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SUPPORTING
INFORMATION

Steric Control of Reactivity of Non-Heme Diiron(II) Model Complexes With Dioxygen: Isolation of a Strongly Coupled μ -Oxo Fe(II)Fe(III) Dimer

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Supporting Information

- Figure S-1.** Structure of $[\text{Fe}_2(\text{OH})(\text{O}_2\text{CCPh}_3)_2(\text{Me}_3\text{tacn})_2](\text{OTf})$ **1-Ph-OTf** showing 30% probability thermal ellipsoids and atom labeling scheme.
- Figure S-2.** Structure of $[\text{Fe}_2(\text{O})(\text{O}_2\text{CCPh}_3)_2(\text{Me}_3\text{tacn})_2](\text{OTf})$ **2-Ph-OTf** showing 30% probability thermal ellipsoids and labeling.
- Figure S-3.** Structure of $[\text{Fe}_2(\text{O})(\text{O}_2\text{CCPh}_3)_2(\text{Me}_3\text{tacn})_2](\text{OTf})$ **(3-Ph-OTf)** showing 30% probability thermal and atom labeling.
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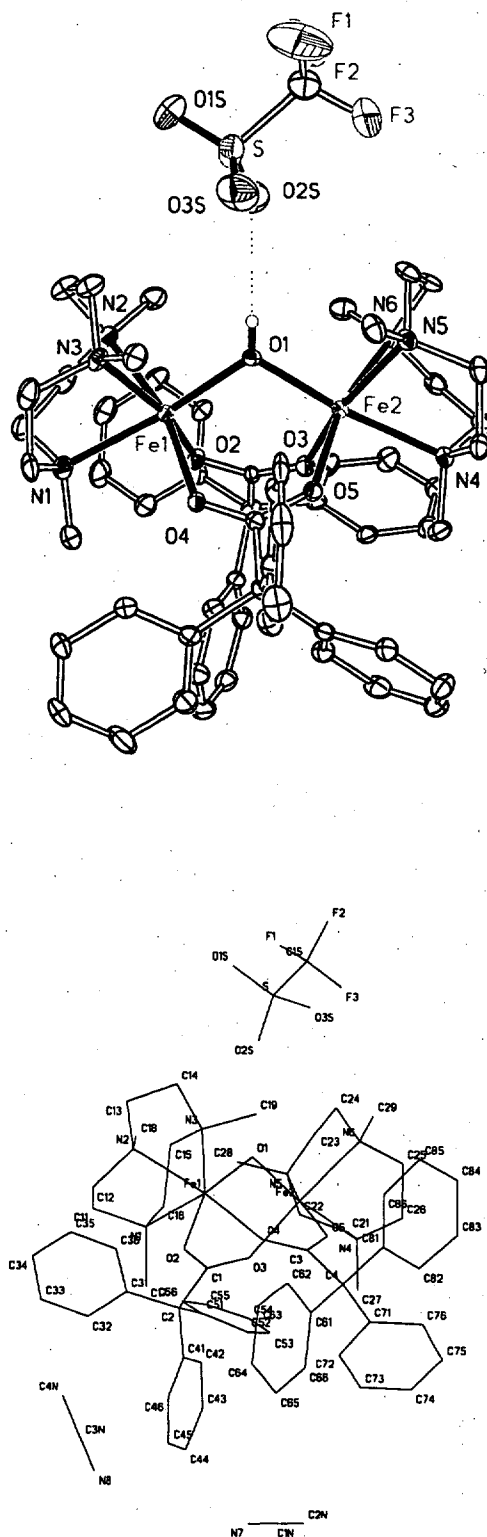


Figure S.1. 30% thermal ellipsoid plot and atom labeling diagram of 1-Ph-OTf

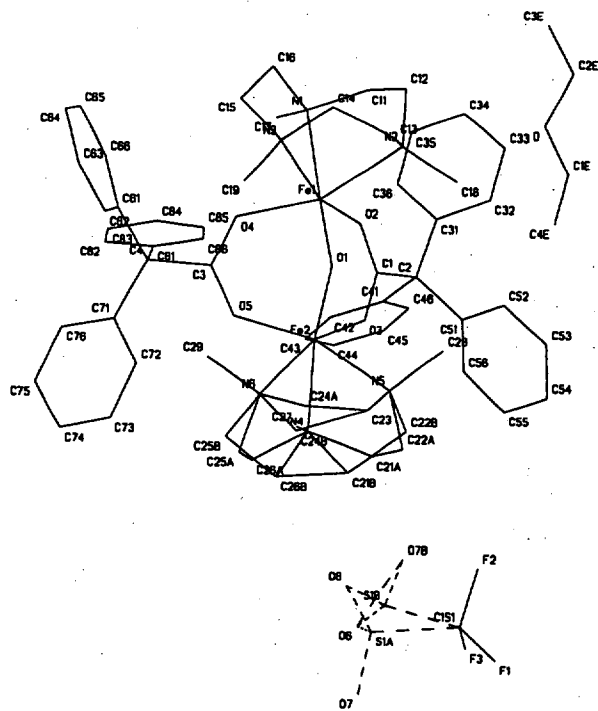
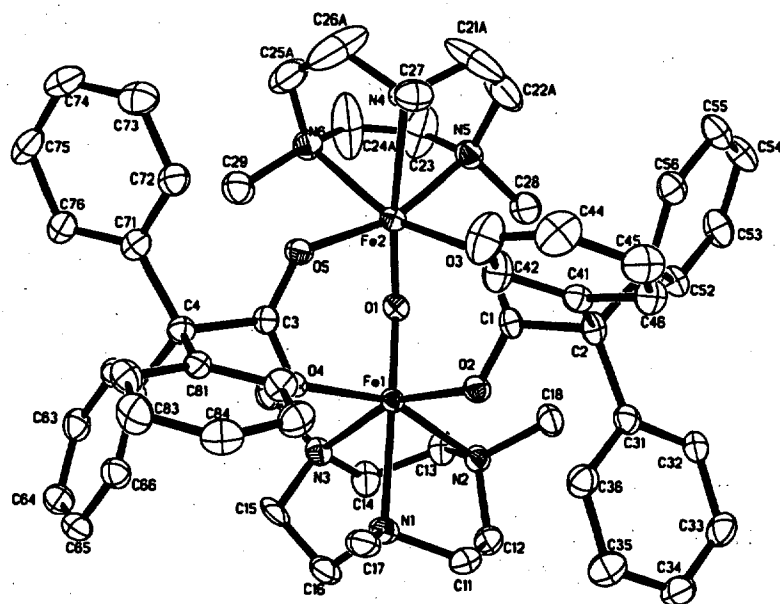


Figure S.2. 30% thermal ellipsoid plot and atom labeling diagram of 2-Ph-OTf

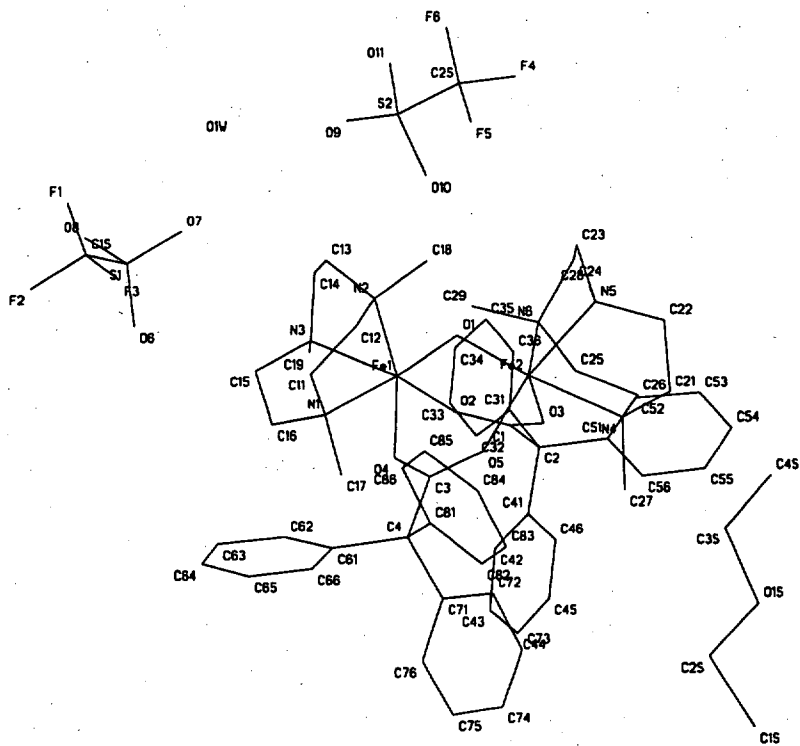
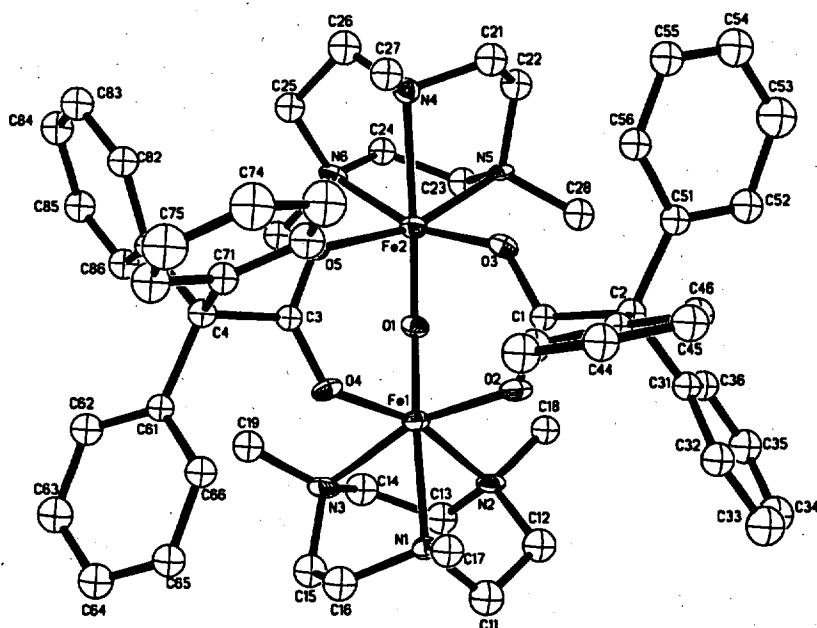


Figure S.3. 30% thermal ellipsoid plot and atom labeling diagram of 3-Ph-OTf

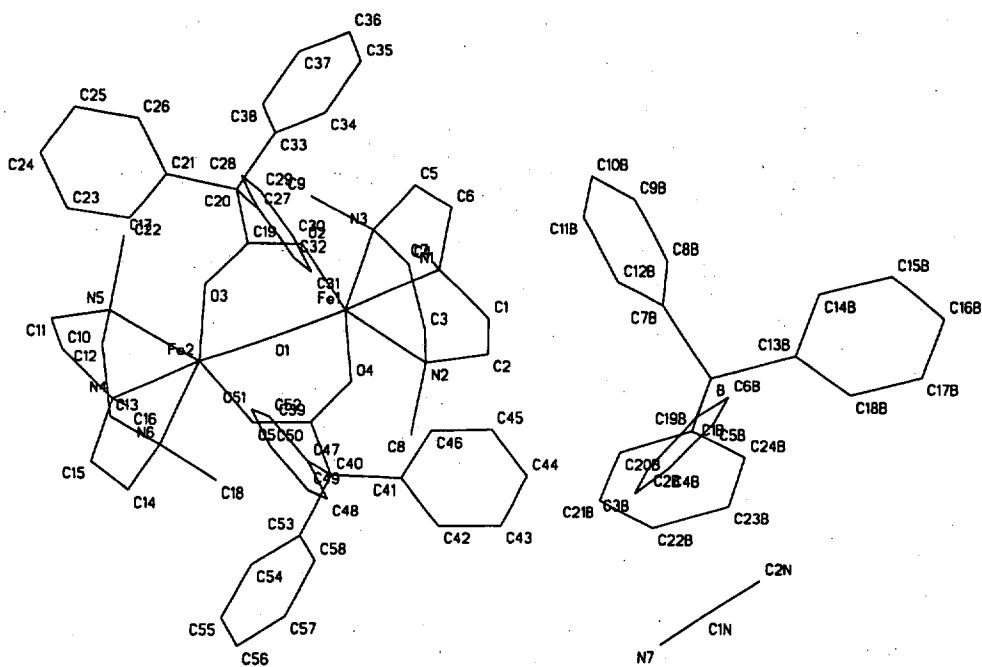


Figure S.5. 30% thermal ellipsoid plot and atom labeling diagram of 2-Ph-BPh₄

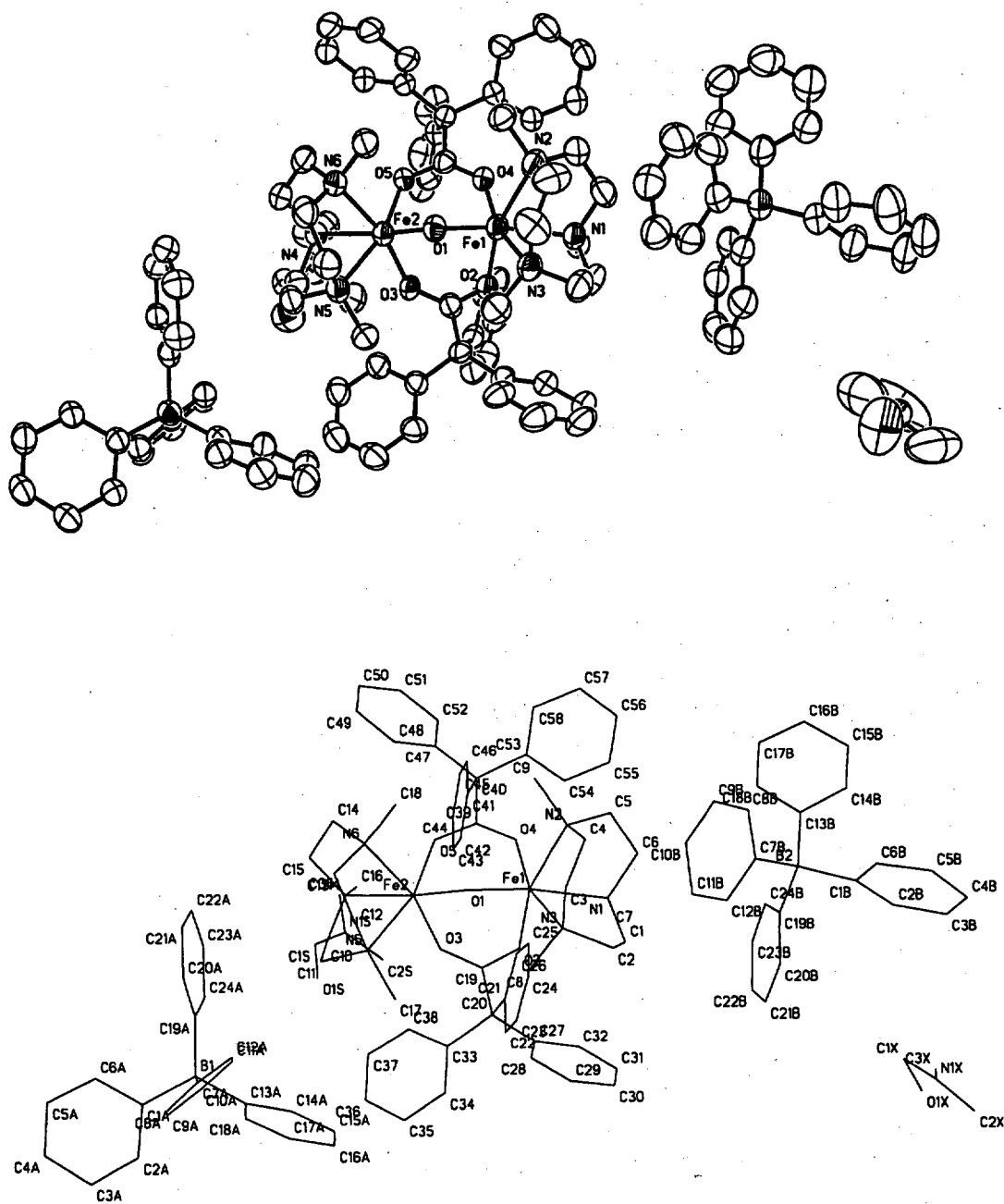


Figure S.6. 30% thermal ellipsoid plot and atom labeling diagram of 3-Ph-BPh₄

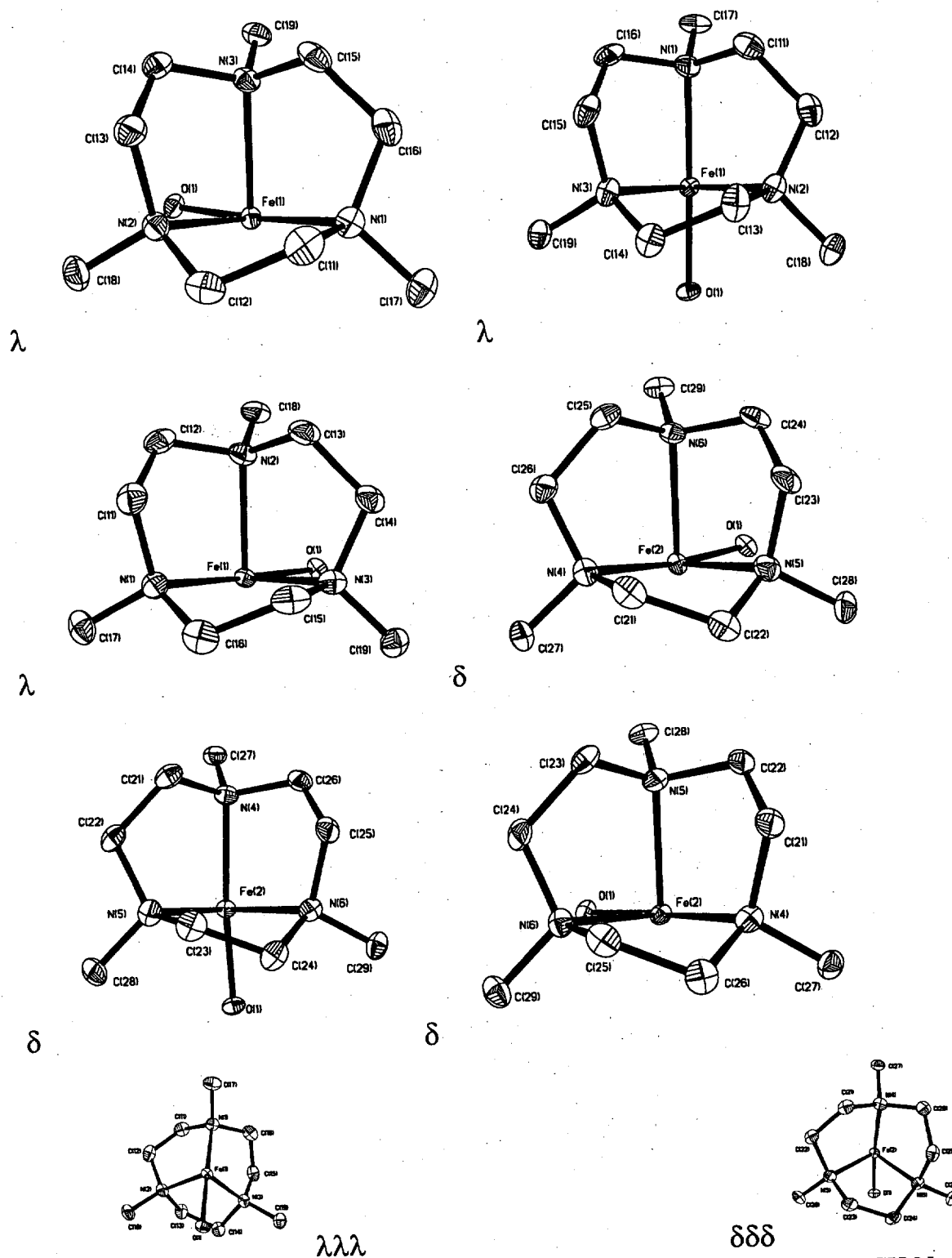


Figure S.7a. 30% thermal ellipsoid plots showing λ or δ configuration of NCH₂CH₂N groups of 1-Ph-OTf. The configuration of the five-membered ring is termed λ if the C-C bond slopes to the left when viewed down the N-Fe-N plane and δ if the C-C bond slopes to the right when viewed down the N-Fe-N plane.

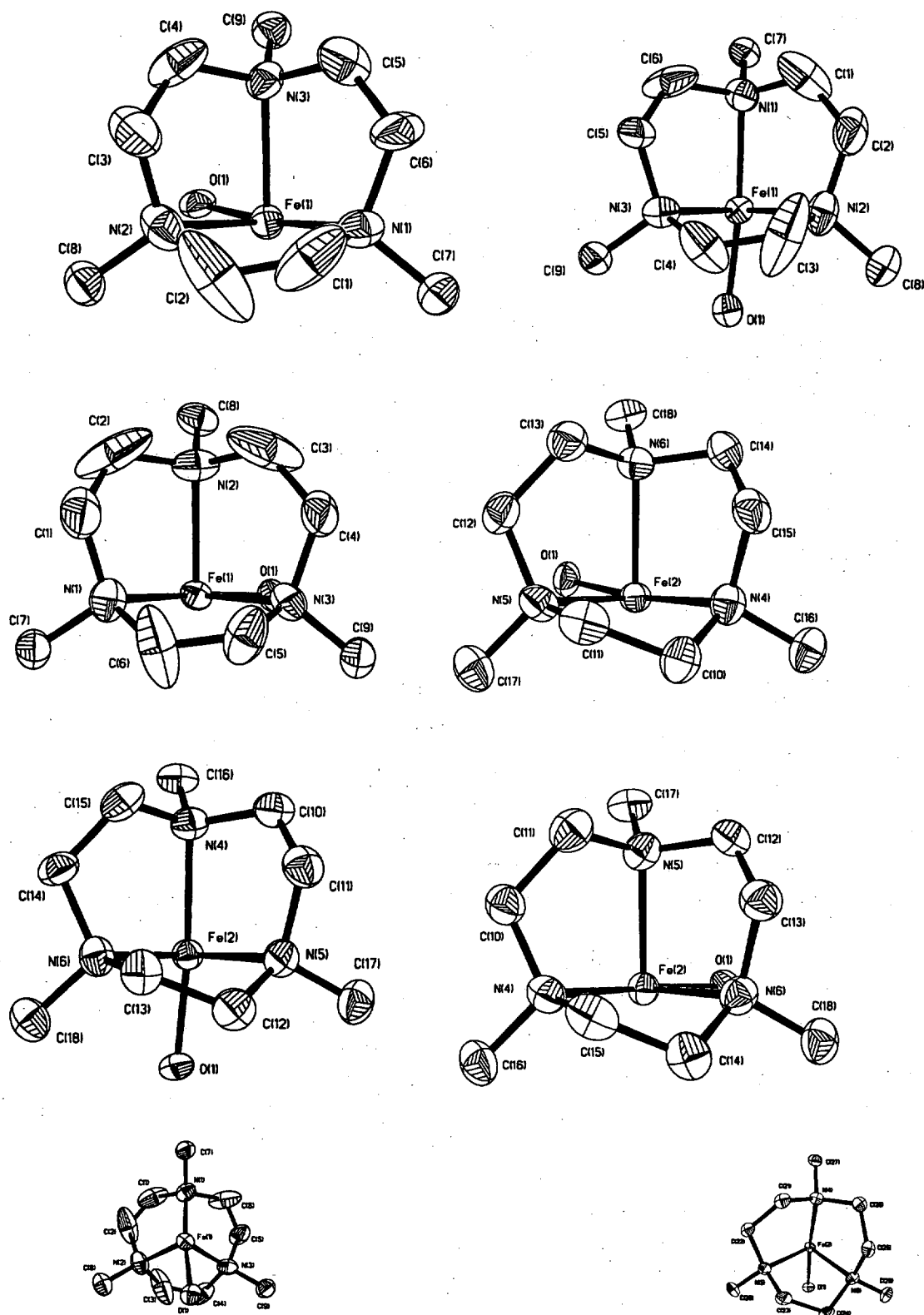


Figure S.7b. 30% thermal ellipsoid plots showing λ or δ configuration of NCH₂CH₂N groups of 1-Ph-BPh₄

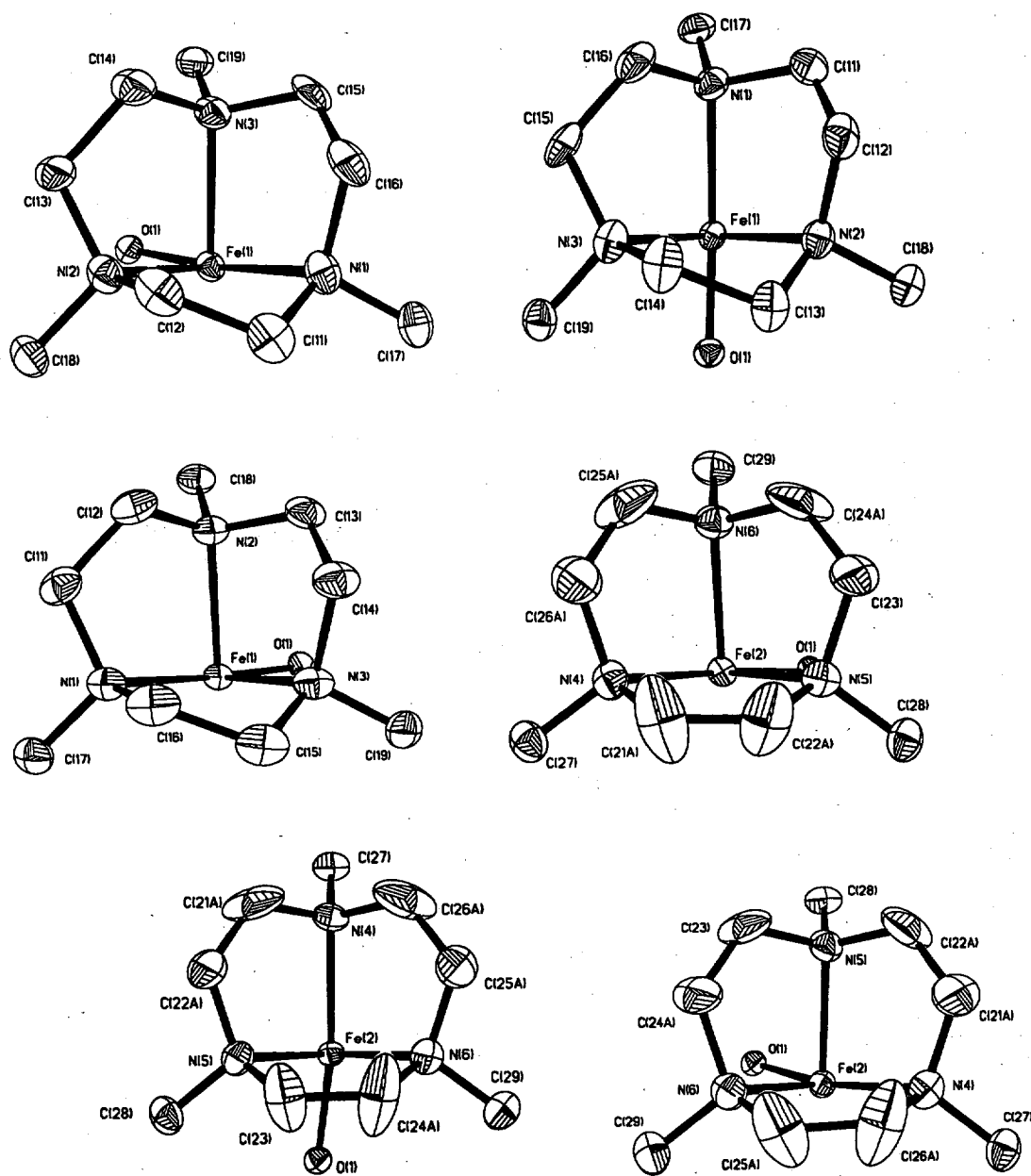


Figure S.7c. 30% thermal ellipsoid plots showing λ or δ configuration of NCH₂CH₂N groups of 2-Ph-OTf

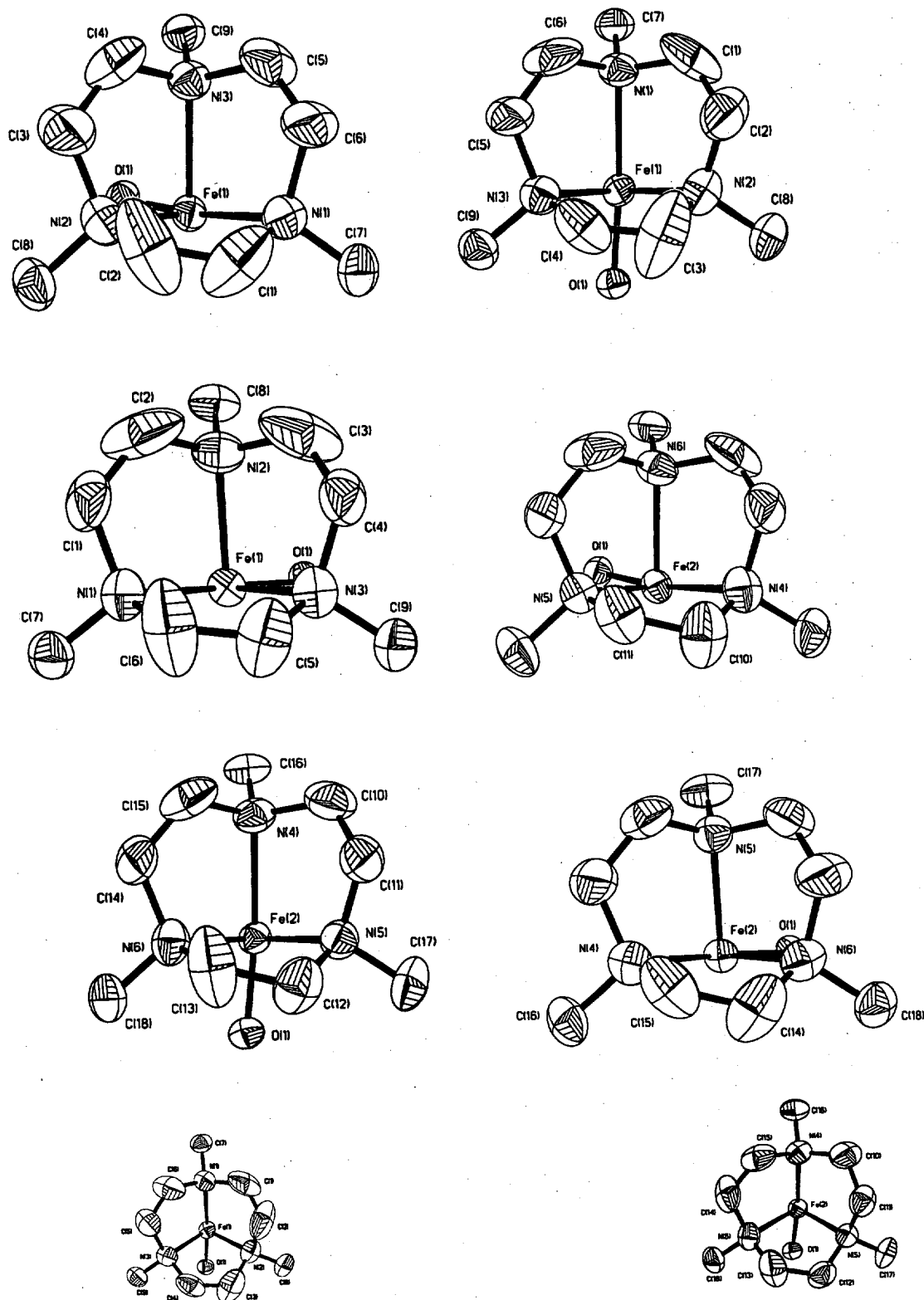


Figure S.7d. 30% thermal ellipsoid plots showing λ or δ configuration of $\text{NCH}_2\text{CH}_2\text{N}$ groups of 2-Ph-BPh₄

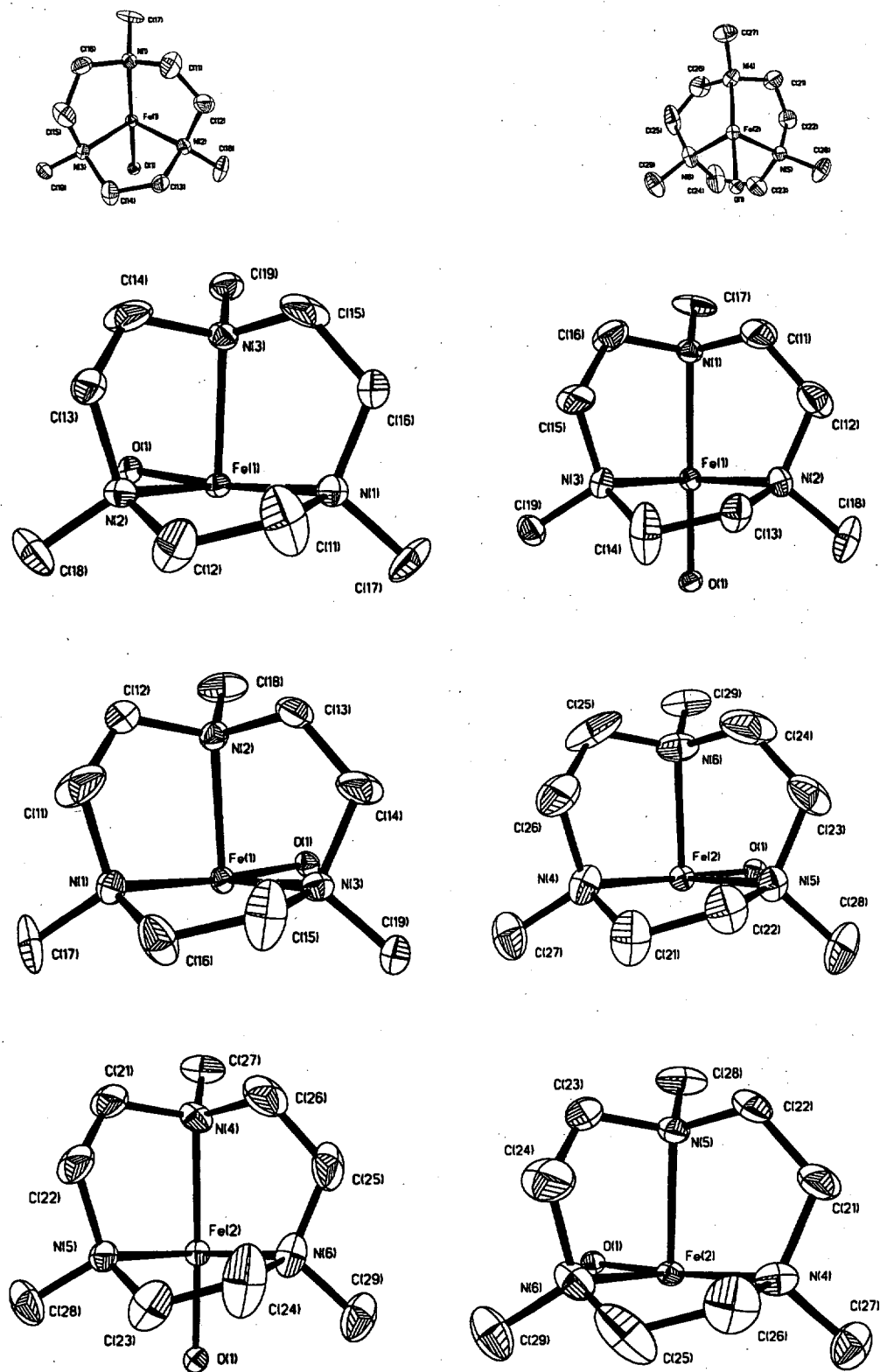


Figure S.7e. 30% thermal ellipsoid plots showing λ or δ configuration of NCH₂CH₂N groups of 2-Me-BPh₄

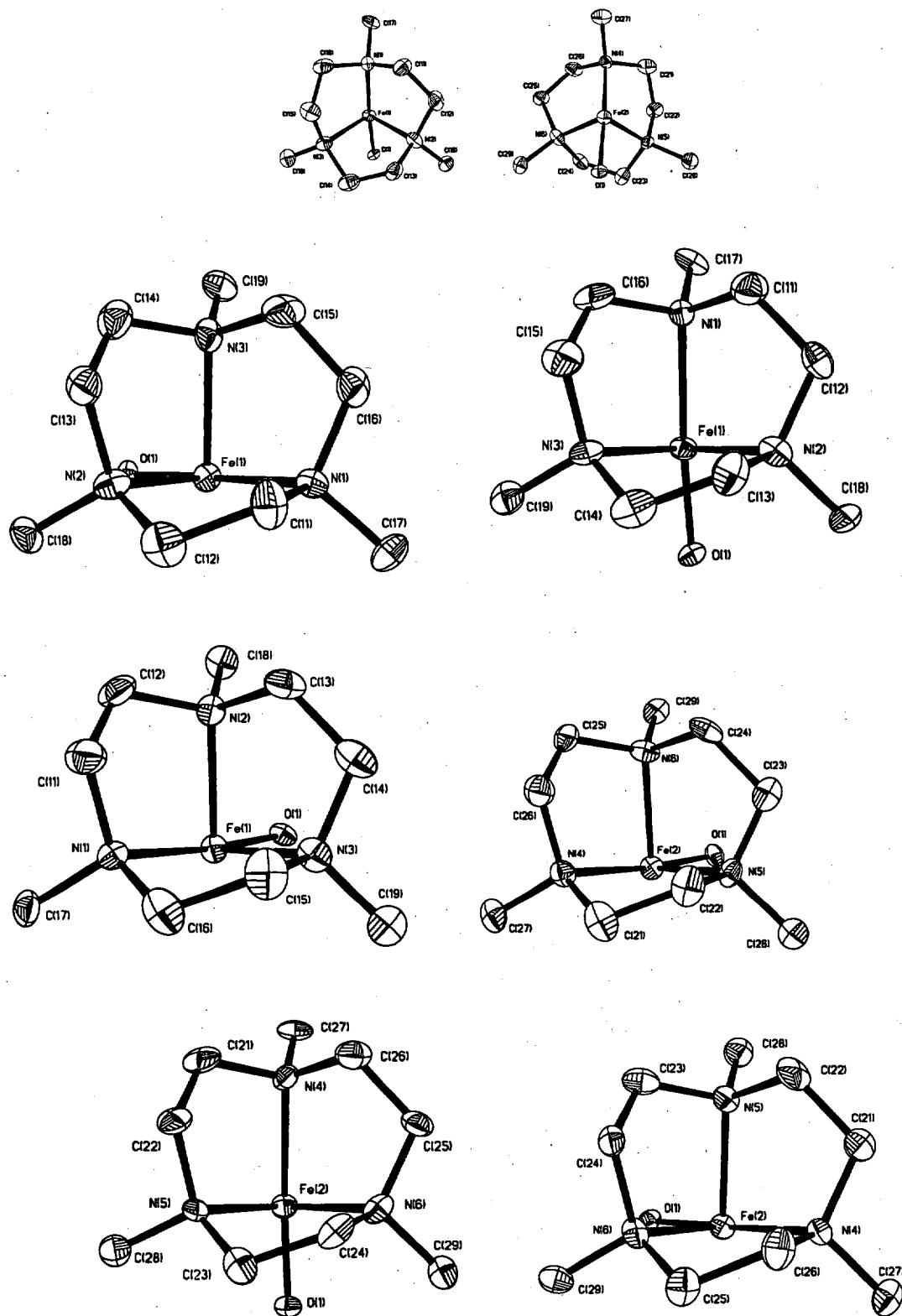


Figure S.7f. 30% thermal ellipsoid plots showing λ or δ configuration of NCH₂CH₂N groups of 3-Ph-OTf

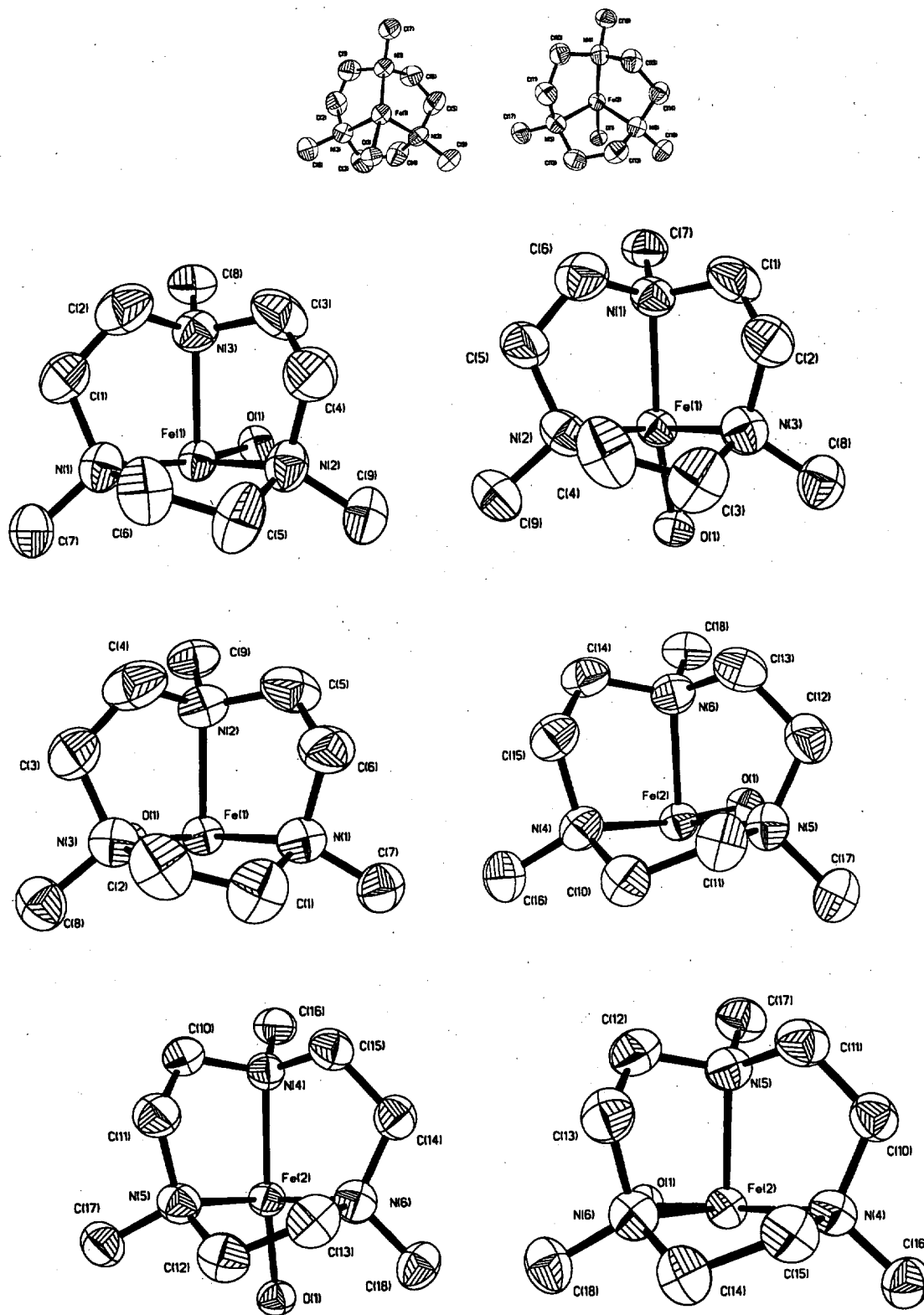


Figure S.7g. 30% thermal ellipsoid plots showing λ or δ configuration of NCH₂CH₂N groups of 3-Ph-BPh₄

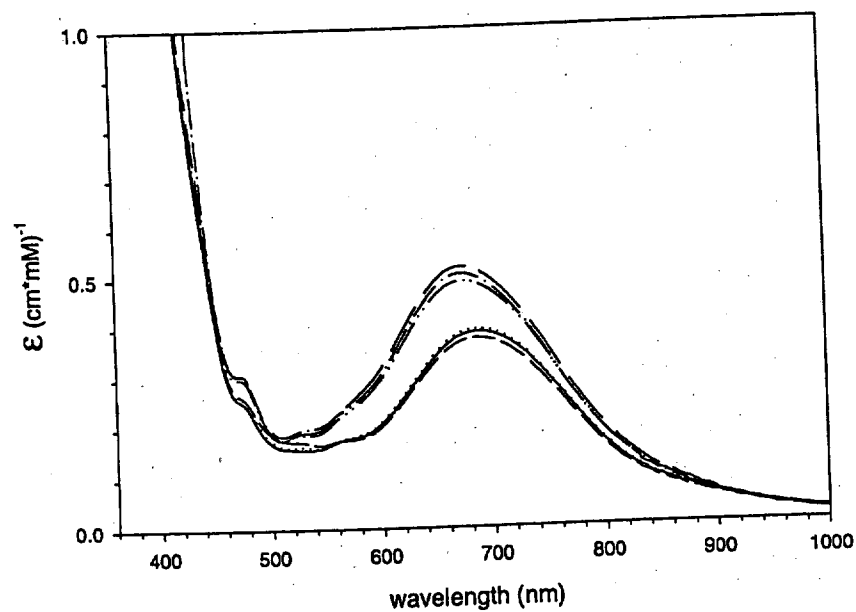


Figure S-8. Visible spectra of 2-Ph-OTf and 2-Me-OTf.
(2.0 mM in CH_3CN ; 2.0 mM in CH_2Cl_2 ; 2.0 mM in THF)

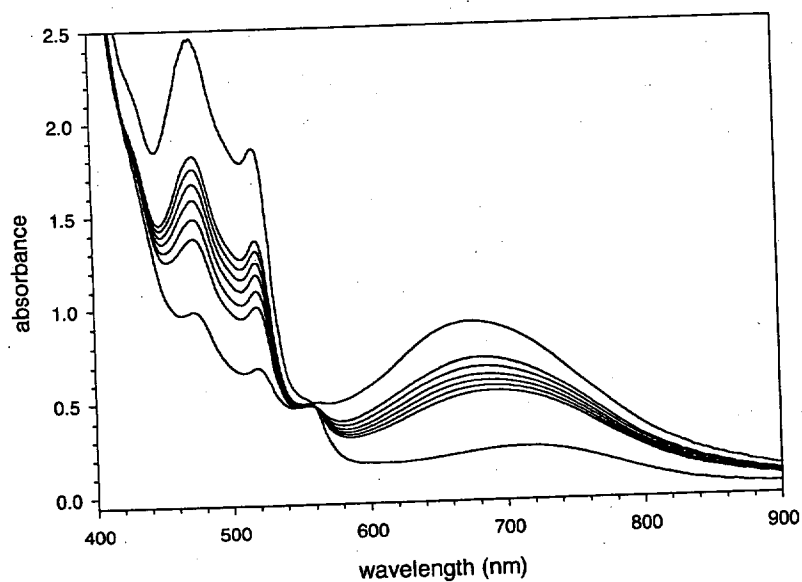
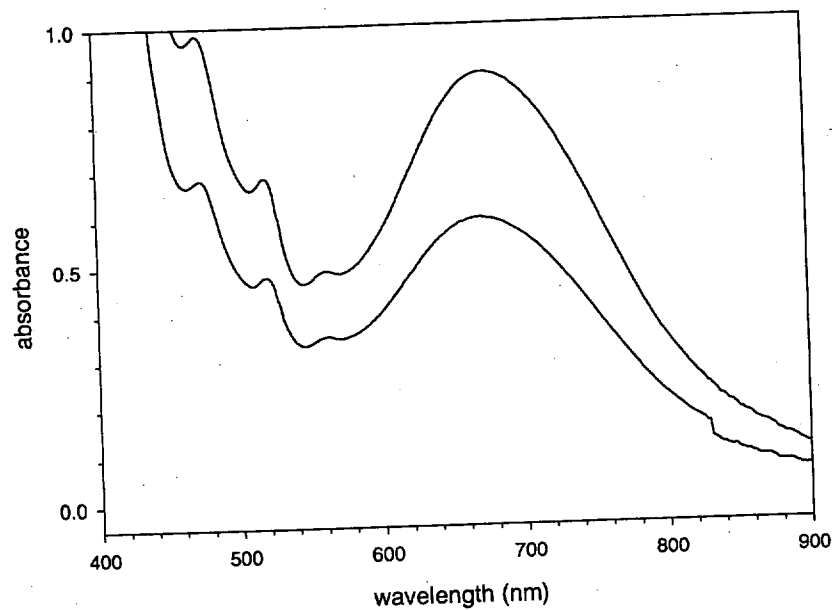


Figure S-9. Visible spectra of reaction of **1-Me-OTf** (2.0 mM in CH_3CN) with dioxygen. Top panel shows maximum formation of **2-Me-OTf** with spectra taken at 20 minute intervals. Bottom panel shows continuation of reaction; conversion of **2-Me-OTf** to **3-Me-OTf** with spectra taken at 10 minute intervals.

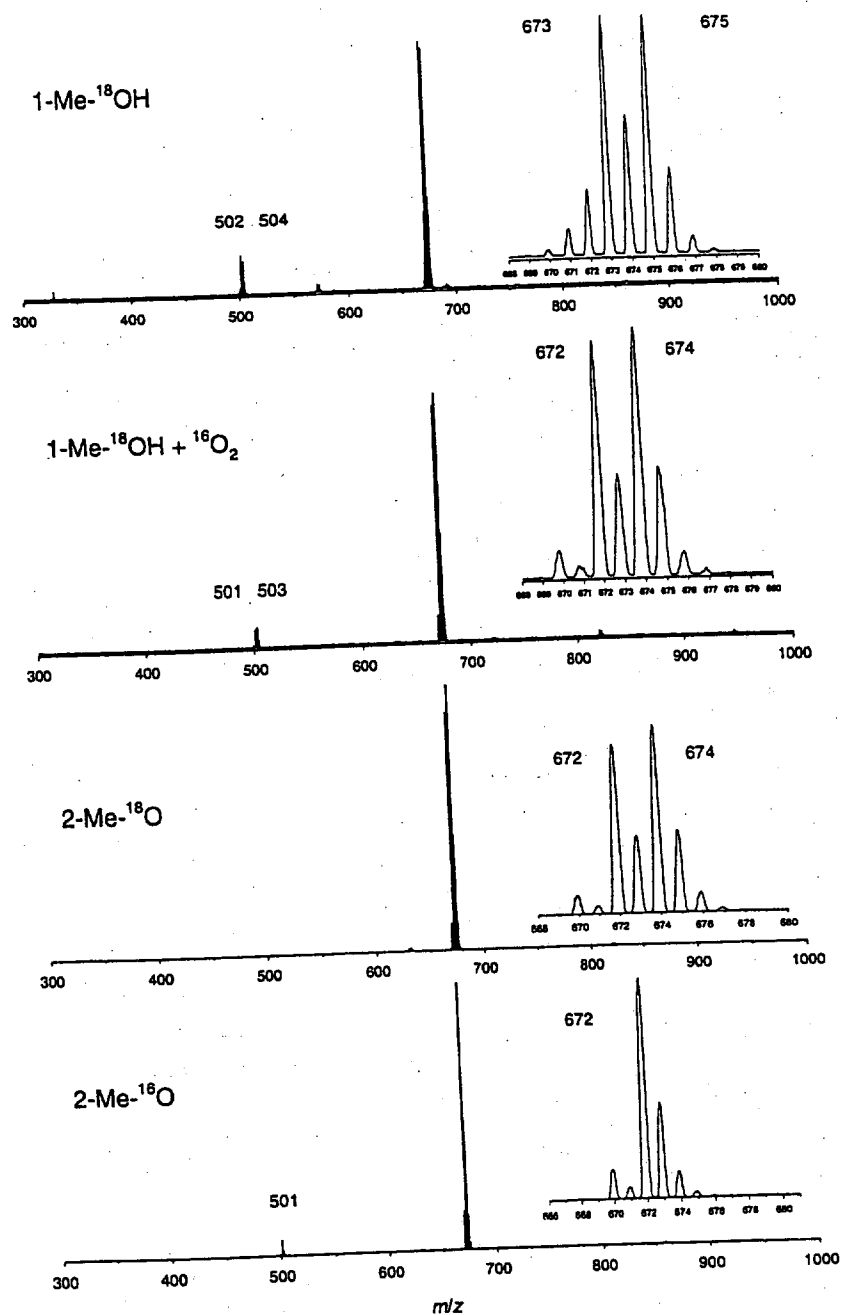


Figure S10.ESI-Mass Spectra of 20 μM solutions of 1-Me- ^{18}OH , 1-Me- $^{18}\text{OH} + ^{16}\text{O}_2$, 2-Me- ^{18}O , and 2-Me- ^{16}O .

Table S-1 . Crystal data and structure refinement for **1-Ph-OTf**.

Empirical formula	C ₆₃ H ₇₉ F ₃ Fe ₂ N ₈ O ₈ S
Formula weight	1277.10
Temperature	173(2) K
Wavelength	Mo K α 0.71073 Å
Crystal system	Monoclinic
Space group, Z	P2(1)/c, 4
Unit cell dimensions	$a = 17.254(4)$ Å $b = 15.452(5)$ Å $c = 24.427(6)$ Å $\beta = 106.280(10)$ deg.
Volume	6251(3) Å ³
Color of crystal	colorless
Density (calculated)	1.357 g/cm ³
Absorption coefficient	0.567 mm ⁻¹
F(000)	2688
Crystal size	0.42 x 0.50 x 0.52 mm
2 θ range for data collection	2.5 to 45 deg.
Limiting indices	$-1 \leq h \leq 18$, $-1 \leq k \leq 16$, $-26 \leq l \leq 25$
Reflections collected	10041
Independent reflections	8151 [$R_{\text{(int)}} = 0.0496$]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.5362 and 0.4884
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8149 / 0 / 769
Goodness-of-fit on F ²	1.038
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0604$, $wR_2 = 0.1609$
R indices (all data)	$R_1 = 0.0834$, $wR_2 = 0.1847$
Largest diff. peak and hole	0.766 and -0.563 e.Å ⁻³

Table S-2. Refined Atom Coordinates ($\times 10^4$) and Temperature Factors ($\text{\AA}^2 \times 10^3$) for **1-OTf**.

	x	y	z	U(eq)
Fe(1)	3263(1)	6353(1)	768(1)	21(1)
Fe(2)	3463(1)	8551(1)	814(1)	21(1)
N(1)	2651(3)	5089(3)	390(2)	31(1)
N(2)	3301(3)	5571(3)	1564(2)	31(1)
N(3)	4340(3)	5474(3)	848(2)	29(1)
N(4)	3138(3)	9907(3)	479(2)	28(1)
N(5)	3458(3)	9267(3)	1618(2)	32(1)
N(6)	4704(2)	9243(3)	1043(2)	28(1)
O(1)	3885(2)	7398(2)	1137(2)	26(1)
O(2)	2105(2)	6813(2)	750(1)	26(1)
O(3)	2205(2)	8238(2)	685(1)	27(1)
O(4)	3150(2)	6761(2)	-96(1)	26(1)
O(5)	3414(2)	8178(2)	-37(1)	26(1)
C(11)	2500(4)	4538(4)	853(2)	41(2)
C(12)	2549(4)	5056(4)	1385(2)	40(1)
C(13)	4036(3)	5024(4)	1739(2)	42(2)
C(14)	4676(3)	5343(4)	1472(2)	38(1)
C(16)	4087(4)	4653(4)	555(2)	40(1)
C(16)	3264(4)	4698(4)	135(2)	40(1)
C(17)	1896(4)	5223(4)	-59(3)	43(2)
C(18)	3270(4)	6163(4)	2031(2)	41(2)
C(19)	4934(3)	5917(4)	622(2)	37(1)
C(21)	2963(3)	10461(4)	932(2)	35(1)
C(22)	2818(3)	9927(3)	1408(2)	32(1)
C(23)	4257(3)	9663(4)	1886(2)	38(1)
C(25)	4618(3)	10122(3)	785(2)	33(1)
C(24)	4918(3)	9277(4)	1668(2)	34(1)
C(26)	3851(3)	10202(3)	311(2)	34(1)
C(27)	2444(3)	9902(3)	-33(2)	32(1)
C(28)	3230(4)	8682(4)	2027(2)	40(1)
C(29)	5310(3)	8742(4)	859(2)	35(1)
C(1)	1826(3)	7562(3)	712(2)	18(1)
C(2)	904(3)	7627(3)	695(2)	23(1)
C(3)	3246(3)	7478(3)	-304(2)	20(1)
C(4)	3185(3)	7529(3)	-957(2)	22(1)
C(31)	763(3)	6923(3)	1101(2)	28(1)
C(32)	254(4)	6218(4)	915(2)	39(1)
C(33)	178(4)	5572(4)	1287(3)	48(2)
C(34)	620(4)	5604(4)	1856(3)	50(2)
C(35)	1125(4)	6301(4)	2043(3)	40(2)
C(36)	1196(3)	6939(4)	1672(2)	31(1)
C(41)	393(3)	7460(3)	78(2)	26(1)
C(42)	704(3)	7133(3)	-342(2)	31(1)
C(43)	216(4)	6957(4)	-883(2)	40(1)
C(44)	-604(4)	7091(4)	-1011(2)	42(2)
C(45)	-925(4)	7418(4)	-606(3)	39(2)
C(46)	-429(3)	7610(3)	-66(2)	33(1)
C(51)	723(3)	8549(3)	861(2)	26(1)
C(52)	770(3)	9222(3)	495(2)	28(1)
C(53)	697(3)	10076(3)	634(2)	33(1)
C(55)	437(4)	9625(4)	1491(3)	42(2)
C(54)	541(3)	10275(4)	1139(2)	38(1)
C(56)	533(3)	8766(4)	1358(2)	35(1)
C(61)	2780(3)	6717(3)	-1283(2)	24(1)

C(62)	3192(3)	5929(3)	-1178(2)	32(1)
C(63)	2900(4)	5187(4)	-1463(2)	39(1)
C(64)	2155(4)	5207(4)	-1868(3)	46(2)
C(65)	1737(4)	5964(4)	-1983(3)	53(2)
C(66)	2048(3)	6712(4)	-1697(2)	37(1)
C(71)	2697(3)	8355(3)	-1177(2)	23(1)
C(72)	1921(3)	8428(4)	-1122(2)	32(1)
C(73)	1449(3)	9154(4)	-1317(2)	39(2)
C(74)	1754(4)	9824(4)	-1563(2)	44(2)
C(75)	2525(4)	9774(4)	-1606(2)	44(2)
C(76)	2995(3)	9051(3)	-1416(2)	33(1)
C(81)	4044(3)	7570(3)	-1020(2)	24(1)
C(82)	4155(4)	7546(3)	-1568(2)	37(1)
C(83)	4910(4)	7556(4)	-1644(3)	44(2)
C(84)	5582(4)	7556(3)	-1182(3)	45(2)
C(85)	5489(3)	7570(3)	-643(3)	37(2)
C(86)	4725(3)	7573(3)	-560(2)	29(1)
N(7)	-411(4)	6553(5)	-2547(3)	72(2)
C(1N)	-468(4)	7258(6)	-2473(3)	53(2)
C(2N)	-542(5)	8187(5)	-2381(4)	78(2)
N(8)	-2466(4)	7595(4)	82(3)	71(2)
C(3N)	-2198(5)	7530(5)	549(4)	61(2)
C(4N)	-1813(8)	7415(9)	1149(4)	152(6)
S	6370(1)	6964(1)	2156(1)	53(1)
O(1S)	6555(5)	6209(4)	2461(3)	115(3)
O(2S)	5550(3)	7267(4)	2104(2)	76(2)
O(3S)	6539(4)	7024(4)	1620(2)	86(2)
C(1S)	6991(4)	7798(5)	2586(3)	50(2)
F(1)	6949(4)	7817(4)	3102(2)	127(2)
F(2)	7738(3)	7672(5)	2619(3)	148(3)
F(3)	6807(4)	8560(3)	2364(3)	119(2)

* $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S-3 . Bond lengths [Å] and Angles [deg] for **1-OTf**.

Fe(1)-O(1)	2.008(4)	C(31)-C(36)	1.386(7)
Fe(1)-O(2)	2.110(3)	C(31)-C(32)	1.392(8)
Fe(1)-O(4)	2.159(3)	C(32)-C(33)	1.380(8)
Fe(1)-N(3)	2.265(4)	C(33)-C(34)	1.387(9)
Fe(1)-N(2)	2.274(4)	C(34)-C(35)	1.379(9)
Fe(1)-N(1)	2.288(4)	C(35)-C(36)	1.367(8)
Fe(2)-O(1)	2.002(4)	C(41)-C(46)	1.382(8)
Fe(2)-O(5)	2.136(3)	C(41)-C(42)	1.380(8)
Fe(2)-O(3)	2.160(3)	C(42)-C(43)	1.380(8)
Fe(2)-N(5)	2.256(4)	C(43)-C(44)	1.376(9)
Fe(2)-N(4)	2.261(4)	C(44)-C(45)	1.358(9)
Fe(2)-N(6)	2.317(4)	C(45)-C(46)	1.389(8)
N(1)-C(17)	1.464(7)	C(51)-C(56)	1.383(7)
N(1)-C(11)	1.495(7)	C(51)-C(52)	1.389(7)
N(1)-C(16)	1.497(7)	C(52)-C(53)	1.377(7)
N(2)-C(18)	1.474(7)	C(53)-C(54)	1.368(8)
N(2)-C(12)	1.479(7)	C(55)-C(54)	1.366(8)
N(2)-C(13)	1.484(7)	C(55)-C(56)	1.388(8)
N(3)-C(16)	1.462(7)	C(61)-C(66)	1.379(7)
N(3)-C(19)	1.464(7)	C(61)-C(62)	1.397(7)
N(3)-C(14)	1.484(7)	C(62)-C(63)	1.362(8)
N(4)-C(27)	1.470(6)	C(63)-C(64)	1.385(8)
N(4)-C(26)	1.475(7)	C(64)-C(65)	1.362(9)
N(4)-C(21)	1.495(7)	C(65)-C(66)	1.379(8)
N(5)-C(28)	1.479(7)	C(71)-C(76)	1.391(7)
N(5)-C(23)	1.483(7)	C(71)-C(72)	1.388(7)
N(5)-C(22)	1.485(7)	C(72)-C(73)	1.390(8)
N(6)-C(29)	1.468(7)	C(73)-C(74)	1.374(9)
N(6)-C(24)	1.467(7)	C(74)-C(75)	1.366(9)
N(6)-C(25)	1.487(7)	C(75)-C(76)	1.382(8)
O(2)-C(1)	1.247(6)	C(81)-C(86)	1.379(7)
O(3)-C(1)	1.244(6)	C(81)-C(82)	1.403(8)
O(4)-C(3)	1.250(6)	C(82)-C(83)	1.368(9)
O(5)-C(3)	1.255(6)	C(83)-C(84)	1.372(9)
C(11)-C(12)	1.508(8)	C(84)-C(85)	1.370(9)
C(13)-C(14)	1.515(8)	C(85)-C(86)	1.389(8)
C(16)-C(16)	1.503(8)	N(7)-C(1N)	1.113(9)
C(21)-C(22)	1.502(8)	C(1N)-C(2N)	1.464(12)
C(23)-C(24)	1.512(8)	N(8)-C(3N)	1.109(10)
C(25)-C(26)	1.498(7)	C(3N)-C(4N)	1.439(14)
C(1)-C(2)	1.584(7)	S-O(1S)	1.373(6)
C(2)-C(51)	1.537(7)	S-O(3S)	1.424(6)
C(2)-C(31)	1.537(7)	S-O(2S)	1.460(5)
C(2)-C(41)	1.539(7)	S-C(1S)	1.811(7)
C(3)-C(4)	1.569(7)	C(1S)-F(1)	1.283(8)
C(4)-C(81)	1.535(7)	C(1S)-F(2)	1.283(8)
C(4)-C(71)	1.541(7)	C(1S)-F(3)	1.299(8)
C(4)-C(61)	1.544(7)		
O(1)-Fe(1)-O(2)	97.05(14)	O(4)-Fe(1)-N(2)	164.6(2)
O(1)-Fe(1)-O(4)	95.40(14)	N(3)-Fe(1)-N(2)	77.4(2)
O(2)-Fe(1)-O(4)	93.15(13)	O(1)-Fe(1)-N(1)	174.9(2)
O(1)-Fe(1)-N(3)	96.9(2)	O(2)-Fe(1)-N(1)	87.2(2)
O(2)-Fe(1)-N(3)	162.41(14)	O(4)-Fe(1)-N(1)	87.11(14)
O(4)-Fe(1)-N(3)	96.09(14)	N(3)-Fe(1)-N(1)	78.3(2)
O(1)-Fe(1)-N(2)	99.2(2)	N(2)-Fe(1)-N(1)	77.9(2)
O(2)-Fe(1)-N(2)	89.87(14)	O(1)-Fe(2)-O(5)	93.12(14)

O(1)-Fe(2)-O(3)	95.63(14)	N(3)-C(14)-C(13)	111.4(5)
O(5)-Fe(2)-O(3)	91.90(13)	N(3)-C(16)-C(16)	112.9(4)
O(1)-Fe(2)-N(5)	100.5(2)	C(16)-C(16)-N(1)	112.2(4)
O(5)-Fe(2)-N(5)	166.1(2)	N(4)-C(21)-C(22)	111.6(4)
O(3)-Fe(2)-N(5)	89.30(14)	N(5)-C(22)-C(21)	112.1(4)
O(1)-Fe(2)-N(4)	173.3(2)	N(5)-C(23)-C(24)	112.4(4)
O(5)-Fe(2)-N(4)	87.73(14)	N(6)-C(25)-C(26)	111.4(4)
O(3)-Fe(2)-N(4)	90.97(14)	N(6)-C(24)-C(23)	112.8(4)
N(5)-Fe(2)-N(4)	78.4(2)	N(4)-C(26)-C(25)	112.6(4)
O(1)-Fe(2)-N(6)	96.1(2)	O(3)-C(1)-O(2)	125.9(4)
O(5)-Fe(2)-N(6)	98.12(14)	O(3)-C(1)-C(2)	119.0(4)
O(3)-Fe(2)-N(6)	164.12(14)	O(2)-C(1)-C(2)	115.1(4)
N(5)-Fe(2)-N(6)	78.1(2)	C(51)-C(2)-C(31)	113.9(4)
N(4)-Fe(2)-N(6)	77.2(2)	C(51)-C(2)-C(41)	108.1(4)
C(17)-N(1)-C(11)	110.0(4)	C(31)-C(2)-C(41)	111.3(4)
C(17)-N(1)-C(16)	109.2(4)	C(51)-C(2)-C(1)	109.2(4)
C(11)-N(1)-C(16)	112.1(4)	C(31)-C(2)-C(1)	106.1(4)
C(17)-N(1)-Fe(1)	113.3(3)	C(41)-C(2)-C(1)	108.1(4)
C(11)-N(1)-Fe(1)	109.8(3)	O(4)-C(3)-O(5)	126.2(4)
C(16)-N(1)-Fe(1)	102.3(3)	O(4)-C(3)-C(4)	118.7(4)
C(18)-N(2)-C(12)	110.1(4)	O(5)-C(3)-C(4)	115.1(4)
C(18)-N(2)-C(13)	110.1(4)	C(81)-C(4)-C(71)	112.3(4)
C(12)-N(2)-C(13)	112.7(4)	C(81)-C(4)-C(61)	107.0(4)
C(18)-N(2)-Fe(1)	109.5(3)	C(71)-C(4)-C(61)	111.6(4)
C(12)-N(2)-Fe(1)	102.7(3)	C(81)-C(4)-C(3)	108.2(4)
C(13)-N(2)-Fe(1)	111.5(3)	C(71)-C(4)-C(3)	105.7(4)
C(16)-N(3)-C(19)	111.4(4)	C(61)-C(4)-C(3)	112.0(4)
C(16)-N(3)-C(14)	111.2(4)	C(36)-C(31)-C(32)	117.1(5)
C(19)-N(3)-C(14)	109.8(4)	C(36)-C(31)-C(2)	119.9(5)
C(16)-N(3)-Fe(1)	110.7(3)	C(32)-C(31)-C(2)	122.8(5)
C(19)-N(3)-Fe(1)	109.3(3)	C(33)-C(32)-C(31)	121.3(5)
C(14)-N(3)-Fe(1)	104.2(3)	C(32)-C(33)-C(34)	120.4(6)
C(27)-N(4)-C(26)	107.9(4)	C(35)-C(34)-C(33)	118.6(5)
C(27)-N(4)-C(21)	110.4(4)	C(36)-C(35)-C(34)	120.6(6)
C(26)-N(4)-C(21)	112.7(4)	C(35)-C(36)-C(31)	122.0(5)
C(27)-N(4)-Fe(2)	111.4(3)	C(46)-C(41)-C(42)	117.2(5)
C(26)-N(4)-Fe(2)	104.2(3)	C(46)-C(41)-C(2)	119.1(5)
C(21)-N(4)-Fe(2)	110.2(3)	C(42)-C(41)-C(2)	123.7(5)
C(28)-N(5)-C(23)	110.1(4)	C(43)-C(42)-C(41)	121.7(5)
C(28)-N(5)-C(22)	109.9(4)	C(42)-C(43)-C(44)	120.0(6)
C(23)-N(5)-C(22)	112.2(4)	C(45)-C(44)-C(43)	119.5(5)
C(28)-N(5)-Fe(2)	110.8(3)	C(44)-C(45)-C(46)	120.2(6)
C(23)-N(5)-Fe(2)	110.9(3)	C(41)-C(46)-C(45)	121.4(5)
C(22)-N(5)-Fe(2)	102.7(3)	C(56)-C(51)-C(52)	117.0(5)
C(29)-N(6)-C(24)	110.1(4)	C(56)-C(51)-C(2)	124.9(5)
C(29)-N(6)-C(25)	110.4(4)	C(52)-C(51)-C(2)	118.1(4)
C(24)-N(6)-C(25)	112.0(4)	C(53)-C(52)-C(51)	122.2(5)
C(29)-N(6)-Fe(2)	111.8(3)	C(54)-C(53)-C(52)	119.5(5)
C(24)-N(6)-Fe(2)	102.3(3)	C(54)-C(55)-C(56)	120.7(5)
C(25)-N(6)-Fe(2)	110.1(3)	C(55)-C(54)-C(53)	119.7(5)
Fe(2)-O(1)-Fe(1)	116.7(2)	C(51)-C(56)-C(55)	120.7(5)
C(1)-O(2)-Fe(1)	131.2(3)	C(66)-C(61)-C(62)	116.4(5)
C(1)-O(3)-Fe(2)	134.6(3)	C(66)-C(61)-C(4)	124.9(5)
C(3)-O(4)-Fe(1)	132.2(3)	C(62)-C(61)-C(4)	118.6(4)
C(3)-O(5)-Fe(2)	132.8(3)	C(63)-C(62)-C(61)	122.9(5)
N(1)-C(11)-C(12)	111.7(5)	C(62)-C(63)-C(64)	118.9(5)
N(2)-C(12)-C(11)	111.9(5)	C(65)-C(64)-C(63)	119.9(5)
N(2)-C(13)-C(14)	110.9(5)	C(64)-C(65)-C(66)	120.5(6)

C(61)-C(66)-C(65)	121.5(6)	C(81)-C(86)-C(85)	120.4(6)
C(76)-C(71)-C(72)	117.3(5)	N(7)-C(1N)-C(2N)	179.4(8)
C(76)-C(71)-C(4)	123.9(5)	N(8)-C(3N)-C(4N)	176.7(10)
C(72)-C(71)-C(4)	118.8(4)	O(1S)-S-O(3S)	118.5(4)
C(73)-C(72)-C(71)	121.4(5)	O(1S)-S-O(2S)	113.1(4)
C(74)-C(73)-C(72)	119.9(5)	O(3S)-S-O(2S)	110.0(4)
C(75)-C(74)-C(73)	119.4(5)	O(1S)-S-C(1S)	106.3(4)
C(74)-C(75)-C(76)	120.9(6)	O(3S)-S-C(1S)	104.3(3)
C(71)-C(76)-C(75)	120.9(5)	O(2S)-S-C(1S)	103.0(3)
C(86)-C(81)-C(82)	117.7(5)	F(1)-C(1S)-F(2)	105.9(7)
C(86)-C(81)-C(4)	122.9(5)	F(1)-C(1S)-F(3)	108.4(7)
C(82)-C(81)-C(4)	119.2(5)	F(2)-C(1S)-F(3)	106.7(7)
C(83)-C(82)-C(81)	121.2(6)	F(1)-C(1S)-S	113.6(5)
C(82)-C(83)-C(84)	120.4(6)	F(2)-C(1S)-S	110.4(6)
C(85)-C(84)-C(83)	119.3(5)	F(3)-C(1S)-S	111.5(5)
C(84)-C(85)-C(86)	120.8(6)		

Table S-4. Anisotropic Temperature Factors ($\text{\AA}^2 \times 10^3$) for **1-OTf**.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	25(1)	18(1)	19(1)	1(1)	5(1)	2(1)
Fe(2)	24(1)	18(1)	19(1)	-2(1)	3(1)	-1(1)
N(1)	34(3)	25(2)	34(3)	3(2)	8(2)	-4(2)
N(2)	37(3)	31(3)	25(2)	6(2)	8(2)	9(2)
N(3)	36(3)	22(2)	29(2)	5(2)	11(2)	10(2)
N(4)	34(3)	19(2)	27(2)	-2(2)	5(2)	-3(2)
N(5)	29(2)	39(3)	25(2)	-8(2)	5(2)	-2(2)
N(6)	24(2)	24(2)	33(2)	-4(2)	4(2)	-2(2)
O(1)	28(2)	22(2)	25(2)	-2(2)	0(2)	3(2)
O(2)	23(2)	21(2)	33(2)	2(2)	8(2)	5(2)
O(3)	19(2)	26(2)	33(2)	0(2)	4(2)	0(2)
O(4)	36(2)	18(2)	22(2)	1(2)	7(2)	0(2)
O(5)	39(2)	20(2)	17(2)	-1(2)	7(2)	0(2)
C(11)	44(4)	28(3)	50(4)	8(3)	11(3)	-3(3)
C(12)	44(4)	33(3)	47(4)	15(3)	21(3)	7(3)
C(13)	41(3)	50(4)	33(3)	13(3)	11(3)	17(3)
C(14)	37(3)	42(4)	34(3)	7(3)	7(3)	15(3)
C(16)	58(4)	27(3)	40(3)	3(3)	24(3)	13(3)
C(16)	58(4)	18(3)	43(3)	-8(3)	13(3)	0(3)
C(17)	46(4)	27(3)	48(4)	-3(3)	0(3)	-10(3)
C(18)	51(4)	48(4)	25(3)	3(3)	13(3)	5(3)
C(19)	37(3)	36(3)	41(3)	0(3)	16(3)	9(3)
C(21)	38(3)	27(3)	37(3)	-10(3)	6(3)	5(3)
C(22)	33(3)	30(3)	32(3)	-13(2)	6(2)	5(2)
C(23)	33(3)	47(4)	26(3)	-13(3)	-3(2)	-6(3)
C(25)	35(3)	24(3)	44(3)	-2(3)	16(3)	-8(2)
C(24)	22(3)	40(3)	34(3)	-11(3)	-2(2)	-5(2)
C(26)	38(3)	23(3)	41(3)	4(2)	12(3)	-4(2)
C(27)	37(3)	29(3)	28(3)	4(2)	6(2)	6(2)
C(28)	48(4)	50(4)	22(3)	-1(3)	12(3)	1(3)
C(29)	26(3)	33(3)	48(3)	-8(3)	13(3)	-4(2)
C(1)	25(3)	17(3)	12(2)	-1(2)	6(2)	-3(2)
C(2)	20(3)	25(3)	24(3)	3(2)	5(2)	2(2)
C(3)	19(3)	21(3)	21(3)	-3(2)	5(2)	3(2)
C(4)	24(3)	18(3)	21(3)	-5(2)	3(2)	0(2)
C(31)	26(3)	22(3)	35(3)	2(2)	9(2)	2(2)
C(32)	44(4)	37(3)	37(3)	6(3)	12(3)	-4(3)
C(33)	51(4)	36(4)	57(4)	14(3)	17(3)	-11(3)
C(34)	65(4)	38(4)	52(4)	18(3)	28(3)	3(3)
C(35)	45(4)	45(4)	35(3)	14(3)	17(3)	10(3)
C(36)	32(3)	33(3)	32(3)	6(2)	13(2)	7(2)
C(41)	23(3)	24(3)	27(3)	2(2)	1(2)	-3(2)
C(42)	37(3)	27(3)	26(3)	8(2)	3(2)	1(2)
C(43)	51(4)	38(3)	28(3)	-4(3)	7(3)	-3(3)
C(44)	41(4)	43(4)	31(3)	8(3)	-7(3)	-10(3)
C(45)	30(3)	37(3)	41(4)	9(3)	-3(3)	-3(3)
C(46)	30(3)	30(3)	40(3)	0(2)	10(3)	-2(2)
C(51)	22(3)	29(3)	26(3)	1(2)	3(2)	7(2)
C(52)	25(3)	30(3)	26(3)	4(2)	1(2)	5(2)
C(53)	30(3)	24(3)	39(3)	7(3)	3(2)	7(2)
C(55)	51(4)	39(4)	38(3)	-3(3)	17(3)	17(3)

C(54)	35(3)	31(3)	45(4)	-1(3)	6(3)	9(3)
C(56)	36(3)	36(3)	35(3)	8(3)	13(3)	11(3)
C(61)	29(3)	28(3)	16(2)	0(2)	9(2)	0(2)
C(62)	37(3)	28(3)	27(3)	1(2)	4(2)	1(3)
C(63)	55(4)	23(3)	36(3)	-11(3)	10(3)	0(3)
C(64)	55(4)	32(4)	46(4)	-17(3)	3(3)	-13(3)
C(65)	45(4)	48(4)	53(4)	-24(3)	-6(3)	-5(3)
C(66)	33(3)	34(3)	37(3)	-4(3)	0(3)	3(3)
C(71)	23(3)	25(3)	19(3)	-4(2)	1(2)	-1(2)
C(72)	33(3)	32(3)	30(3)	-1(2)	8(2)	2(2)
C(73)	30(3)	41(4)	40(3)	-11(3)	-1(3)	12(3)
C(74)	54(4)	30(3)	35(3)	-3(3)	-9(3)	14(3)
C(75)	69(5)	27(3)	33(3)	10(3)	9(3)	2(3)
C(76)	40(3)	28(3)	29(3)	0(2)	7(2)	-5(3)
C(81)	28(3)	16(3)	27(3)	-1(2)	8(2)	2(2)
C(82)	43(4)	36(3)	34(3)	-6(3)	18(3)	-3(3)
C(83)	53(4)	39(4)	52(4)	-5(3)	37(4)	-5(3)
C(84)	36(4)	20(3)	90(6)	-6(3)	38(4)	-2(3)
C(85)	30(3)	13(3)	67(4)	-1(3)	13(3)	-3(2)
C(86)	31(3)	14(3)	40(3)	-7(2)	8(3)	-1(2)
N(7)	81(5)	69(5)	69(4)	-12(4)	29(4)	9(4)
C(1N)	53(4)	69(5)	41(4)	-4(4)	19(3)	-11(4)
C(2N)	95(6)	68(5)	80(6)	-17(5)	39(5)	-18(5)
N(8)	51(4)	71(5)	82(5)	9(4)	7(4)	-5(3)
C(3N)	48(4)	63(5)	72(6)	-10(4)	15(4)	-9(4)
C(4N)	122(10)	258(19)	67(7)	-7(8)	13(6)	-27(10)
S	72(1)	35(1)	53(1)	1(1)	22(1)	4(1)
O(1S)	152(6)	61(4)	96(5)	39(3)	-24(4)	0(4)
O(2S)	52(3)	79(4)	91(4)	-4(3)	10(3)	4(3)
O(3S)	108(5)	96(5)	56(3)	-15(3)	24(3)	0(4)
C(1S)	44(4)	59(5)	48(4)	-1(3)	14(3)	-1(3)
F(1)	182(6)	143(5)	71(4)	-50(4)	60(4)	-64(5)
F(2)	47(3)	243(9)	142(6)	-41(5)	7(3)	-6(4)
F(3)	147(5)	57(3)	121(5)	1(3)	-13(4)	-33(3)

*The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

Table S-5. Calculated Hydrogen coordinates($\times 10^4$) and Temperature Factors ($\text{\AA}^2 \times 10^3$) for **1-OTf**.

	x	y	z	U(eq)
H(1)	4236(42)	7367(45)	1353(30)	50
H(11A)	2904(4)	4066(4)	945(2)	49
H(11B)	1959(4)	4271(4)	717(2)	49
H(12A)	2078(4)	5450(4)	1314(2)	47
H(12B)	2525(4)	4658(4)	1697(2)	47
H(13A)	3894(3)	4418(4)	1621(2)	50
H(13B)	4253(3)	5035(4)	2160(2)	50
H(14A)	4901(3)	5896(4)	1652(2)	46
H(14B)	5121(3)	4916(4)	1542(2)	46
H(16A)	4086(4)	4200(4)	842(2)	47
H(16B)	4485(4)	4480(4)	352(2)	47
H(16C)	3089(4)	4106(4)	-1(2)	48
H(16D)	3294(4)	5046(4)	-198(2)	48
H(17A)	2000(4)	5585(4)	-361(3)	65
H(17B)	1504(4)	5511(4)	101(3)	65
H(17C)	1680(4)	4663(4)	-220(3)	65
H(18A)	3771(4)	6499(4)	2147(2)	61
H(18B)	3209(4)	5826(4)	2356(2)	61
H(18C)	2810(4)	6556(4)	1900(2)	61
H(19A)	5089(3)	6465(4)	825(2)	55
H(19B)	4698(3)	6034(4)	215(2)	55
H(19C)	5412(3)	5550(4)	674(2)	55
H(21A)	2481(3)	10821(4)	762(2)	42
H(21B)	3425(3)	10855(4)	1089(2)	42
H(22A)	2796(3)	10312(3)	1727(2)	39
H(22B)	2288(3)	9633(3)	1271(2)	39
H(23A)	4394(3)	9581(4)	2305(2)	45
H(23B)	4225(3)	10293(4)	1810(2)	45
H(25A)	5083(3)	10241(3)	634(2)	40
H(25B)	4620(3)	10558(3)	1082(2)	40
H(24A)	5415(3)	9626(4)	1810(2)	41
H(24B)	5035(3)	8684(4)	1821(2)	41
H(26A)	3773(3)	10815(3)	190(2)	40
H(26B)	3899(3)	9857(3)	-19(2)	40
H(27A)	1961(3)	9707(3)	68(2)	48
H(27B)	2554(3)	9509(3)	-317(2)	48
H(27C)	2354(3)	10488(3)	-192(2)	48
H(28A)	2701(4)	8424(4)	1845(2)	59
H(28B)	3202(4)	9012(4)	2363(2)	59
H(28C)	3635(4)	8223(4)	2142(2)	59
H(29A)	5162(3)	8723(4)	442(2)	53
H(29B)	5332(3)	8152(4)	1010(2)	53
H(29C)	5840(3)	9017(4)	1005(2)	53
H(32A)	-46(4)	6182(4)	525(2)	47
H(33A)	-180(4)	5103(4)	1152(3)	57
H(34A)	577(4)	5156(4)	2112(3)	59
H(35A)	1427(4)	6337(4)	2432(3)	48
H(36A)	1552(3)	7408(4)	1811(2)	37
H(42A)	1267(3)	7025(3)	-257(2)	37
H(43A)	446(4)	6744(4)	-1168(2)	48
H(44A)	-943(4)	6955(4)	-1380(2)	50

H(45A)	-1490(4)	7515(4)	-693(3)	46
H(46A)	-660(3)	7850(3)	210(2)	40
H(52A)	855(3)	9088(3)	137(2)	33
H(53A)	755(3)	10523(3)	382(2)	39
H(55A)	298(4)	9763(4)	1830(3)	50
H(54A)	504(3)	10862(4)	1244(2)	46
H(56A)	468(3)	8322(4)	1611(2)	42
H(62A)	3699(3)	5910(3)	-896(2)	38
H(63A)	3202(4)	4665(4)	-1385(2)	46
H(64A)	1937(4)	4694(4)	-2066(3)	56
H(65A)	1228(4)	5977(4)	-2263(3)	63
H(66A)	1752(3)	7236(4)	-1788(2)	44
H(72A)	1707(3)	7971(4)	-947(2)	38
H(73A)	916(3)	9187(4)	-1280(2)	47
H(74A)	1431(4)	10319(4)	-1701(2)	53
H(75A)	2741(4)	10242(4)	-1768(2)	53
H(76A)	3530(3)	9030(3)	-1450(2)	39
H(82A)	3696(4)	7522(3)	-1891(2)	44
H(83A)	4970(4)	7564(4)	-2019(3)	52
H(84A)	6107(4)	7546(3)	-1236(3)	54
H(85A)	5953(3)	7578(3)	-323(3)	44
H(86A)	4671(3)	7578(3)	-183(2)	35
H(2NA)	-500(5)	8511(5)	-2707(4)	94
H(2NB)	-126(5)	8376(5)	-2052(4)	94
H(2NC)	-1084(5)	8267(5)	-2320(4)	94
H(4NB)	-1662(8)	6818(9)	1211(4)	182
H(4NC)	-2181(8)	7549(9)	1368(4)	182
H(4NA)	-1342(8)	7775(9)	1272(4)	182

Table S-6 . Crystal data and structure refinement for 2-Ph-OTf.

Empirical formula	C ₆₃ H ₆₇ F ₃ Fe ₂ N ₆ O ₉ S
Formula weight	1252.99
Temperature	173(2) K
Wavelength	Mo K α 0.71073 Å
Crystal system	Orthorhombic
Space group, Z	Pbca, 8
Unit cell dimensions	$a = 20.7008(3)$ Å $b = 19.61610(10)$ Å $c = 30.3179(5)$ Å
Volume	12311.2(3) Å ³
Color	dark green
Density (calculated)	1.352 g/cm ³
Absorption coefficient	0.575 mm ⁻¹
F(000)	5232
Crystal size	0.50 x 0.19 x 0.12 mm
2 θ range for data collection	2.7 to 48.3°
Limiting indices	$-23 \leq h \leq 16$, $-22 \leq k \leq 22$, $-27 \leq l \leq 34$
Reflections collected	47851
Independent reflections	9750 [$R_{\text{int}} = 0.0680$]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.7720 and 0.7163
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9750 / 0 / 802
Goodness-of-fit on F ²	1.165
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0887$, $wR_2 = 0.2261$
R indices (all data)	$R_1 = 0.1087$, $wR_2 = 0.2409$
Largest diff. peak and hole	1.002 and -0.657 e.Å ⁻³

Table S-7. Refined Atom Coordinates ($\times 10^4$) and Temperature Factors ($\text{\AA}^2 \times 10^3$) for **2-OTf**.

	x	y	z	U(eq)
Fe(1)	-880(1)	8110(1)	743(1)	31(1)
Fe(2)	112(1)	7098(1)	1159(1)	32(1)
O(1)	-150(2)	7621(2)	685(1)	35(1)
O(2)	-1509(2)	7389(2)	1008(1)	34(1)
O(3)	-801(2)	6609(2)	1247(1)	36(1)
O(4)	-684(2)	8583(2)	1333(1)	35(1)
O(5)	-65(2)	7820(2)	1682(1)	37(1)
N(1)	-1774(3)	8813(3)	732(2)	43(1)
N(2)	-1296(3)	7934(3)	66(2)	41(1)
N(3)	-516(3)	9029(2)	384(2)	42(1)
N(4)	462(3)	6311(3)	1675(2)	47(1)
N(5)	529(3)	6267(3)	732(2)	44(1)
N(6)	1184(3)	7323(3)	1215(2)	48(1)
C(1)	-1361(3)	6809(3)	1154(2)	30(1)
C(2)	-1916(3)	6274(3)	1234(2)	33(1)
C(3)	-338(3)	8386(3)	1653(2)	32(1)
C(4)	-286(3)	8909(3)	2045(2)	34(1)
C(11)	-2229(3)	8459(4)	430(2)	51(2)
C(12)	-1925(3)	8285(4)	0(2)	52(2)
C(13)	-777(4)	8214(3)	-218(2)	51(2)
C(14)	-632(4)	8952(4)	-102(2)	57(2)
C(15)	-874(4)	9607(3)	574(2)	53(2)
C(16)	-1589(4)	9502(3)	561(2)	54(2)
C(17)	-2073(3)	8888(4)	1171(2)	52(2)
C(18)	-1372(4)	7199(3)	-21(2)	48(2)
C(19)	186(3)	9100(3)	470(2)	50(2)
C(21A)	432(17)	5625(9)	1409(7)	70(6)
C(22A)	675(17)	5636(9)	968(7)	70(6)
C(24A)	1433(13)	7034(13)	800(11)	104(11)
C(25A)	1485(11)	6990(12)	1587(11)	83(7)
C(26A)	1064(8)	6642(21)	1876(6)	90(8)
C(21B)	750(20)	5752(15)	1492(12)	38(9)
C(22B)	363(20)	5646(15)	1026(10)	28(8)
C(24B)	1670(25)	6940(37)	883(22)	116(24)
C(25B)	1291(17)	7147(16)	1715(9)	34(9)
C(26B)	1144(16)	6348(15)	1768(12)	40(9)
C(23)	1174(4)	6506(6)	590(3)	92(3)
C(27)	13(3)	6233(4)	2047(2)	53(2)
C(28)	118(4)	6171(4)	346(2)	55(2)
C(29)	1312(4)	8064(4)	1211(3)	60(2)
C(31)	-2553(3)	6522(3)	1027(2)	36(1)
C(32)	-2852(3)	6237(3)	662(2)	41(2)
C(33)	-3424(3)	6503(4)	489(2)	51(2)
C(34)	-3716(3)	7067(4)	688(2)	53(2)
C(35)	-3439(3)	7352(4)	1062(2)	51(2)
C(36)	-2868(3)	7084(3)	1227(2)	43(2)
C(41)	-2028(3)	6191(3)	1736(2)	34(1)
C(42)	-1679(3)	6532(4)	2050(2)	49(2)
C(43)	-1786(4)	6419(4)	2500(2)	65(2)
C(44)	-2249(4)	5950(4)	2631(2)	63(2)
C(45)	-2603(3)	5614(4)	2323(2)	53(2)
C(46)	-2501(3)	5737(3)	1878(2)	43(2)

C(51)	-1648(3)	5597(3)	1046(2)	36(1)
C(52)	-1546(3)	5526(3)	588(2)	42(2)
C(53)	-1277(4)	4938(3)	413(2)	53(2)
C(54)	-1095(4)	4408(3)	688(2)	55(2)
C(55)	-1161(3)	4479(3)	1136(2)	49(2)
C(56)	-1441(3)	5069(3)	1311(2)	41(2)
C(61)	-248(3)	9623(3)	1831(2)	36(1)
C(62)	292(3)	9799(3)	1573(2)	40(1)
C(63)	338(3)	10423(3)	1363(2)	46(2)
C(64)	-164(4)	10891(3)	1400(2)	52(2)
C(65)	-709(3)	10729(3)	1641(2)	49(2)
C(66)	-749(3)	10094(3)	1857(2)	42(2)
C(71)	297(3)	8742(3)	2346(2)	37(1)
C(72)	292(3)	8117(3)	2568(2)	43(2)
C(73)	807(4)	7917(4)	2834(2)	56(2)
C(74)	1339(3)	8346(4)	2881(2)	55(2)
C(75)	1338(3)	8975(4)	2677(2)	56(2)
C(76)	818(3)	9175(3)	2418(2)	46(2)
C(81)	-905(3)	8841(3)	2327(2)	34(1)
C(82)	-963(3)	9233(3)	2707(2)	44(2)
C(83)	-1514(3)	9208(4)	2970(2)	50(2)
C(84)	-2016(3)	8780(4)	2857(2)	49(2)
C(85)	-1953(3)	8366(3)	2491(2)	48(2)
C(86)	-1411(3)	8401(3)	2226(2)	40(1)
O(6)	3192(7)	5401(10)	754(6)	290(10)
S(1A)	2791(2)	5006(2)	1021(2)	66(1)
O(7)	3181(4)	4603(4)	1308(3)	94(3)
O(8)	2274(3)	5321(3)	1256(2)	80(2)
C(1S1)	2342(6)	4306(7)	705(3)	94(4)
F(1)	2712(6)	3993(5)	443(3)	215(6)
F(2)	1886(8)	4577(8)	479(4)	382(14)
F(3)	2145(5)	3876(5)	986(3)	164(3)
S(1B)	2642(8)	5126(9)	843(6)	82(5)
O(7B)	2494(12)	5447(12)	487(8)	67(8)
O	-786(9)	7383(7)	-1198(4)	111(6)
C(1E)	-436(10)	6936(10)	-1237(7)	79(6)
C(2E)	-1085(11)	7583(12)	-1514(5)	95(7)
C(3E)	-1720(9)	7983(13)	-1358(5)	95(7)
C(4E)	-221(11)	6626(19)	-976(7)	161(15)

* $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S-8 . Bond lengths [Å] and Angles [deg] for **2-OTf**.

Fe(1)-O(1)	1.800(4)	C(24B)-C(23)	1.60(5)
Fe(1)-O(4)	2.055(4)	C(25B)-C(26B)	1.60(4)
Fe(1)-O(2)	2.084(4)	C(31)-C(32)	1.386(8)
Fe(1)-N(3)	2.236(5)	C(31)-C(36)	1.417(9)
Fe(1)-N(2)	2.253(5)	C(32)-C(33)	1.395(9)
Fe(1)-N(1)	2.307(5)	C(33)-C(34)	1.396(10)
Fe(1)-Fe(2)	3.1227(11)	C(34)-C(35)	1.388(10)
Fe(2)-O(1)	1.847(4)	C(35)-C(36)	1.388(9)
Fe(2)-O(3)	2.135(4)	C(41)-C(42)	1.370(9)
Fe(2)-O(5)	2.157(4)	C(41)-C(46)	1.392(8)
Fe(2)-N(5)	2.254(5)	C(42)-C(43)	1.399(9)
Fe(2)-N(6)	2.270(5)	C(43)-C(44)	1.387(11)
Fe(2)-N(4)	2.314(5)	C(44)-C(45)	1.359(10)
O(2)-C(1)	1.259(7)	C(45)-C(46)	1.386(9)
O(3)-C(1)	1.255(7)	C(51)-C(56)	1.380(8)
O(4)-C(3)	1.269(7)	C(51)-C(52)	1.410(8)
O(5)-C(3)	1.249(7)	C(52)-C(53)	1.387(9)
N(1)-C(17)	1.474(8)	C(53)-C(54)	1.385(10)
N(1)-C(11)	1.486(8)	C(54)-C(55)	1.371(9)
N(1)-C(16)	1.498(8)	C(55)-C(56)	1.399(9)
N(2)-C(18)	1.476(8)	C(61)-C(66)	1.391(8)
N(2)-C(13)	1.482(8)	C(61)-C(62)	1.407(8)
N(2)-C(12)	1.485(8)	C(62)-C(63)	1.382(9)
N(3)-C(15)	1.473(8)	C(63)-C(64)	1.390(10)
N(3)-C(19)	1.483(8)	C(64)-C(65)	1.380(10)
N(3)-C(14)	1.499(8)	C(65)-C(66)	1.411(9)
N(4)-C(21B)	1.36(3)	C(71)-C(76)	1.389(9)
N(4)-C(26B)	1.44(3)	C(71)-C(72)	1.398(9)
N(4)-C(27)	1.471(8)	C(72)-C(73)	1.395(9)
N(4)-C(26A)	1.53(2)	C(73)-C(74)	1.393(11)
N(4)-C(21A)	1.57(2)	C(74)-C(75)	1.381(11)
N(5)-C(22A)	1.46(2)	C(75)-C(76)	1.389(9)
N(5)-C(28)	1.459(9)	C(81)-C(86)	1.391(8)
N(5)-C(23)	1.479(10)	C(81)-C(82)	1.391(8)
N(5)-C(22B)	1.55(3)	C(82)-C(83)	1.392(9)
N(6)-C(25A)	1.44(2)	C(83)-C(84)	1.379(10)
N(6)-C(29)	1.476(9)	C(84)-C(85)	1.381(9)
N(6)-C(24A)	1.47(2)	C(85)-C(86)	1.383(9)
N(6)-C(25B)	1.57(3)	O(6)-S(1B)	1.29(2)
N(6)-C(24B)	1.61(6)	O(6)-S(1A)	1.394(11)
C(1)-C(2)	1.575(7)	O(6)-O(7B)	1.66(3)
C(2)-C(31)	1.539(8)	S(1A)-O(8)	1.426(6)
C(2)-C(51)	1.548(8)	S(1A)-O(7)	1.428(9)
C(2)-C(41)	1.551(8)	S(1A)-C(1S1)	1.914(13)
C(3)-C(4)	1.574(8)	O(8)-S(1B)	1.52(2)
C(4)-C(81)	1.546(8)	C(1S1)-F(1)	1.263(11)
C(4)-C(61)	1.547(8)	C(1S1)-F(3)	1.266(13)
C(4)-C(71)	1.548(8)	C(1S1)-F(2)	1.281(12)
C(11)-C(12)	1.489(10)	C(1S1)-S(1B)	1.77(2)
C(13)-C(14)	1.520(9)	S(1B)-O(7B)	1.29(3)
C(15)-C(16)	1.494(10)	O-C(1E)	1.14(2)
C(21A)-C(22A)	1.43(3)	O-C(2E)	1.21(2)
C(24A)-C(23)	1.33(2)	C(1E)-C(4E)	1.09(3)
C(25A)-C(26A)	1.41(3)	C(1E)-C(2E)	2.03(3)
C(21B)-C(22B)	1.64(6)	C(2E)-C(3E)	1.60(3)
C(21B)-C(26B)	1.65(6)		

O(1)-Fe(1)-O(4)	99.2(2)	C(12)-N(2)-Fe(1)	112.7(4)
O(1)-Fe(1)-O(2)	101.5(2)	C(15)-N(3)-C(19)	110.5(5)
O(4)-Fe(1)-O(2)	95.4(2)	C(15)-N(3)-C(14)	112.4(5)
O(1)-Fe(1)-N(3)	95.7(2)	C(19)-N(3)-C(14)	109.9(5)
O(4)-Fe(1)-N(3)	89.6(2)	C(15)-N(3)-Fe(1)	105.1(4)
O(2)-Fe(1)-N(3)	161.0(2)	C(19)-N(3)-Fe(1)	108.7(4)
O(1)-Fe(1)-N(2)	98.6(2)	C(14)-N(3)-Fe(1)	110.1(4)
O(4)-Fe(1)-N(2)	159.6(2)	C(21B)-N(4)-C(26B)	72(3)
O(2)-Fe(1)-N(2)	90.5(2)	C(21B)-N(4)-C(27)	120.3(14)
N(3)-Fe(1)-N(2)	78.9(2)	C(26B)-N(4)-C(27)	118(2)
O(1)-Fe(1)-N(1)	172.3(2)	C(27)-N(4)-C(26A)	104.7(9)
O(4)-Fe(1)-N(1)	84.3(2)	C(27)-N(4)-C(21A)	106.2(10)
O(2)-Fe(1)-N(1)	84.8(2)	C(26A)-N(4)-C(21A)	127(3)
N(3)-Fe(1)-N(1)	77.4(2)	C(21B)-N(4)-Fe(2)	113.5(14)
N(2)-Fe(1)-N(1)	76.8(2)	C(26B)-N(4)-Fe(2)	113.9(13)
O(1)-Fe(1)-Fe(2)	31.56(12)	C(27)-N(4)-Fe(2)	113.0(4)
O(4)-Fe(1)-Fe(2)	78.78(11)	C(26A)-N(4)-Fe(2)	103.9(11)
O(2)-Fe(1)-Fe(2)	79.79(11)	C(21A)-N(4)-Fe(2)	102.3(8)
N(3)-Fe(1)-Fe(2)	119.18(14)	C(22A)-N(5)-C(28)	113.8(10)
N(2)-Fe(1)-Fe(2)	121.49(13)	C(22A)-N(5)-C(23)	103(2)
N(1)-Fe(1)-Fe(2)	155.88(13)	C(28)-N(5)-C(23)	109.5(6)
O(1)-Fe(2)-O(3)	95.0(2)	C(28)-N(5)-C(22B)	103.3(14)
O(1)-Fe(2)-O(5)	99.2(2)	C(23)-N(5)-C(22B)	128(2)
O(3)-Fe(2)-O(5)	93.1(2)	C(22A)-N(5)-Fe(2)	114.2(11)
O(1)-Fe(2)-N(5)	93.8(2)	C(28)-N(5)-Fe(2)	109.3(4)
O(3)-Fe(2)-N(5)	94.9(2)	C(23)-N(5)-Fe(2)	106.5(5)
O(5)-Fe(2)-N(5)	164.2(2)	C(22B)-N(5)-Fe(2)	98.8(12)
O(1)-Fe(2)-N(6)	103.7(2)	C(25A)-N(6)-C(29)	112.0(10)
O(3)-Fe(2)-N(6)	160.6(2)	C(25A)-N(6)-C(24A)	110.0(14)
O(5)-Fe(2)-N(6)	89.1(2)	C(29)-N(6)-C(24A)	108.0(11)
N(5)-Fe(2)-N(6)	79.0(2)	C(29)-N(6)-C(25B)	101.5(12)
O(1)-Fe(2)-N(4)	171.1(2)	C(29)-N(6)-C(24B)	110(3)
O(3)-Fe(2)-N(4)	83.9(2)	C(25B)-N(6)-C(24B)	114(3)
O(5)-Fe(2)-N(4)	89.7(2)	C(25A)-N(6)-Fe(2)	113.0(10)
N(5)-Fe(2)-N(4)	77.6(2)	C(29)-N(6)-Fe(2)	111.4(4)
N(6)-Fe(2)-N(4)	76.9(2)	C(24A)-N(6)-Fe(2)	101.8(11)
O(1)-Fe(2)-Fe(1)	30.67(12)	C(25B)-N(6)-Fe(2)	99.6(13)
O(3)-Fe(2)-Fe(1)	75.77(10)	C(24B)-N(6)-Fe(2)	118(2)
O(5)-Fe(2)-Fe(1)	76.62(10)	O(3)-C(1)-O(2)	125.8(5)
N(5)-Fe(2)-Fe(1)	118.64(14)	O(3)-C(1)-C(2)	115.7(5)
N(6)-Fe(2)-Fe(1)	123.3(2)	O(2)-C(1)-C(2)	118.5(5)
N(4)-Fe(2)-Fe(1)	154.63(14)	C(31)-C(2)-C(51)	115.4(5)
Fe(1)-O(1)-Fe(2)	117.8(2)	C(31)-C(2)-C(41)	107.8(5)
C(1)-O(2)-Fe(1)	126.7(4)	C(51)-C(2)-C(41)	109.0(5)
C(1)-O(3)-Fe(2)	130.5(4)	C(31)-C(2)-C(1)	110.6(4)
C(3)-O(4)-Fe(1)	129.8(4)	C(51)-C(2)-C(1)	104.7(4)
C(3)-O(5)-Fe(2)	127.5(4)	C(41)-C(2)-C(1)	109.2(4)
C(17)-N(1)-C(11)	109.7(5)	O(5)-C(3)-O(4)	125.5(5)
C(17)-N(1)-C(16)	109.3(5)	O(5)-C(3)-C(4)	119.7(5)
C(11)-N(1)-C(16)	111.7(5)	O(4)-C(3)-C(4)	114.7(5)
C(17)-N(1)-Fe(1)	112.5(4)	C(81)-C(4)-C(61)	110.6(5)
C(11)-N(1)-Fe(1)	103.8(4)	C(81)-C(4)-C(71)	107.7(5)
C(16)-N(1)-Fe(1)	109.8(4)	C(61)-C(4)-C(71)	113.6(5)
C(18)-N(2)-C(13)	109.6(5)	C(81)-C(4)-C(3)	107.7(5)
C(18)-N(2)-C(12)	109.6(5)	C(61)-C(4)-C(3)	106.0(4)
C(13)-N(2)-C(12)	112.7(5)	C(71)-C(4)-C(3)	111.1(5)
C(18)-N(2)-Fe(1)	110.7(4)	N(1)-C(11)-C(12)	112.2(6)
C(13)-N(2)-Fe(1)	101.2(4)	N(2)-C(12)-C(11)	111.1(5)

N(2)-C(13)-C(14)	111.2(6)	C(65)-C(64)-C(63)	120.1(6)
N(3)-C(14)-C(13)	110.8(5)	C(64)-C(65)-C(66)	119.8(6)
N(3)-C(15)-C(16)	112.4(5)	C(61)-C(66)-C(65)	121.0(6)
C(15)-C(16)-N(1)	111.7(5)	C(76)-C(71)-C(72)	117.9(6)
C(22A)-C(21A)-N(4)	117(2)	C(76)-C(71)-C(4)	124.6(6)
N(5)-C(22A)-C(21A)	114(2)	C(72)-C(71)-C(4)	117.5(5)
C(23)-C(24A)-N(6)	124.6(12)	C(73)-C(72)-C(71)	121.3(6)
C(26A)-C(25A)-N(6)	116(2)	C(74)-C(73)-C(72)	119.6(7)
C(25A)-C(26A)-N(4)	117(2)	C(75)-C(74)-C(73)	119.5(6)
N(4)-C(21B)-C(22B)	104(3)	C(74)-C(75)-C(76)	120.5(7)
N(4)-C(21B)-C(26B)	56(2)	C(75)-C(76)-C(71)	121.2(7)
C(22B)-C(21B)-C(26B)	140(2)	C(86)-C(81)-C(82)	117.4(6)
N(5)-C(22B)-C(21B)	107(3)	C(86)-C(81)-C(4)	123.8(5)
C(23)-C(24B)-N(6)	101(3)	C(82)-C(81)-C(4)	118.8(5)
N(6)-C(25B)-C(26B)	107(2)	C(83)-C(82)-C(81)	121.7(6)
N(4)-C(26B)-C(25B)	103(3)	C(84)-C(83)-C(82)	119.8(6)
N(4)-C(26B)-C(21B)	52(2)	C(85)-C(84)-C(83)	119.1(6)
C(25B)-C(26B)-C(21B)	137(3)	C(84)-C(85)-C(86)	121.0(6)
C(24A)-C(23)-N(5)	118.1(10)	C(85)-C(86)-C(81)	120.9(6)
N(5)-C(23)-C(24B)	126(3)	S(1B)-O(6)-O(7B)	49.8(13)
C(32)-C(31)-C(36)	116.8(6)	O(6)-S(1A)-O(8)	119.7(9)
C(32)-C(31)-C(2)	125.5(5)	O(6)-S(1A)-O(7)	109.0(8)
C(36)-C(31)-C(2)	117.7(5)	O(8)-S(1A)-O(7)	111.1(6)
C(31)-C(32)-C(33)	121.9(6)	O(6)-S(1A)-C(1S1)	113.4(10)
C(32)-C(33)-C(34)	120.1(6)	O(8)-S(1A)-C(1S1)	101.3(5)
C(35)-C(34)-C(33)	119.6(6)	O(7)-S(1A)-C(1S1)	100.5(5)
C(36)-C(35)-C(34)	119.6(7)	F(1)-C(1S1)-F(3)	107.2(11)
C(35)-C(36)-C(31)	122.1(6)	F(1)-C(1S1)-F(2)	108.1(10)
C(42)-C(41)-C(46)	118.0(6)	F(3)-C(1S1)-F(2)	113(2)
C(42)-C(41)-C(2)	123.6(5)	F(1)-C(1S1)-S(1B)	112.1(12)
C(46)-C(41)-C(2)	118.4(5)	F(3)-C(1S1)-S(1B)	124.0(10)
C(41)-C(42)-C(43)	121.0(6)	F(2)-C(1S1)-S(1B)	90.5(12)
C(44)-C(43)-C(42)	119.7(7)	F(1)-C(1S1)-S(1A)	111.7(11)
C(45)-C(44)-C(43)	119.8(6)	F(3)-C(1S1)-S(1A)	107.4(7)
C(44)-C(45)-C(46)	120.2(6)	F(2)-C(1S1)-S(1A)	109.2(10)
C(45)-C(46)-C(41)	121.3(6)	O(7B)-S(1B)-O(6)	80(2)
C(56)-C(51)-C(52)	117.0(5)	O(7B)-S(1B)-O(8)	117(2)
C(56)-C(51)-C(2)	122.8(5)	O(6)-S(1B)-O(8)	120.8(14)
C(52)-C(51)-C(2)	120.0(5)	O(7B)-S(1B)-C(1S1)	99.4(14)
C(53)-C(52)-C(51)	121.2(6)	O(6)-S(1B)-C(1S1)	130(2)
C(54)-C(53)-C(52)	120.2(6)	O(8)-S(1B)-C(1S1)	104.3(10)
C(55)-C(54)-C(53)	119.5(6)	S(1B)-O(7B)-O(6)	49.9(11)
C(54)-C(55)-C(56)	120.2(6)	C(1E)-O-C(2E)	119(2)
C(51)-C(56)-C(55)	121.8(6)	C(4E)-C(1E)-O	128(2)
C(66)-C(61)-C(62)	117.5(6)	C(4E)-C(1E)-C(2E)	157(2)
C(66)-C(61)-C(4)	122.7(5)	O-C(1E)-C(2E)	31.2(10)
C(62)-C(61)-C(4)	119.7(5)	O-C(2E)-C(3E)	110(2)
C(63)-C(62)-C(61)	121.8(6)	O-C(2E)-C(1E)	29.4(11)
C(62)-C(63)-C(64)	119.8(6)	C(3E)-C(2E)-C(1E)	136.7(12)

Table S-9. Anisotropic Temperature Factors ($\text{\AA}^2 \times 10^3$) for **2-OTf**.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	36(1)	27(1)	30(1)	2(1)	-2(1)	0(1)
Fe(2)	33(1)	31(1)	33(1)	1(1)	2(1)	3(1)
O(1)	38(2)	34(2)	33(2)	0(2)	6(2)	1(2)
O(2)	34(2)	32(2)	37(2)	4(2)	1(2)	-1(2)
O(3)	34(2)	34(2)	41(2)	8(2)	1(2)	0(2)
O(4)	40(2)	30(2)	34(2)	-3(2)	-3(2)	5(2)
O(5)	41(2)	35(2)	35(2)	-2(2)	-3(2)	8(2)
N(1)	49(3)	38(3)	41(3)	0(2)	-7(2)	6(2)
N(2)	49(3)	39(3)	35(3)	0(2)	-7(2)	0(2)
N(3)	60(3)	33(3)	34(3)	9(2)	-6(2)	-5(2)
N(4)	42(3)	53(3)	45(3)	9(3)	-3(3)	13(3)
N(5)	42(3)	40(3)	50(3)	-4(2)	4(3)	3(2)
N(6)	37(3)	47(3)	60(4)	-5(3)	0(3)	1(2)
C(1)	36(3)	28(3)	26(3)	0(2)	3(2)	-3(2)
C(2)	34(3)	31(3)	34(3)	0(2)	8(2)	-8(2)
C(3)	34(3)	32(3)	30(3)	-1(2)	0(3)	0(3)
C(4)	32(3)	37(3)	34(3)	-2(3)	1(2)	3(3)
C(11)	49(4)	52(4)	51(4)	1(3)	-17(3)	7(3)
C(12)	60(4)	46(4)	51(4)	3(3)	-20(4)	2(3)
C(13)	72(5)	52(4)	29(3)	2(3)	4(3)	-18(4)
C(14)	79(5)	50(4)	41(4)	8(3)	-7(4)	-17(4)
C(15)	85(5)	19(3)	53(4)	9(3)	-9(4)	3(3)
C(16)	72(5)	33(4)	59(4)	1(3)	-16(4)	15(3)
C(17)	51(4)	51(4)	53(4)	-7(3)	-4(3)	17(3)
C(18)	63(4)	38(4)	43(4)	-4(3)	-7(3)	-5(3)
C(19)	59(4)	44(4)	46(4)	4(3)	3(3)	-11(3)
C(21A)	104(19)	27(7)	79(12)	-5(7)	11(11)	7(9)
C(22A)	96(17)	43(7)	72(10)	-4(6)	9(11)	17(10)
C(24A)	42(13)	107(15)	163(24)	-88(15)	78(14)	-47(11)
C(25A)	65(11)	82(11)	102(16)	24(11)	-36(11)	6(9)
C(26A)	50(8)	160(25)	61(10)	11(13)	-15(7)	-4(11)
C(21B)	46(19)	14(12)	53(17)	9(10)	-11(13)	-16(12)
C(22B)	35(18)	15(10)	32(15)	0(8)	20(12)	15(12)
C(24B)	36(26)	189(50)	123(33)	-117(33)	-24(27)	29(28)
C(23)	47(5)	139(9)	91(7)	-61(7)	30(5)	-25(5)
C(27)	54(4)	58(4)	49(4)	17(3)	2(3)	6(3)
C(28)	61(5)	54(4)	50(4)	-15(3)	0(4)	8(4)
C(29)	52(4)	49(4)	80(6)	3(4)	0(4)	-3(3)
C(31)	36(3)	30(3)	42(3)	3(3)	4(3)	-2(3)
C(32)	48(4)	33(3)	42(4)	-2(3)	-3(3)	-7(3)
C(33)	52(4)	52(4)	49(4)	1(3)	-17(3)	-8(3)
C(34)	41(4)	57(4)	60(4)	5(4)	-8(3)	2(3)
C(35)	44(4)	61(4)	49(4)	-2(3)	5(3)	2(3)
C(36)	39(4)	48(4)	40(3)	-2(3)	0(3)	0(3)
C(41)	37(3)	32(3)	33(3)	4(2)	4(3)	1(3)
C(42)	50(4)	55(4)	43(4)	-7(3)	10(3)	-16(3)
C(43)	72(5)	89(6)	35(4)	-10(4)	6(4)	-22(5)
C(44)	63(5)	92(6)	35(4)	11(4)	8(4)	-6(4)
C(45)	43(4)	63(5)	54(4)	18(4)	14(3)	-3(3)
C(46)	42(4)	47(4)	39(3)	3(3)	5(3)	-7(3)
C(51)	36(3)	32(3)	39(3)	-4(3)	5(3)	-4(2)
C(52)	49(4)	35(3)	41(4)	-4(3)	3(3)	-2(3)

C(53)	74(5)	42(4)	44(4)	-11(3)	9(4)	-4(3)
C(54)	75(5)	28(3)	61(5)	-4(3)	15(4)	5(3)
C(55)	56(4)	30(3)	61(5)	-4(3)	10(4)	2(3)
C(56)	46(4)	36(3)	41(3)	3(3)	3(3)	-2(3)
C(61)	39(3)	31(3)	38(3)	-7(3)	-3(3)	0(3)
C(62)	39(3)	38(3)	41(4)	-7(3)	-3(3)	-3(3)
C(63)	45(4)	42(4)	52(4)	2(3)	-1(3)	-10(3)
C(64)	60(4)	34(4)	63(5)	8(3)	-9(4)	-4(3)
C(65)	48(4)	34(3)	66(5)	1(3)	-7(3)	4(3)
C(66)	37(3)	38(3)	51(4)	-2(3)	3(3)	3(3)
C(71)	34(3)	48(4)	28(3)	-7(3)	1(2)	6(3)
C(72)	42(4)	52(4)	34(3)	-5(3)	-2(3)	6(3)
C(73)	68(5)	66(5)	34(4)	7(3)	-3(3)	14(4)
C(74)	42(4)	84(6)	40(4)	0(4)	-10(3)	16(4)
C(75)	38(4)	87(6)	44(4)	-14(4)	-11(3)	1(4)
C(76)	42(4)	49(4)	46(4)	-3(3)	-5(3)	-2(3)
C(81)	35(3)	33(3)	33(3)	-2(2)	-3(3)	3(3)
C(82)	52(4)	42(4)	37(3)	-8(3)	6(3)	-1(3)
C(83)	56(4)	54(4)	39(4)	-11(3)	10(3)	1(3)
C(84)	44(4)	61(4)	43(4)	8(3)	10(3)	11(3)
C(85)	37(4)	55(4)	51(4)	6(3)	1(3)	-4(3)
C(86)	38(3)	45(4)	36(3)	-2(3)	4(3)	0(3)
O(6)	169(12)	390(23)	310(18)	207(17)	80(12)	-48(13)
S(1A)	52(2)	60(2)	85(3)	37(2)	25(2)	12(1)
O(7)	57(5)	66(5)	158(9)	9(5)	-44(5)	9(4)
O(8)	75(4)	84(4)	82(4)	-13(3)	1(3)	21(3)
C(1S1)	118(9)	129(10)	35(5)	-10(5)	-11(5)	50(8)
F(1)	353(15)	198(9)	95(5)	-30(6)	33(7)	142(10)
F(2)	481(22)	378(18)	287(14)	-224(14)	-311(16)	334(18)
F(3)	185(9)	150(7)	158(8)	-56(6)	2(7)	-41(6)
O	216(19)	66(8)	49(7)	-23(6)	-17(9)	19(10)
C(1E)	82(13)	69(12)	86(14)	4(10)	45(12)	30(10)
C(2E)	114(16)	155(19)	16(7)	-21(9)	-21(9)	-62(14)
C(3E)	70(12)	186(22)	28(8)	32(11)	-13(8)	-2(13)
C(4E)	109(18)	310(38)	63(13)	-11(18)	2(12)	174(24)

*The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

Table S-10. Calculated Hydrogen coordinates ($\times 10^4$) and Temperature Factors ($\text{\AA}^2 \times 10^3$) for **2-Ph-OTf**.

	x	y	z	U(eq)
H(11A)	-2604(3)	8739(4)	386(2)	61
H(11B)	-2366(3)	8042(4)	568(2)	61
H(12A)	-2206(3)	7997(4)	-170(2)	63
H(12B)	-1857(3)	8699(4)	-162(2)	63
H(13A)	-904(4)	8180(3)	-522(2)	61
H(13B)	-390(4)	7951(3)	-179(2)	61
H(14A)	-263(4)	9111(4)	-264(2)	68
H(14B)	-997(4)	9227(4)	-183(2)	68
H(15A)	-765(4)	10012(3)	412(2)	63
H(15B)	-742(4)	9674(3)	874(2)	63
H(16A)	-1794(4)	9848(3)	735(2)	65
H(16B)	-1738(4)	9545(3)	263(2)	65
H(17A)	-2440(3)	9184(4)	1148(2)	78
H(17B)	-2210(3)	8448(4)	1274(2)	78
H(17C)	-1768(3)	9077(4)	1376(2)	78
H(18A)	-1549(4)	7131(3)	-311(2)	72
H(18B)	-959(4)	6978(3)	-2(2)	72
H(18C)	-1659(4)	7008(3)	194(2)	72
H(19A)	351(3)	9492(3)	318(2)	75
H(19B)	261(3)	9149(3)	781(2)	75
H(19C)	400(3)	8698(3)	365(2)	75
H(27A)	185(3)	5900(4)	2248(2)	80
H(27B)	-35(3)	6661(4)	2197(2)	80
H(27C)	-401(3)	6083(4)	1942(2)	80
H(28A)	290(4)	5815(4)	163(2)	83
H(28B)	-310(4)	6049(4)	440(2)	83
H(28C)	101(4)	6589(4)	182(2)	83
H(29A)	1768(4)	8144(4)	1233(3)	91
H(29B)	1153(4)	8253(4)	940(3)	91
H(29C)	1096(4)	8275(4)	1455(3)	91
H(32A)	-2662(3)	5846(3)	522(2)	49
H(33A)	-3619(3)	6295(4)	235(2)	61
H(34A)	-4105(3)	7249(4)	564(2)	64
H(35A)	-3637(3)	7739(4)	1201(2)	62
H(36A)	-2679(3)	7277(3)	1488(2)	51
H(42A)	-1358(3)	6857(4)	1958(2)	59
H(43A)	-1540(4)	6666(4)	2715(2)	78
H(44A)	-2311(4)	5855(4)	2939(2)	76
H(45A)	-2934(3)	5300(4)	2413(2)	64
H(46A)	-2760(3)	5505(3)	1662(2)	51
H(52A)	-1671(3)	5889(3)	394(2)	50
H(53A)	-1215(4)	4901(3)	101(2)	64
H(54A)	-916(4)	3997(3)	567(2)	66
H(55A)	-1023(3)	4122(3)	1330(2)	59
H(56A)	-1484(3)	5111(3)	1625(2)	49
H(62A)	639(3)	9478(3)	1545(2)	47
H(63A)	712(3)	10528(3)	1189(2)	55
H(64A)	-125(4)	11331(3)	1264(2)	63
H(65A)	-1061(3)	11046(3)	1654(2)	59
H(66A)	-1127(3)	9984(3)	2026(2)	50
H(72A)	-77(3)	7824(3)	2537(2)	51

H(73A)	792(4)	7483(4)	2981(2)	67
H(74A)	1704(3)	8198(4)	3051(2)	66
H(75A)	1696(3)	9278(4)	2720(2)	67
H(76A)	817(3)	9617(3)	2283(2)	55
H(82A)	-616(3)	9534(3)	2785(2)	52
H(83A)	-1542(3)	9485(4)	3230(2)	60
H(84A)	-2402(3)	8765(4)	3033(2)	59
H(85A)	-2291(3)	8052(3)	2417(2)	57
H(86A)	-1382(3)	8122(3)	1966(2)	48

Table S-11 . Crystal data and structure refinement for **3-Ph-OTf**.

Identification code	3-Ph-OTf
Empirical formula	C ₆₄ H ₈₂ F ₆ Fe ₂ N ₆ O ₁₃ S ₂
Formula weight	1433.18
Temperature	173(2) K
Wavelength	Cu K α 1.54178 Å
Crystal system	Monoclinic
Space group, Z	P2(1)/c, 4
Unit cell dimensions	$a = 16.171(5)$ Å $b = 15.182(2)$ Å $c = 27.989(6)$ Å $\beta = 105.23(2)$ deg.
Volume	6630.2(27) Å ³
Color	orange-red
Density (calculated)	1.436 g/cm ³
Absorption coefficient	4.810 mm ⁻¹
F(000)	3000
Crystal size	0.56 x 0.44 x 0.09 mm
2 θ range for data collection	2 to 97°
Limiting indices	$-1 \leq h \leq 12$, $-1 \leq k \leq 14$, $-27 \leq l \leq 26$
Reflections collected	7517
Independent reflections	5961 [$R_{\text{(int)}} = 0.0695$]
Absorption correction	Integration
Max. and min. transmission	0.8239 and 0.1931
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5961 / 0 / 648
Goodness-of-fit on F^2	1.020
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0802$, $wR_2 = 0.1790$
R indices (all data)	$R_1 = 0.1463$, $wR_2 = 0.2191$
Largest diff. peak and hole	0.704 and -0.468 e.Å ⁻³

Table S-12. Refined Atom Coordinates ($\times 10^4$) and Temperature Factors ($\text{\AA}^2 \times 10^3$) for **3-OTf**.

	x	y	z	U(eq)
Fe(1)	7059(1)	7711(1)	1850(1)	29(1)
Fe(2)	6922(1)	5642(1)	1757(1)	29(1)
O(1)	6444(4)	6704(4)	1763(2)	28(2)
O(2)	7949(4)	7293(5)	2471(3)	34(2)
O(3)	7962(4)	5828(5)	2353(3)	31(2)
O(4)	7841(4)	7404(5)	1400(3)	29(2)
O(5)	7592(5)	5969(5)	1261(2)	29(2)
N(1)	7747(6)	8997(5)	2002(3)	27(2)
N(2)	6289(6)	8392(6)	2270(3)	33(3)
N(3)	6248(6)	8543(6)	1257(4)	36(3)
N(4)	7387(6)	4254(6)	1705(3)	31(2)
N(6)	5870(6)	5086(6)	1165(3)	32(3)
N(5)	6237(6)	4946(6)	2218(3)	31(2)
C(1)	8195(7)	6529(8)	2616(4)	30(3)
C(2)	8846(8)	6432(7)	3130(4)	33(3)
C(3)	7886(7)	6688(9)	1168(4)	29(3)
C(4)	8351(7)	6698(7)	744(4)	32(3)
C(11)	7408(9)	9531(8)	2347(5)	52(4)
C(12)	6903(8)	8998(8)	2614(4)	51(4)
C(13)	5581(8)	8872(8)	1936(4)	48(4)
C(14)	5444(8)	8602(9)	1416(5)	54(4)
C(15)	6650(8)	9423(8)	1245(5)	53(4)
C(16)	7554(8)	9427(8)	1512(5)	51(4)
C(17)	8701(7)	8919(8)	2191(4)	43(4)
C(18)	5933(7)	7777(8)	2569(4)	41(3)
C(19)	6079(8)	8134(7)	768(4)	44(4)
C(26)	6806(8)	3779(8)	1279(4)	48(4)
C(23)	5337(8)	5026(8)	1927(4)	42(3)
C(24)	5218(7)	4729(8)	1396(4)	38(3)
C(22)	6499(9)	3994(7)	2290(5)	48(4)
C(25)	6282(8)	4410(8)	921(4)	41(3)
C(21)	7353(8)	3853(8)	2182(5)	46(4)
C(27)	8279(8)	4203(7)	1665(5)	43(4)
C(29)	5467(7)	5763(7)	797(4)	38(3)
C(28)	6327(8)	5348(8)	2713(4)	45(4)
C(31)	8585(7)	7131(7)	3460(4)	32(3)
C(32)	9111(8)	7837(8)	3656(4)	43(3)
C(33)	8857(9)	8495(9)	3945(5)	60(4)
C(34)	8060(8)	8441(9)	4014(5)	56(4)
C(35)	7503(8)	7768(8)	3820(4)	48(4)
C(36)	7791(7)	7130(8)	3551(4)	38(3)
C(41)	9761(7)	6587(7)	3082(4)	28(3)
C(42)	9955(7)	6820(7)	2654(4)	37(3)
C(43)	10809(8)	6888(8)	2633(5)	47(4)
C(44)	11460(8)	6746(7)	3048(4)	39(3)
C(45)	11280(8)	6525(8)	3473(4)	44(3)
C(46)	10444(7)	6435(7)	3502(4)	40(3)
C(51)	8828(7)	5481(7)	3340(4)	35(3)
C(52)	8513(7)	5275(8)	3739(4)	44(4)
C(53)	8497(8)	4356(9)	3882(5)	63(4)
C(54)	8798(8)	3728(9)	3624(5)	52(4)