.3(8)	45.1(10)	56.2(10)	13.3(8)	23.5(8)	6.2(7)
C1T	30.6(11)	25.1(11)	26.7(10)	2.1(9)	11.7(9)	0.7(9)
O1S	71.6(13)	39.1(10)	51.6(11)	6.0(8)	35.7(10)	3.0(9)
C1S	116(3)	57.3(19)	65(2)	12.9(16)	54(2)	6.5(19)
C2S	64.8(19)	54.9(17)	58.1(17)	3.5(14)	37.1(15)	3.4(14)
C3S	57.2(17)	38.0(14)	78(2)	11.6(14)	36.9(16)	9.2(13)
C4S	142(4)	82(3)	113(3)	43(2)	74(3)	-1(3)

Table S4. Bond Lengths for $[Fe(TrIm)_4(OTf)_2]$ (**1**).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	N1	2.1823(15)	N2A	C3A	1.384(2)
Fe1	N1[1]	2.1823(15)	N2A	C4A	1.502(2)
Fe1	N1A	2.1807(15)	C2A	C3A	1.352(3)
Fe1	N1A[1]	2.1808(15)	C4A	C5A	1.543(3)
Fe1	O1T[1]	2.1843(13)	C4A	C11A	1.541(3)
Fe1	O1T	2.1843(13)	C4A	C17A	1.549(3)
N1	C1	1.318(2)	C5A	C6A	1.395(3)
N1	C2	1.374(2)	C5A	C10A	1.388(3)
N2	C1	1.355(2)	C6A	C7A	1.377(3)
N2	C3	1.375(2)	C7A	C8A	1.380(3)
N2	C4	1.503(2)	C8A	C9A	1.379(3)
C2	C3	1.353(3)	C9A	C10A	1.391(3)
C4	C5	1.539(3)	C11A	C12A	1.383(3)
C4	C11	1.547(2)	C11A	C16A	1.390(3)
C4	C17	1.542(3)	C12A	C13A	1.392(3)
C5	C6	1.391(3)	C13A	C14A	1.372(4)
C5	C10	1.395(3)	C14A	C15A	1.379(3)
C6	C7	1.386(3)	C15A	C16A	1.380(3)
C7	C8	1.374(3)	C17A	C18A	1.391(3)
C8	C9	1.372(3)	C17A	C22A	1.387(3)
C9	C10	1.381(3)	C18A	C19A	1.387(3)
C11	C12	1.390(3)	C19A	C20A	1.372(3)
C11	C16	1.398(3)	C20A	C21A	1.374(3)
C12	C13	1.390(3)	C21A	C22A	1.385(3)
C13	C14	1.379(3)	S1T	O1T	1.4524(14)
C14	C15	1.380(3)	S1T	O2T	1.4288(14)
C15	C16	1.382(3)	S1T	O3T	1.4284(15)
C17	C18	1.397(3)	S1T	C1T	1.821(2)
C17	C22	1.385(3)	F1T	C1T	1.332(2)
C18	C19	1.376(3)	F2T	C1T	1.330(2)
C19	C20	1.383(3)	F3T	C1T	1.332(2)
C20	C21	1.374(3)	O1S	C2S	1.388(3)
C21	C22	1.393(3)	O1S	C3S	1.388(3)
N1A	C1A	1.320(2)	C1S	C2S	1.471(4)
N1A	C2A	1.376(2)	C3S	C4S	1.444(4)
N2A	C1A	1.348(2)			

[1]1-X,1-Y,2-Z

Table S5. Bond Angles for [Fe(TrIm)$_4$(OTf)$_2$] (**1**).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1[1]	Fe1	N1	180.00(8)	C1A	N1A	C2A	105.30(15)
N1[1]	Fe1	O1T[1]	93.07(5)	C2A	N1A	Fe1	132.42(12)
N1	Fe1	O1T	93.07(5)	C1A	N2A	C3A	106.12(15)
N1	Fe1	O1T[1]	86.93(5)	C1A	N2A	C4A	127.81(15)
N1[1]	Fe1	O1T	86.93(5)	C3A	N2A	C4A	126.02(15)
N1A[1]	Fe1	N1	86.87(6)	N1A	C1A	N2A	112.17(16)
N1A	Fe1	N1	93.13(6)	C3A	C2A	N1A	109.88(17)
N1A[1]	Fe1	N1[1]	93.13(6)	C2A	C3A	N2A	106.53(17)
N1A	Fe1	N1[1]	86.87(6)	N2A	C4A	C5A	106.37(15)
N1A	Fe1	N1A[1]	180.00(9)	N2A	C4A	C11A	109.76(14)
N1A	Fe1	O1T[1]	84.76(6)	N2A	C4A	C17A	107.30(14)
N1A[1]	Fe1	O1T	84.76(6)	C5A	C4A	C17A	112.07(15)
N1A	Fe1	O1T	95.24(6)	C11A	C4A	C5A	112.55(15)
N1A[1]	Fe1	O1T[1]	95.24(6)	C11A	C4A	C17A	108.64(15)
O1T[1]	Fe1	O1T	180.0	C6A	C5A	C4A	119.08(17)
C1	N1	Fe1	125.92(12)	C10A	C5A	C4A	122.95(17)
C1	N1	C2	105.15(15)	C10A	C5A	C6A	117.95(18)
C2	N1	Fe1	128.82(12)	C7A	C6A	C5A	121.23(19)
C1	N2	C3	106.06(15)	C6A	C7A	C8A	120.4(2)
C1	N2	C4	125.24(15)	C9A	C8A	C7A	119.13(19)
C3	N2	C4	128.02(15)	C8A	C9A	C10A	120.68(19)
N1	C1	N2	112.12(16)	C5A	C10A	C9A	120.51(19)
C3	C2	N1	109.97(17)	C12A	C11A	C4A	123.21(18)
C2	C3	N2	106.70(16)	C12A	C11A	C16A	118.32(19)
N2	C4	C5	106.93(14)	C16A	C11A	C4A	118.45(17)
N2	C4	C11	108.20(14)	C11A	C12A	C13A	120.5(2)
N2	C4	C17	109.14(15)	C14A	C13A	C12A	120.3(2)
C5	C4	C11	112.26(15)	C13A	C14A	C15A	120.0(2)
C5	C4	C17	111.09(15)	C14A	C15A	C16A	119.7(2)
C17	C4	C11	109.11(15)	C15A	C16A	C11A	121.3(2)
C6	C5	C4	122.33(18)	C18A	C17A	C4A	118.78(17)
C6	C5	C10	117.75(19)	C22A	C17A	C4A	123.32(18)
C10	C5	C4	119.92(17)	C22A	C17A	C18A	117.89(18)
C7	C6	C5	120.3(2)	C19A	C18A	C17A	121.1(2)
C8	C7	C6	121.0(2)	C20A	C19A	C18A	119.9(2)
C9	C8	C7	119.5(2)	C19A	C20A	C21A	120.0(2)
C8	C9	C10	120.1(2)	C20A	C21A	C22A	120.2(2)
C9	C10	C5	121.4(2)	C21A	C22A	C17A	120.9(2)
C12	C11	C4	123.21(17)	O1T	S1T	C1T	101.31(9)

C12	C11	C16	117.51(18)	O2T	S1T	O1T	114.11(9)
C16	C11	C4	119.27(17)	O2T	S1T	C1T	104.07(9)
C13	C12	C11	120.9(2)	O3T	S1T	O1T	113.88(9)
C14	C13	C12	120.6(2)	O3T	S1T	O2T	116.88(9)
C13	C14	C15	119.24(19)	O3T	S1T	C1T	104.09(9)
C14	C15	C16	120.3(2)	S1T	O1T	Fe1	136.70(8)
C15	C16	C11	121.4(2)	F1T	C1T	S1T	111.09(14)
C18	C17	C4	119.02(18)	F2T	C1T	S1T	111.02(14)
C22	C17	C4	122.60(17)	F2T	C1T	F1T	107.67(16)
C22	C17	C18	118.35(19)	F2T	C1T	F3T	107.87(16)
C19	C18	C17	121.3(2)	F3T	C1T	S1T	111.19(13)
C18	C19	C20	120.0(2)	F3T	C1T	F1T	107.85(17)
C21	C20	C19	119.4(2)	C2S	O1S	C3S	115.3(2)
C20	C21	C22	121.0(2)	O1S	C2S	C1S	112.6(2)
C17	C22	C21	120.0(2)	O1S	C3S	C4S	113.4(3)
C1A	N1A	Fe1	121.76(13)				

[1]1-X,1-Y,2-Z

Table S6. Torsion Angles for $[Fe(TrIm)_4(OTf)_2]$ (**1**).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Fe1	N1	C1	N2	-177.03(12)	N2A	C4A	C17A	C18A	-78.0(2)
Fe1	N1	C2	C3	176.77(13)	N2A	C4A	C17A	C22A	100.6(2)
Fe1	N1A	C1A	N2A	-172.88(12)	C1A	N1A	C2A	C3A	0.2(2)
Fe1	N1A	C2A	C3A	171.75(14)	C1A	N2A	C3A	C2A	0.0(2)
N1	C2	C3	N2	-0.2(2)	C1A	N2A	C4A	C5A	138.07(18)
N2	C4	C5	C6	-130.97(18)	C1A	N2A	C4A	C11A	-99.9(2)
N2	C4	C5	C10	49.3(2)	C1A	N2A	C4A	C17A	18.0(2)
N2	C4	C11	C12	-104.2(2)	C2A	N1A	C1A	N2A	-0.2(2)
N2	C4	C11	C16	76.8(2)	C3A	N2A	C1A	N1A	0.1(2)
N2	C4	C17	C18	-163.55(17)	C3A	N2A	C4A	C5A	-45.0(2)
N2	C4	C17	C22	18.5(2)	C3A	N2A	C4A	C11A	77.1(2)
C1	N1	C2	C3	0.5(2)	C3A	N2A	C4A	C17A	-165.07(17)
C1	N2	C3	C2	-0.1(2)	C4A	N2A	C1A	N1A	177.58(16)
C1	N2	C4	C5	35.0(2)	C4A	N2A	C3A	C2A	-177.52(17)
C1	N2	C4	C11	156.16(17)	C4A	C5A	C6A	C7A	-175.84(18)
C1	N2	C4	C17	-85.2(2)	C4A	C5A	C10A	C9A	176.04(17)
C2	N1	C1	N2	-0.6(2)	C4A	C11A	C12A	C13A	179.5(2)
C3	N2	C1	N1	0.5(2)	C4A	C11A	C16A	C15A	-179.49(19)
C3	N2	C4	C5	-155.72(18)	C4A	C17A	C18A	C19A	176.89(18)
C3	N2	C4	C11	-34.6(2)	C4A	C17A	C22A	C21A	-177.54(19)
C3	N2	C4	C17	84.0(2)	C5A	C4A	C11A	C12A	107.6(2)

C4	N2	C1	N1	171.71(16)	C5A	C4A	C11A	C16A	-74.1(2)
C4	N2	C3	C2	-171.02(17)	C5A	C4A	C17A	C18A	165.55(17)
C4	C5	C6	C7	-178.88(18)	C5A	C4A	C17A	C22A	-15.8(3)
C4	C5	C10	C9	179.14(18)	C5A	C6A	C7A	C8A	-0.8(3)
C4	C11	C12	C13	179.90(18)	C6A	C5A	C10A	C9A	-2.2(3)
C4	C11	C16	C15	-179.46(18)	C6A	C7A	C8A	C9A	-1.1(3)
C4	C17	C18	C19	-177.49(19)	C7A	C8A	C9A	C10A	1.4(3)
C4	C17	C22	C21	177.85(19)	C8A	C9A	C10A	C5A	0.3(3)
C5	C4	C11	C12	13.6(2)	C10A	C5A	C6A	C7A	2.5(3)
C5	C4	C11	C16	-165.46(17)	C11A	C4A	C5A	C6A	-163.85(17)
C5	C4	C17	C18	78.8(2)	C11A	C4A	C5A	C10A	17.9(2)
C5	C4	C17	C22	-99.2(2)	C11A	C4A	C17A	C18A	40.6(2)
C5	C6	C7	C8	-0.5(3)	C11A	C4A	C17A	C22A	-140.75(19)
C6	C5	C10	C9	-0.6(3)	C11A	C12A	C13A	C14A	-0.6(4)
C6	C7	C8	C9	-0.2(3)	C12A	C11A	C16A	C15A	-1.1(3)
C7	C8	C9	C10	0.4(3)	C12A	C13A	C14A	C15A	-0.1(4)
C8	C9	C10	C5	0.0(3)	C13A	C14A	C15A	C16A	0.2(4)
C10	C5	C6	C7	0.9(3)	C14A	C15A	C16A	C11A	0.4(3)
C11	C4	C5	C6	110.5(2)	C16A	C11A	C12A	C13A	1.2(3)
C11	C4	C5	C10	-69.2(2)	C17A	C4A	C5A	C6A	73.4(2)
C11	C4	C17	C18	-45.5(2)	C17A	C4A	C5A	C10A	-104.9(2)
C11	C4	C17	C22	136.53(19)	C17A	C4A	C11A	C12A	-127.7(2)
C11	C12	C13	C14	0.1(3)	C17A	C4A	C11A	C16A	50.6(2)
C12	C11	C16	C15	1.4(3)	C17A	C18A	C19A	C20A	1.3(3)
C12	C13	C14	C15	0.5(3)	C18A	C17A	C22A	C21A	1.2(3)
C13	C14	C15	C16	-0.2(3)	C18A	C19A	C20A	C21A	0.1(4)
C14	C15	C16	C11	-0.8(3)	C19A	C20A	C21A	C22A	-0.8(4)
C16	C11	C12	C13	-1.0(3)	C20A	C21A	C22A	C17A	0.2(4)
C17	C4	C5	C6	-12.0(2)	C22A	C17A	C18A	C19A	-1.9(3)
C17	C4	C5	C10	168.28(16)	O1T	S1T	C1T	F1T	65.28(15)
C17	C4	C11	C12	137.20(19)	O1T	S1T	C1T	F2T	-174.94(13)
C17	C4	C11	C16	-41.9(2)	O1T	S1T	C1T	F3T	-54.84(15)
C17	C18	C19	C20	-0.8(3)	O2T	S1T	O1T	Fe1	40.17(15)
C18	C17	C22	C21	-0.1(3)	O2T	S1T	C1T	F1T	-176.06(13)
C18	C19	C20	C21	0.5(4)	O2T	S1T	C1T	F2T	-56.28(15)
C19	C20	C21	C22	-0.1(4)	O2T	S1T	C1T	F3T	63.82(15)
C20	C21	C22	C17	-0.1(3)	O3T	S1T	O1T	Fe1	-97.55(13)
C22	C17	C18	C19	0.6(3)	O3T	S1T	C1T	F1T	-53.14(16)
N1A	C2A	C3A	N2A	-0.1(2)	O3T	S1T	C1T	F2T	66.64(16)
N2A	C4A	C5A	C6A	-43.6(2)	O3T	S1T	C1T	F3T	-173.26(14)
N2A	C4A	C5A	C10A	138.13(17)	C1T	S1T	O1T	Fe1	151.34(12)
N2A	C4A	C11A	C12A	-10.7(3)	C2S	O1S	C3S	C4S	179.9(3)

N2A C4A C11A C16A 167.64(17) C3S O1S C2S C1S -175.9(3)

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for CF316a.

Atom	***x***	***y***	***z***	**U(eq)**
H1	5705	3626	8287	28
H2	6257	6598	9009	31
H3	7046	6072	7721	31
H6	7252	1933	7129	36
H7	5946	471	6327	48
H8	4017	557	5348	50
H9	3379	2121	5172	45
H10	4666	3588	5953	36
H12	5630	3642	4860	35
H13	5813	4475	3556	42
H14	7296	5774	4099	43
H15	8617	6223	5962	40
H16	8455	5386	7265	34
H18	8571	3197	6707	39
H19	10350	2822	7856	48
H20	11019	3143	9775	53
H21	9878	3811	10517	52
H22	8072	4174	9367	39
H1A	4207	6837	8740	28
H2A	2029	4667	8665	31
H3A	909	5927	7681	31
H6A	1758	6100	5980	34
H7A	307	5640	4192	38
H8A	-1193	6591	3540	38
H9A	-1249	7981	4722	37
H10A	214	8459	6520	31
H12A	1856	7490	9390	43
H13A	1478	8690	10545	60
H14A	1353	10334	10239	60
H15A	1605	10795	8775	48
H16A	1975	9603	7621	36
H18A	4099	8759	9156	36
H19A	5765	9409	9149	46
H20A	5910	9218	7505	52
H21A	4393	8378	5869	53
H22A	2740	7697	5874	39

H1SA	7503	7831	6882	112
H1SB	8124	8104	8205	112
H1SC	8844	7821	7551	112
H2SA	7781	9572	7529	68
H2SB	9123	9543	8129	68
H3SA	9462	10634	7091	66
H3SB	8139	10748	6520	66
H4SA	8048	10140	4809	156
H4SB	9392	10115	5410	156
H4SC	8899	11168	5424	156