Supporting Information

Halogen Transfer to Carbon Radicals by High-Valent Iron Chloride and Iron Fluoride Corroles

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Table S1. Crystallographic data for **3**.

Chemical formula	$C_{93}H_{59}AgF_6FeN_4O_6S_2 \cdot 2(C_7H_8)$
M_r	1854.55
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	110
a, *b*, *c* (Å)	15.6092 (2), 17.3033 (3), 21.2276 (3)
α, β, γ (°)	67.0780 (15), 74.1580 (15), 64.7220 (15)
V (Å^3)	4735.68 (15)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	3.86
Crystal size (mm)	0.36 × 0.31 × 0.24
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Analytical *CrysAlis PRO* 1.171.39.29c (Rigaku Oxford Diffraction, 2017) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.389, 0.542
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	61006, 18548, 17160
R_{int}	0.028
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.124, 1.06
No. of reflections	18548
No. of parameters	1339
No. of restraints	761
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.46, -0.99

Single Crystal X-ray Crystallography

3: All reflection intensities were measured at 110(2) K using a SuperNova diffractometer (equipped with Atlas detector) with Cu *K*α radiation (λ = 1.54178 Å) under the program CrysAlisPro (Version CrysAlisPro 1.171.39.29c, Rigaku OD, 2017). The same program was used to refine the cell dimensions and for data reduction. The structure was solved with the program SHELXS-2018/3[1] and was refined on F^2 with SHELXL-2018/3[1]. Analytical numeric absorption correction using a multifaceted crystal model was applied using CrysAlisPro. The temperature of the data collection was controlled using the system Cryojet (manufactured by Oxford Instruments). The H atoms were placed at calculated positions using the instructions AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 U_{eq} of the attached C atoms. The coordinated triflate anion and two lattice toluene solvent molecules were found to be disordered over two orientations. The occupancy factors of the major components of the disorder refine to 0.664(3), 0.691(5) and 0.769(5), respectively. The crystal lattice contains some remaining amount of very disordered lattice solvent molecules (toluene), and their contribution has been removed using the SQUEEZE procedure in Platon[2].

Computer programs: *CrysAlis PRO* 1.171.39.29c (Rigaku OD, 2017), *SHELXS2018*/3 (Sheldrick, 2018), *SHELXL2018*/3 (Sheldrick, 2018), *SHELXTL* v6.10 (Sheldrick, 2008).

Table S2. Metrical parameters obtained from X-Ray Crystallography for **3**.

Bond Lengths (Å)	
Fe1-N1	1.883(2)
Fe1-N2	1.9140(19)
Fe1-N3	1.925(2)
Fe1-N4	1.882(2)
Fe1-O1	1.9908(19)
Ag1-O4	2.4562(18)
Ag1-C12	2.468(2)
Ag1-C13	2.554(2)
Ag1-C63	2.552(2)
Ag1-C64	2.629(2)
Ag1-C90	2.539(2)
Ag1-C91	2.572(2)
Bond Angles (o)	
N1-Fe-N3	156.54(9)
N4-Fe-N2	155.81(8)
N1-Fe1-N2	88.24(9)
N1-Fe1-N4	80.09(9)
N2-Fe1-N3	94.24(8)
N3-Fe1-N4	88.53(8)
N1-Fe1-O1	105.47(9)
N2-Fe1-O1	101.18(9)
N3-Fe1-O1	96.93(8)
N4-Fe1-O1	102.33(9)
O4-Ag1-C12	107.77(7)
O4-Ag1-C13	109.27(7)
O4-Ag1-C63	82.37(7)
O4-Ag1-C64	86.18(8)
O4-Ag1-C90	85.30(8)
O4-Ag1-C91	84.57(7)

Table S3. Crystallographic data for **4**.

Crystal data	
Chemical formula	$C_{91}H_{59}FFeN_4 \cdot C_7H_8$
M_r	1375.40
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	110
a, *b*, *c* (Å)	14.2616 (3), 16.0010 (4), 21.0841 (4)
α, β, γ (°)	95.1405 (16), 105.0505 (15), 110.8099 (19)
V (Å^3)	4254.19 (17)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	1.79
Crystal size (mm)	0.24 × 0.18 × 0.14
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Analytical *CrysAlis PRO* 1.171.40.67a (Rigaku Oxford Diffraction, 2019) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.751, 0.837
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	51718, 20056, 12291
R_{int}	0.036
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.609
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.107, 0.84
No. of reflections	20056
No. of parameters	1078
No. of restraints	446
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, -0.29

Single Crystal X-ray Crystallography

4: All reflection intensities were measured at 110(2) K using a SuperNova diffractometer (equipped with Atlas detector) with Cu *K*α radiation (λ = 1.54178 Å) under the program CrysAlisPro (Version CrysAlisPro 1.171.39.29c, Rigaku OD, 2017). The same program was used to refine the cell dimensions and for data reduction. The structure was solved with the program SHELXS-2018/3[1] and was refined on F^2 with SHELXL-2018/3[1]. Analytical numeric absorption correction using a multifaceted crystal model was applied using CrysAlisPro. The temperature of the data collection was controlled using the Cryojet system (manufactured by Oxford Instruments). The H atoms were placed at calculated positions using the instructions AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 U_{eq} of the attached C atoms. The Fe–F bond is disordered over two orientations (above and below the corrole plane). The major component of the disorder refines to 0.723(3). One phenyl group and one lattice toluene solvent molecule are disordered over two orientations, and the occupancy factors of the major components of the disorder refine to 0.641(8) and 0.645(4), respectively. The asymmetric unit also contains some very disordered lattice solvent molecules (toluene), and their contributions were removed from the final refinement using the SQUEEZE procedure in Platon[2]. The crystal that was mounted on the diffractometer was a composite of two crystal components, and the two components are related by a *ca.* 5.18° rotation along the –0.8172 **a*** + 0.5707 **b*** – 0.0811**c*** reciprocal direction. The BASF scale factor refines to 0.0583(10).

Computer programs: *CrysAlis PRO* 1.171.39.29c (Rigaku OD, 2017), *SHELXS2018*/3 (Sheldrick, 2018), *SHELXL2018*/3 (Sheldrick, 2018), *SHELXTL* v6.10 (Sheldrick, 2008).

Table S4. Comparison of metrical parameters obtained from X-Ray Crystallography and DFT for **4**.

Bond Lengths (Å)	**1 (72%)**	**1' (28%)**	**DFT**
Fe-N1	1.8793(16)	1.880(2)	1.901
Fe-N2	1.9100(16)	1.903(2)	1.918
Fe-N3	1.9010(16)	1.913(2)	1.917
Fe-N4	1.8821(17)	1.873(2)	1.895
Fe-F	1.972(2)	1.815(5)	1.806
Bond Angles (o)			
N1-Fe-N3	160.52(11)	158.38(19)	154
N4-Fe-N2	157.87(11)	160.65(19)	154.6
N1-Fe-N2	89.04(7)	89.25(10)	88.2
N1-Fe-N4	80.55(7)	80.78(10)	79.5
N3-Fe-N2	94.04(7)	93.89(11)	93.2
N4-Fe-N3	89.71(7)	89.62(11)	88.5
N1-Fe-F	99.83(9)	102.1(2)	102.2
N2-Fe-F	100.11(9)	100.19(19)	102.5
N3-Fe-F	98.47(9)	98.41(19)	102.8
N4-Fe-F	100.88(9)	98.10(19)	101.8

Table S5. Selected distances (Å) for Fe(X)(ttppc) from XRD.

X	OTf	Cl[3]	OH[3]	F (72%)	F' (28%)
Fe – X	1.9908(19)	2.2559(11)	1.857(3)	1.972(2)	1.815(5)
Fe – N_1	1.883(2)	1.872(3)	1.876(3)	1.8793(16)	1.880(2)
Fe – N_2	1.9140(19)	1.895(3)	1.902(3)	1.9100(16)	1.903(2)
Fe – N_3	1.925(2)	1.904(2)	1.905(3)	1.9010(16)	1.913(2)
Fe – N_4	1.882(2)	1.880(3)	1.882(3)	1.8821(17)	1.873(2)
Fe – $(N_{pyrrole})_{plane}$	0.374	0.341	0.383	0.323	0.318
C_β – C_β (av)	1.369(4)	1.370(4)	1.366(4)	1.367(3)	1.367(3)
C_α – C_β (av)	1.430(9)	1.428(4)	1.427(4)	1.425(3)	1.425(3)
C_α – C_α (C1–C19)	1.410(4)	1.407(4)	1.429(4)	1.425(3)	1.425(3)
C_α – N (av)	1.374(3)	1.382(4)	1.377(4)	1.376(2)	1.376(2)
C_α – C_{meso} (av)	1.407(7)	1.404(4)	1.399(4)	1.401(3)	1.401(3)

Table S6. Mössbauer Parameters (δ [mm s^{-1}] and $|\Delta E_Q|$ [mm s^{-1}]): Experimental Data (80 K, $C_6H_5CH_3$) and Theoretical Values

Complex	δ_{exp}	δ (B3LYP)	δ (TPSSh)	$\|\Delta E_Q\|_{exp}$	$\|\Delta E_Q\|$ (B3LYP)	$\|\Delta E_Q\|$ (TPSSh)
1	0.17	0.178	0.184	2.76	2.730	2.781
3	0.22	0.220	0.231	3.36	3.273	3.172
4	0.18	0.202	0.197	2.33	2.343	2.472

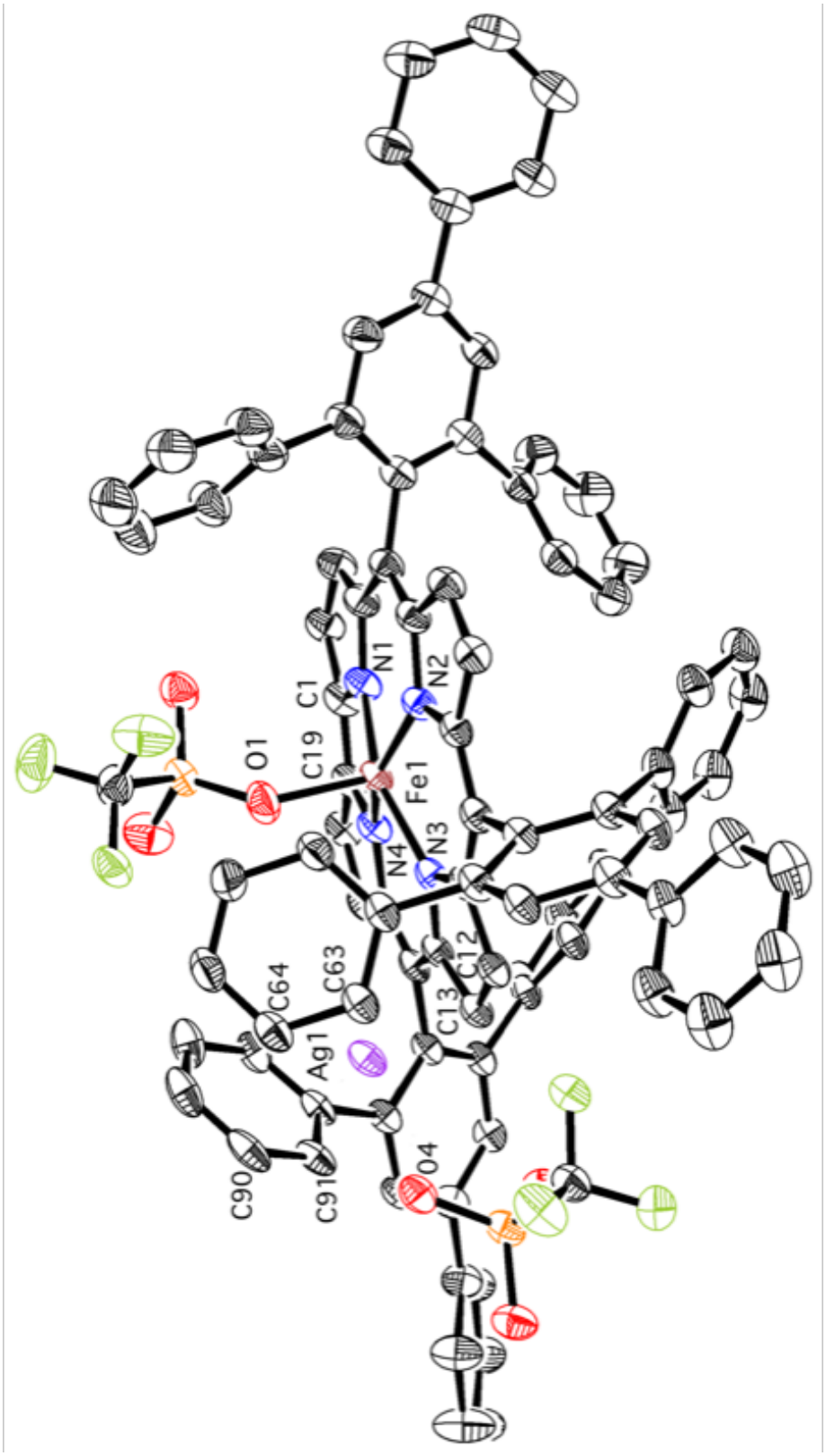

Figure S1. Displacement ellipsoid plot (40% probability) of **3** at 110 K. Hydrogen atoms omitted for clarity.

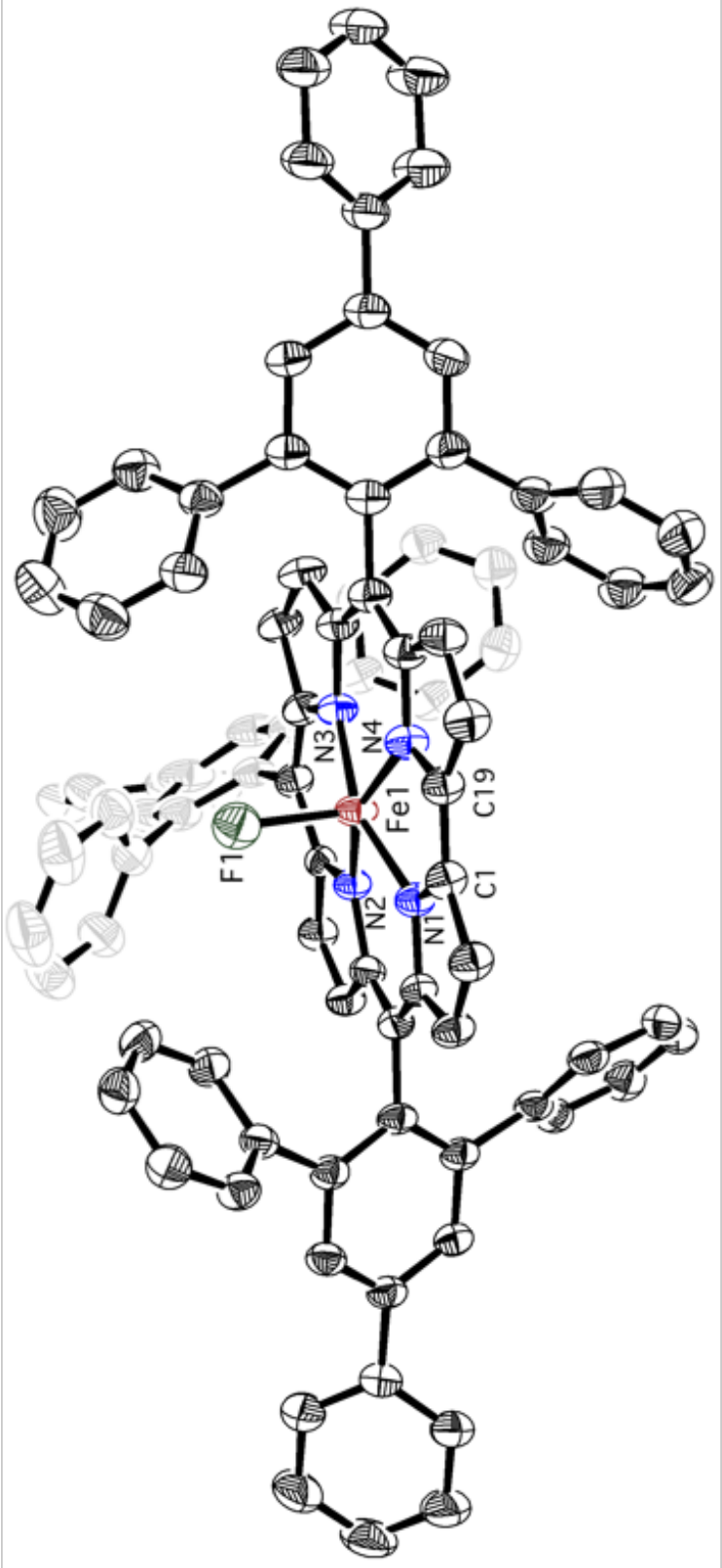

Figure S2. Displacement ellipsoid plot (50% probability) of **4** at 110 K. Hydrogen atoms omitted for clarity.

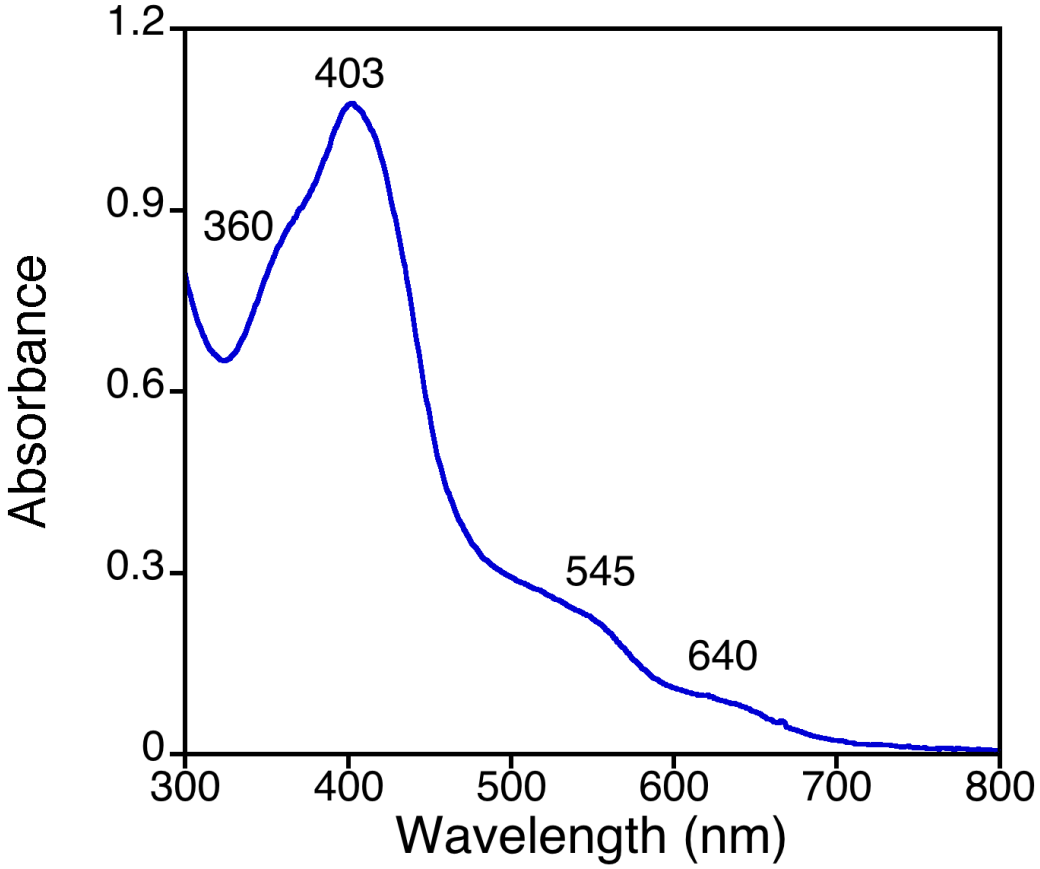

Figure S3. UV-vis spectrum of **2** in 1/1 (v/v) $CH_3CN/C_6H_5CH_3$ at 23 °C.

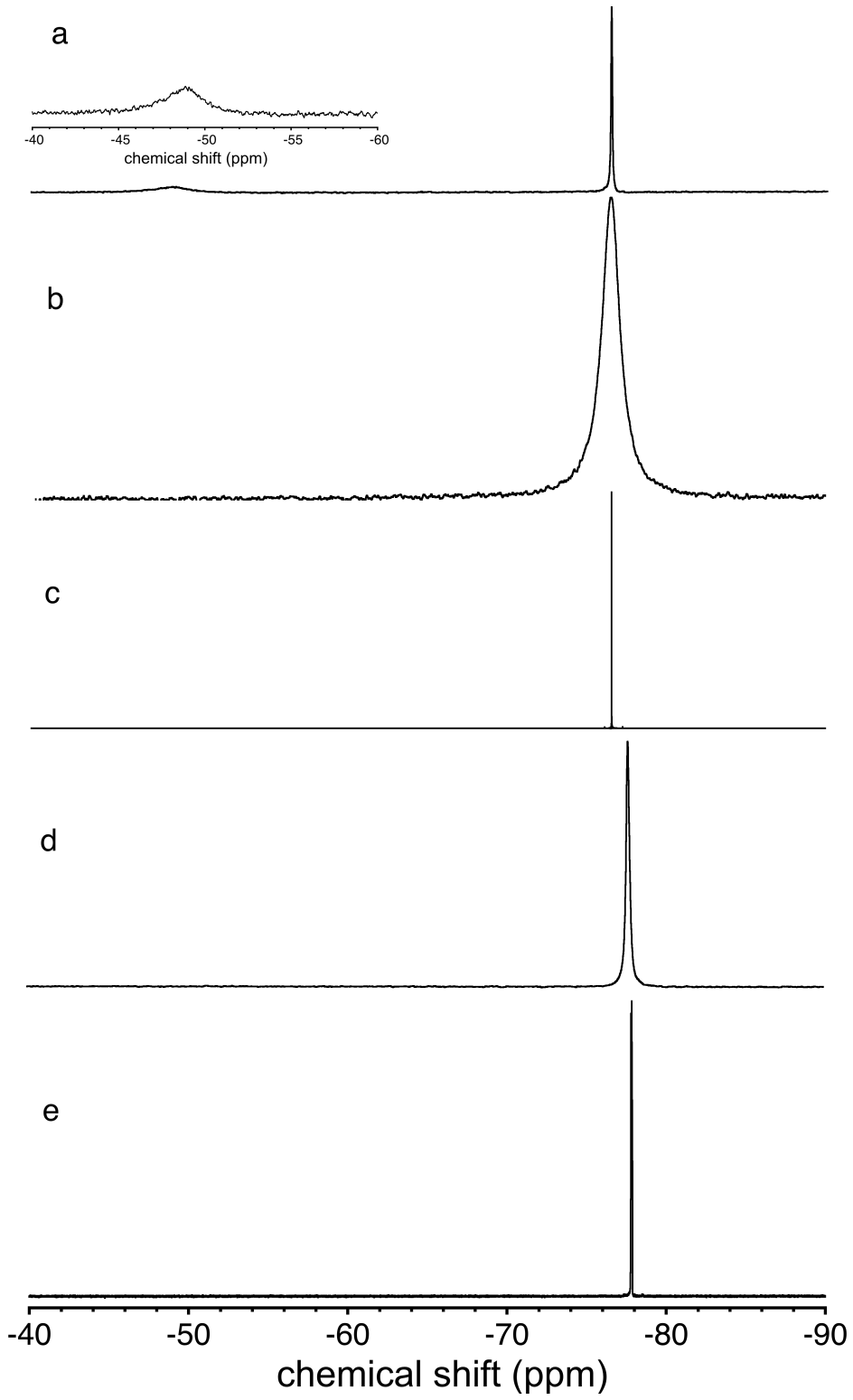

Figure S4. ^{19}F $\{^{1}H\}$ NMR spectra (300 MHz, 23 °C) of (a) crystalline **3** in $C_6D_5CD_3$, (b) **2** in $C_6D_5CD_3$, (c) AgOTf in $C_6D_5CD_3$, (d) **2** in 1/1 (v/v) $C_6D_5CD_3/CD_3CN$, and (e) AgOTf in 1/1 (v/v) $C_6D_5CD_3/CD_3CN$.

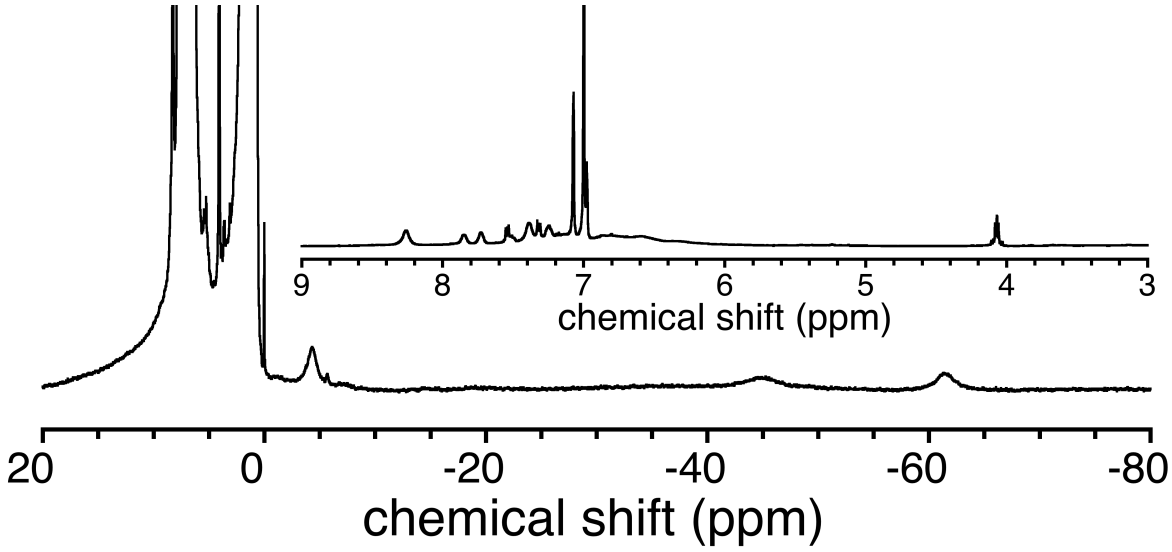

Figure S5. ^{1}H NMR spectrum (400 MHz) of **2** in 1/1 (v/v) $C_6D_5CD_3/CD_3CN$ at 23 °C. Inset: expanded region from 3 – 9 ppm.

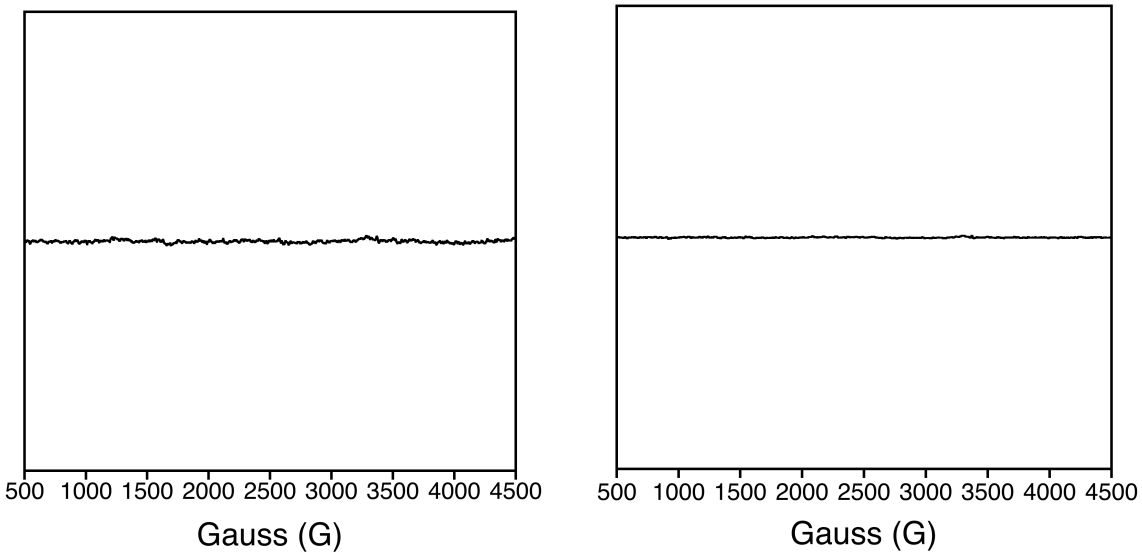

Figure S6. X-band EPR spectrum of **2** (2 mM) in 1/1 (v/v) $C_6H_5CH_3/CH_3CN$ (left), and $C_6H_5CH_3$ (right). EPR parameters: T = 20 K, freq. = 9.439 GHz, power = 0.2012 mW, mod. amp. = 10 G, mod. freq. = 100 kHz, receiver gain = 5.02 x 10^3.

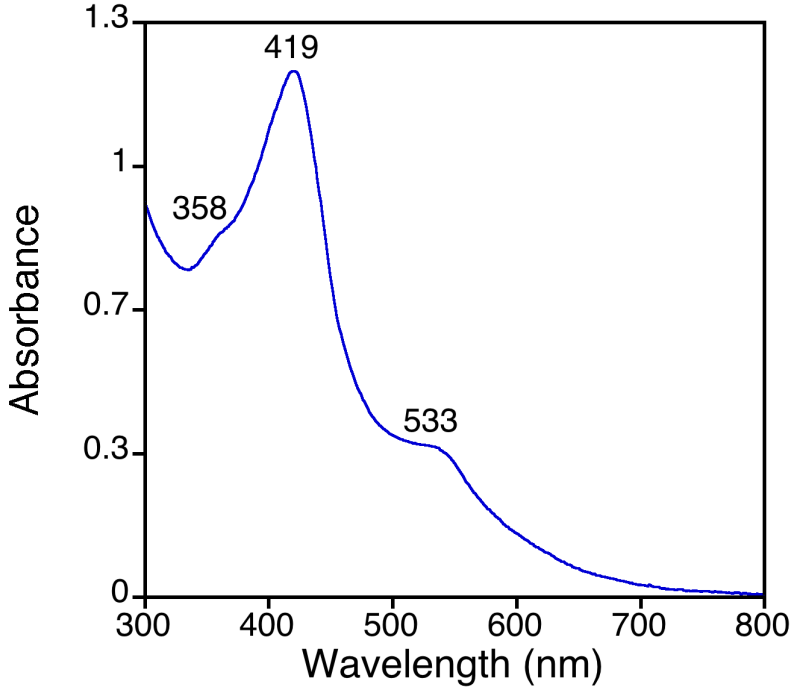

Figure S7. UV-vis spectrum of **3** in $C_6H_5CH_3$ at 23 °C.

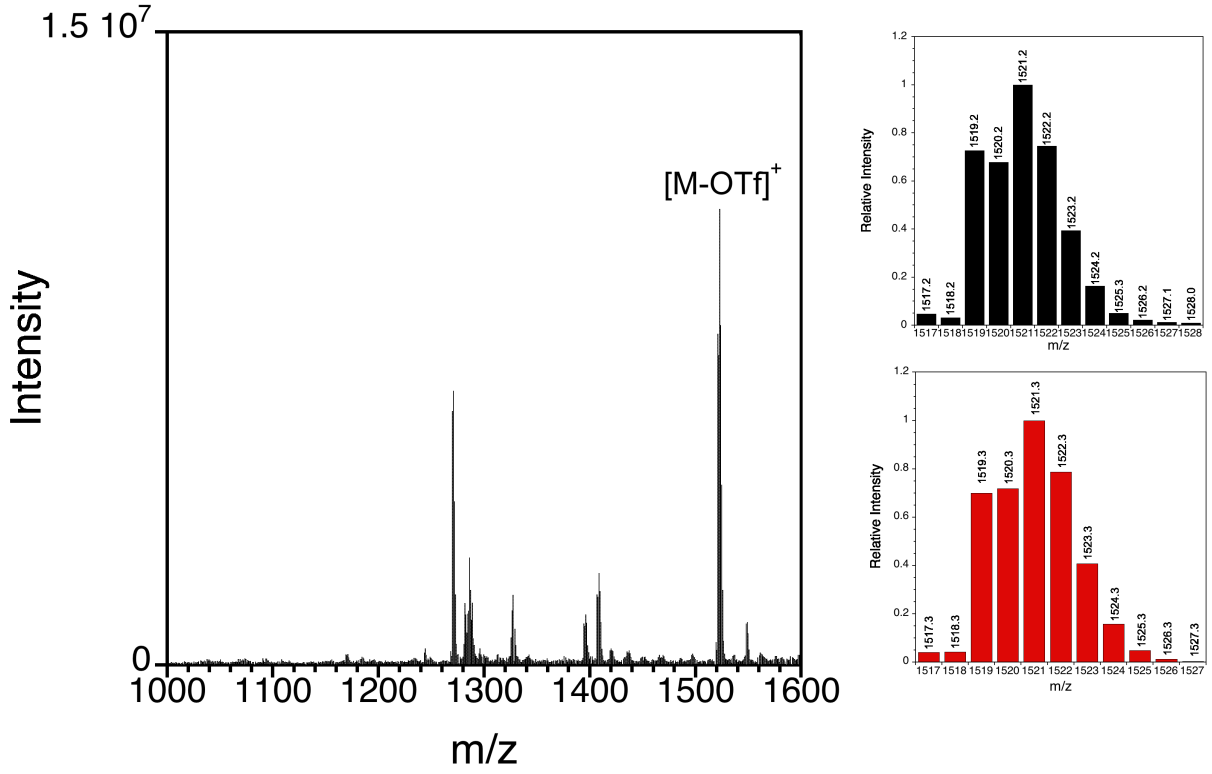

Figure S8. ESI-MS(+) spectrum of **3** in 1/1 (v/v) $CH_3C(O)CH_3/C_6H_5CH_3$ at 23 °C. ESI-MS: m/z = 1521.2, (M+) (black); 1521.27 calculated most probable mass for $C_{92}H_{59}AgF_3FeN_4O_3S$ (red).

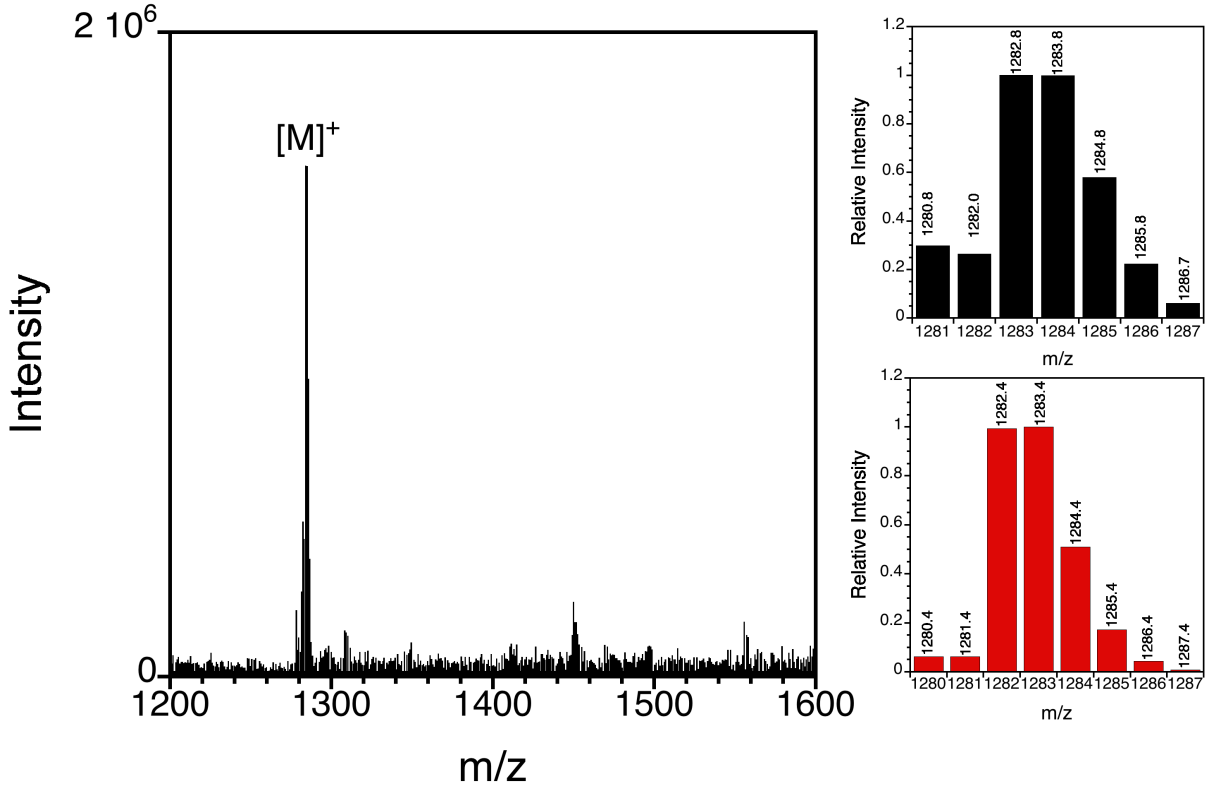

Figure S9. ESI-MS(+) spectrum of **4** in 1/1 (v/v) $CH_3CN/C_6H_5CH_3$ at 23 °C. ESI-MS: m/z = 1283.8 (M+) (black); 1283.4 calculated most probable mass for $C_{91}H_{59}N_4FeF$ (red).

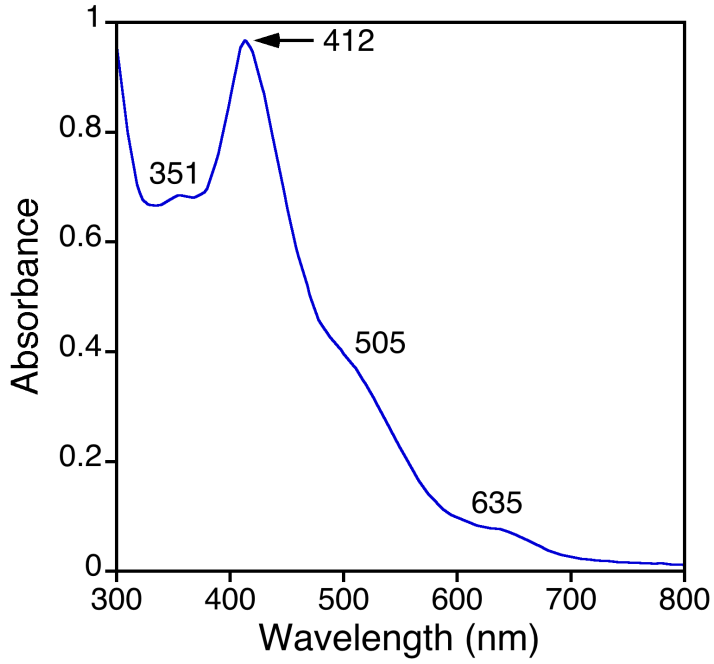

Figure S10. UV-vis spectrum of crystalline **4** in $C_6H_5CH_3$ at 23 °C.

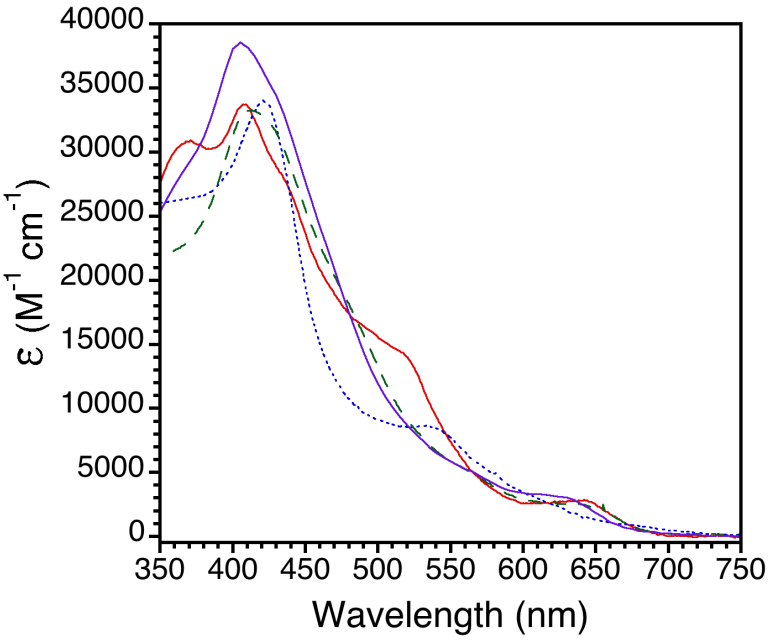

Figure S11. UV-vis spectra of **1** (red, solid line), **2** (blue, dotted line), **4** (green, dashed line), and Fe(OH)(ttppc) (purple, solid line) in toluene at 23 °C.

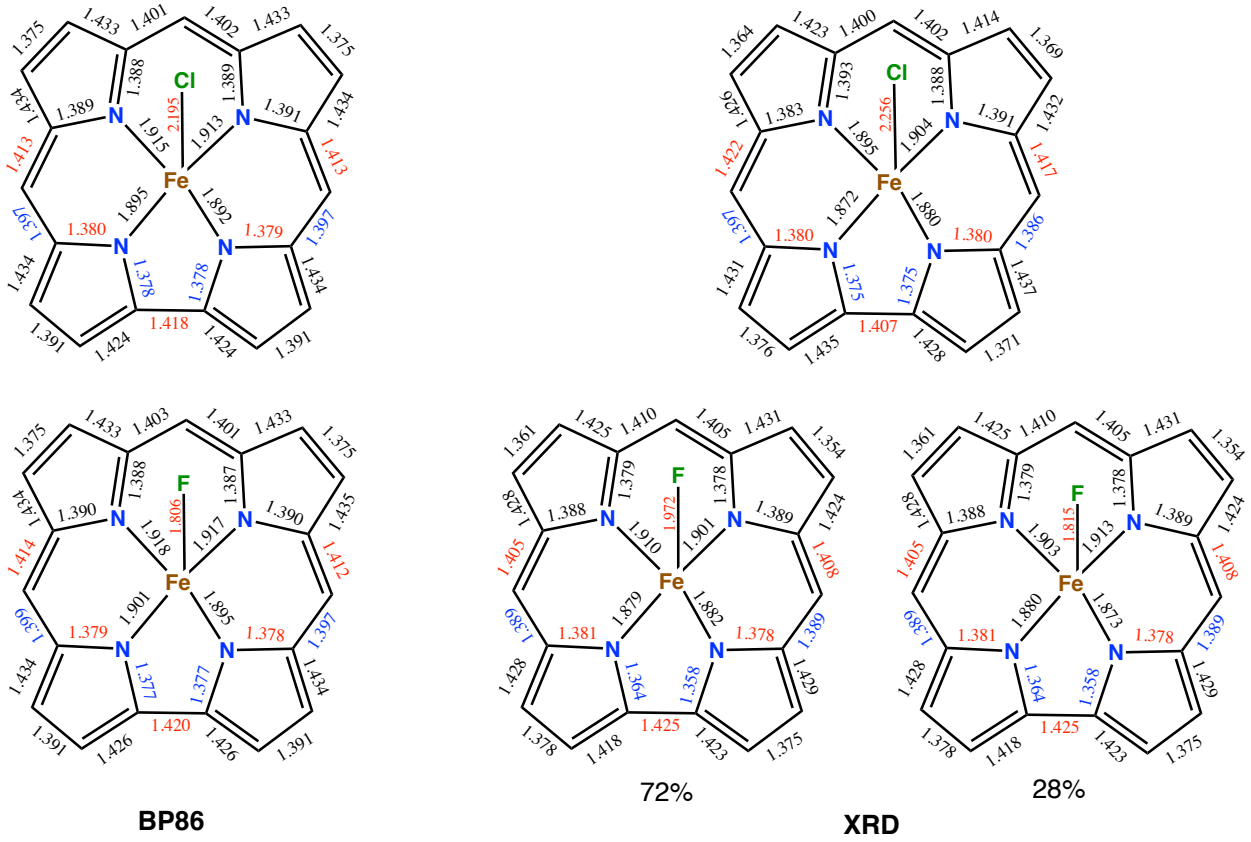

Figure S12. Comparison of DFT geometry-optimized structures for Fe(X)(ttppc) (X = Cl, F) with structures obtained from single crystal XRD.

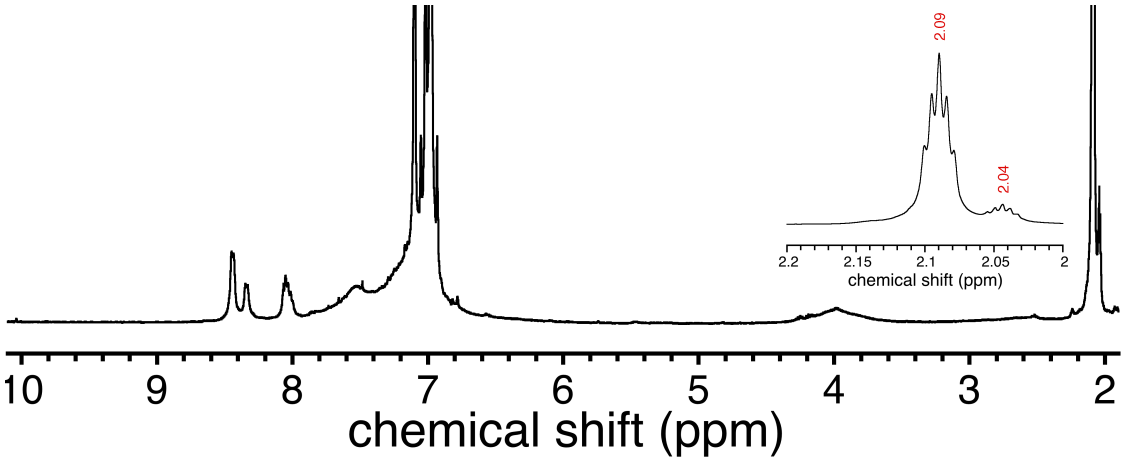

Figure S13. Evans Method for measuring the spin magnetic moment for **4**. ^{1}H NMR spectrum (400 MHz) of **4** (4 mM) in $C_6D_5CD_3$ at 297.1 K. Inset: expanded region from 2 – 2.2 ppm. Red peak labels mark the chemical shifts for the residual proteo-toluene signals coming from the inner and outer coaxial tubes. A spectrum of 20 Hz was observed leading to $\mu_{eff} = 2.63\ \mu_B$.

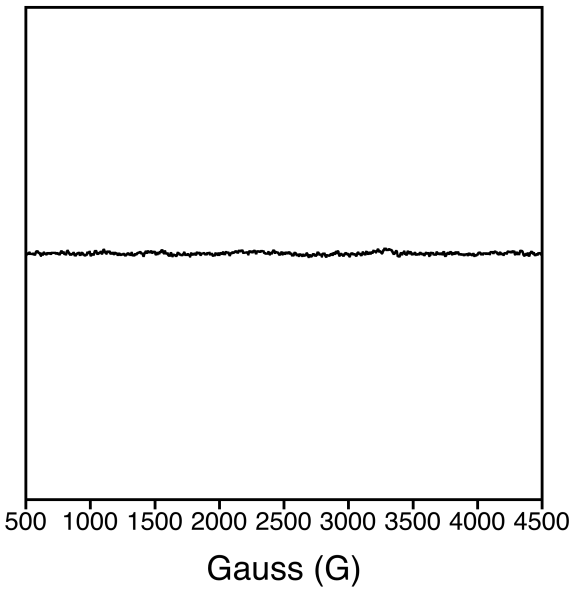

Figure S14. X-band EPR spectrum of **4** (2 mM) in $C_6H_5CH_3$. EPR parameters: T = 20 K, freq. = 9.439 GHz, power = 0.2012 mW, mod. amp. = 10 G, mod. freq. = 100 kHz, receiver gain = 5.02 x 10^3.

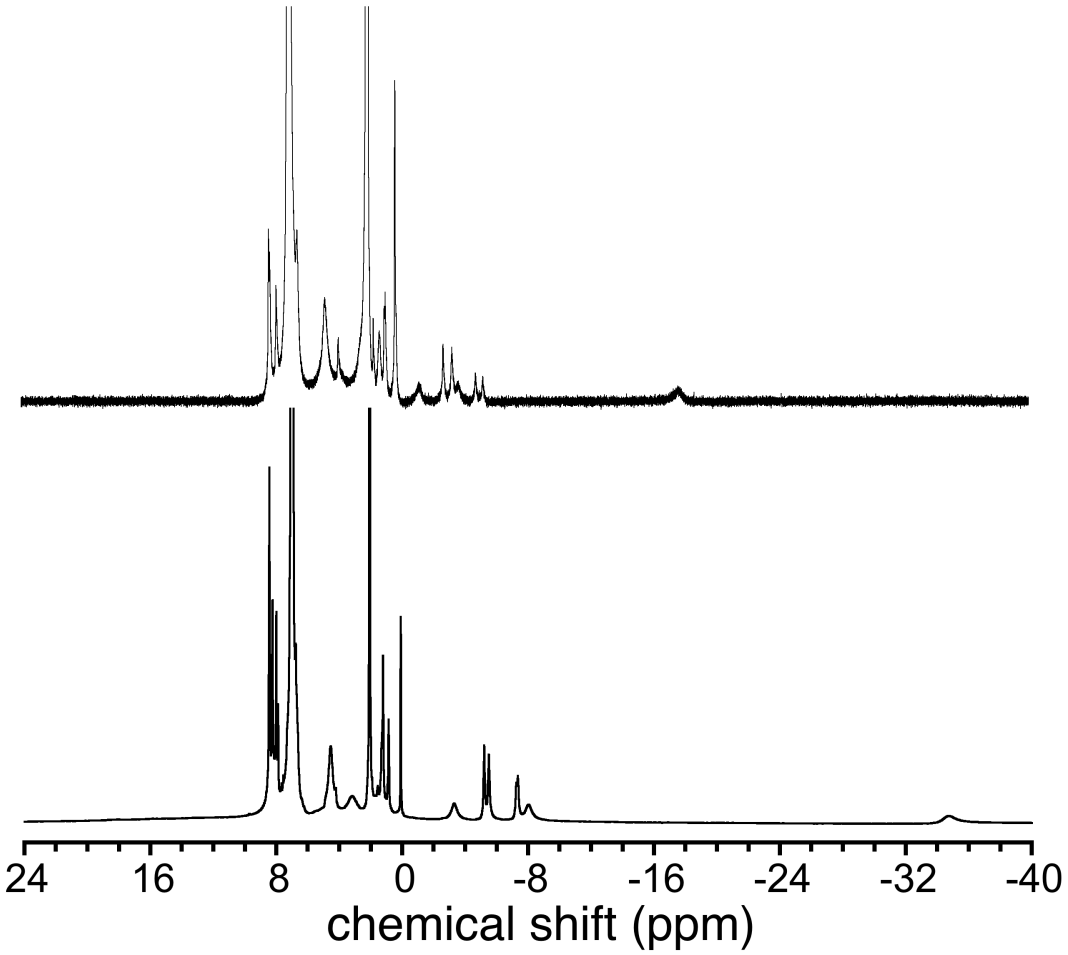

Figure S15. ^{1}H NMR spectra (400 MHz, $C_6D_5CD_3$, 23 °C) of Fe(X)(ttppc) with X = OH (top) and Cl (bottom) for comparison of the paramagnetic peaks.

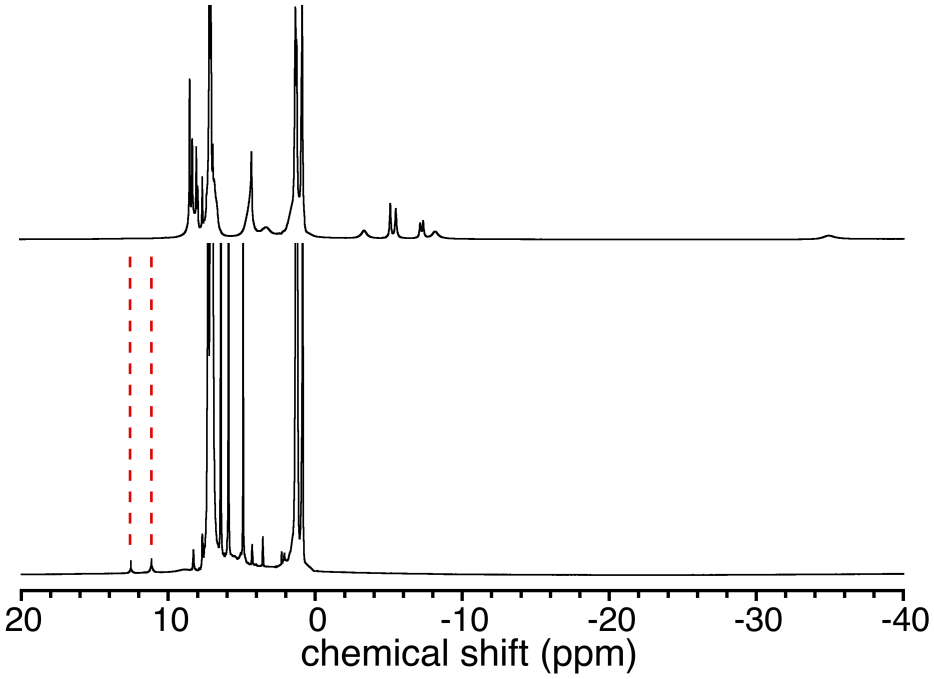

Figure S16. ^{1}H NMR spectra (400 MHz, C_6D_6, 23 °C) of **1** (top), and **1** + Ph_3C• (bottom). Appearance of the peaks at +11.2 and +12.5 ppm (red, dashed lines) in the reaction mixture are characteristic of Fe^{III}(ttppc).[3]

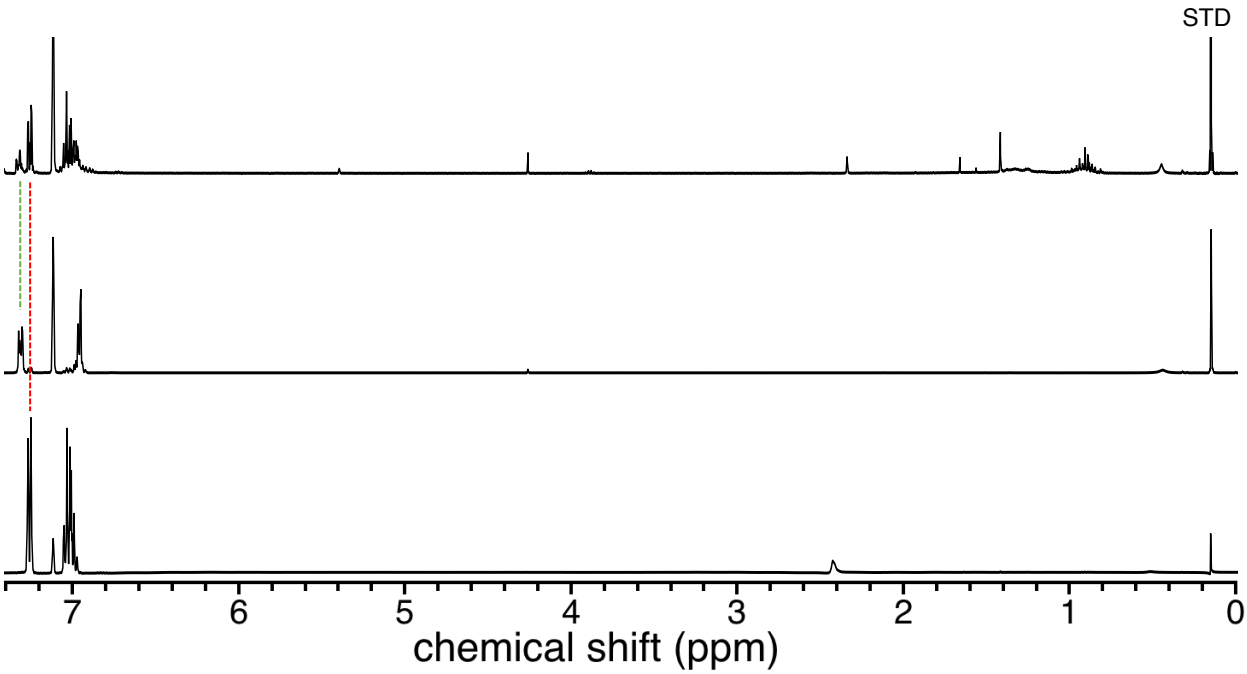

Figure S17. Quantification by ^{1}H NMR spectroscopy (400 MHz, C_6D_6, 23 °C) of Ph_3CCl (6 H, m, 7.34 – 7.39 ppm) isolated from the reaction of **1** and $Ph_2C{=}C_6H_5{-}CPh_3$, shown by green dotted line, with aerobic byproduct[4], Ph_3COH, shown by red dotted line (top), Ph_3CCl (middle), and Ph_3COH (bottom).

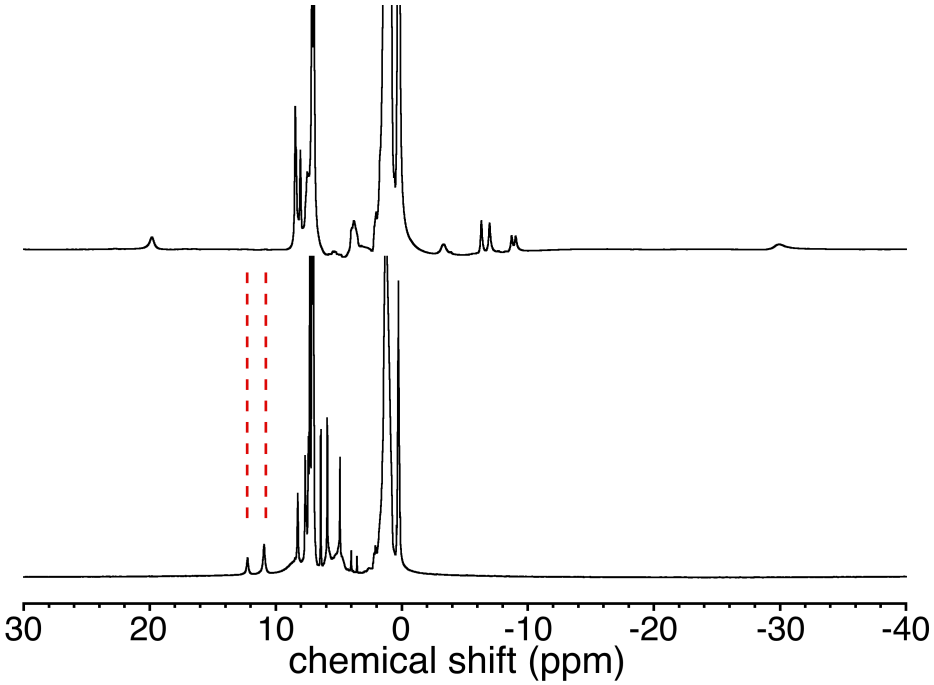

Figure S18. ^{1}H NMR spectra (400 MHz, C_6D_6, 23 °C) of **4** (top), and **4** with $Ph_2C{=}C_6H_5{-}CPh_3$. (bottom) Appearance of the peaks highlighted by red, dashed lines in the reaction mixture are characteristic of Fe^{III}(ttppc).[3]

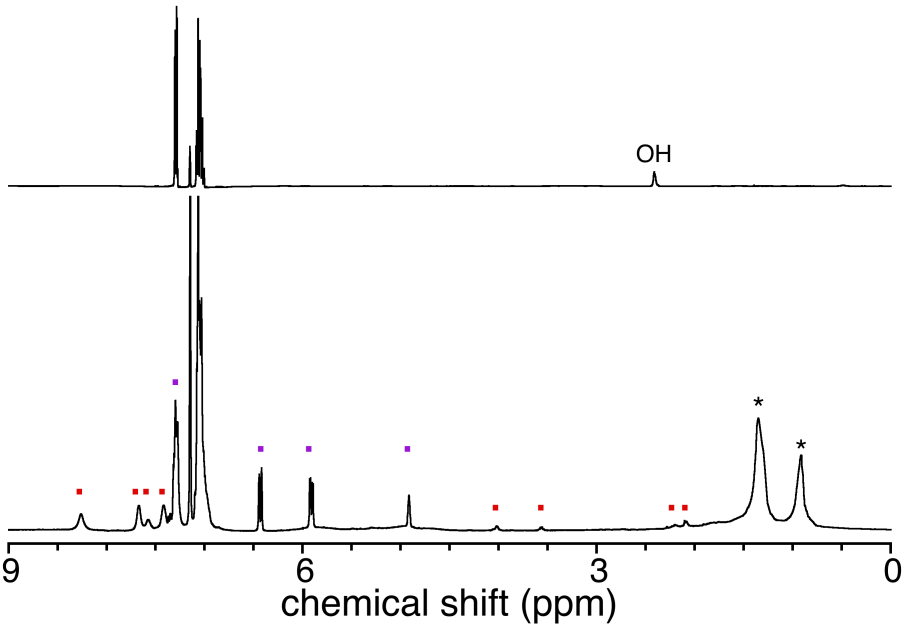

Figure S19. ^{1}H NMR spectra (400 MHz, C_6D_6 (S), 23 °C) of Ph_3COH (top), and **4** with $Ph_2C{=}C_6H_5{-}CPh_3$ (purple dot) (bottom) to show no aerobic oxidation. Appearance of the peaks highlighted by a red dot are characteristic of Fe^{III}(ttppc).[3] Residual solvent peaks for hexane from the synthesis of **4** are marked with a black asterisk (*).

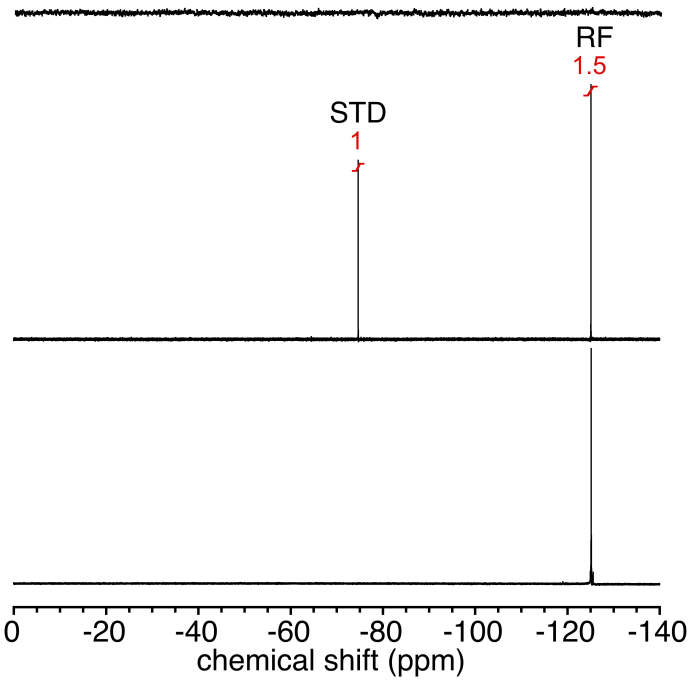

Figure S20. ^{19}F $\{^{1}H\}$ NMR spectra (300 MHz, C_6D_6, 23 °C) of **4** (top); **4** + Ph_3C• with $CF_3C(O)OC_2H_5$ (0.44 μmol) added as an internal standard (STD) (middle); and the fluorinated product, $(C_6H_5)_3CF$ (RF) (bottom).

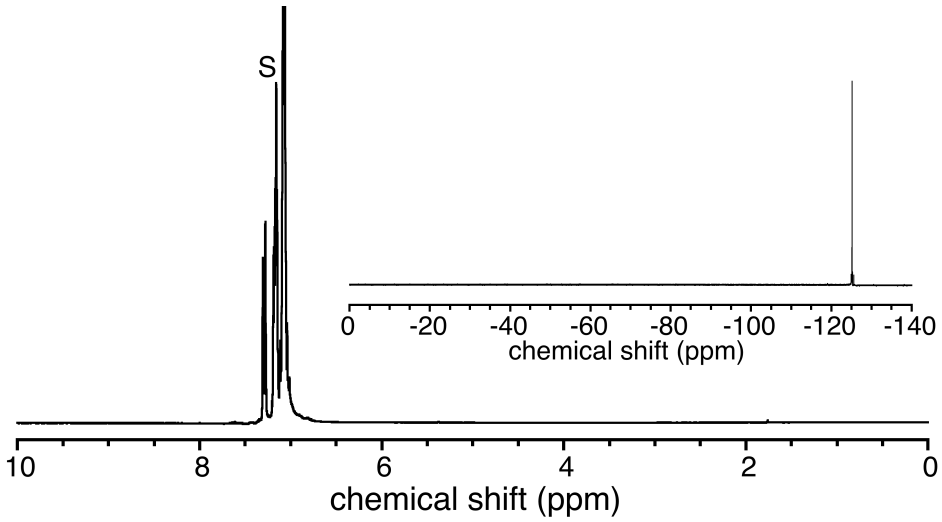

Figure S21. ^{1}H NMR (400 MHz) of Ph_3CF in C_6D_6 at 23 °C. Inset: ^{19}F $\{^{1}H\}$ NMR (300 MHz) of Ph_3CF in C_6D_6, at 23 °C. S denotes C_6D_6.

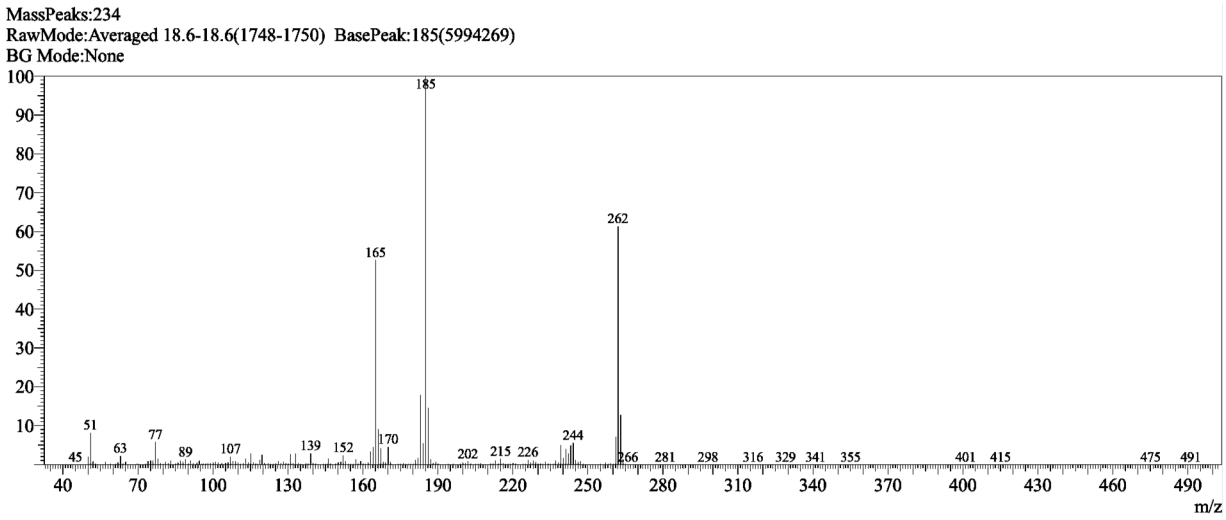

Figure S22. GC-MS (C_6H_6) of Ph_3CF at R_T = 18.6 min for $[M]^+$.

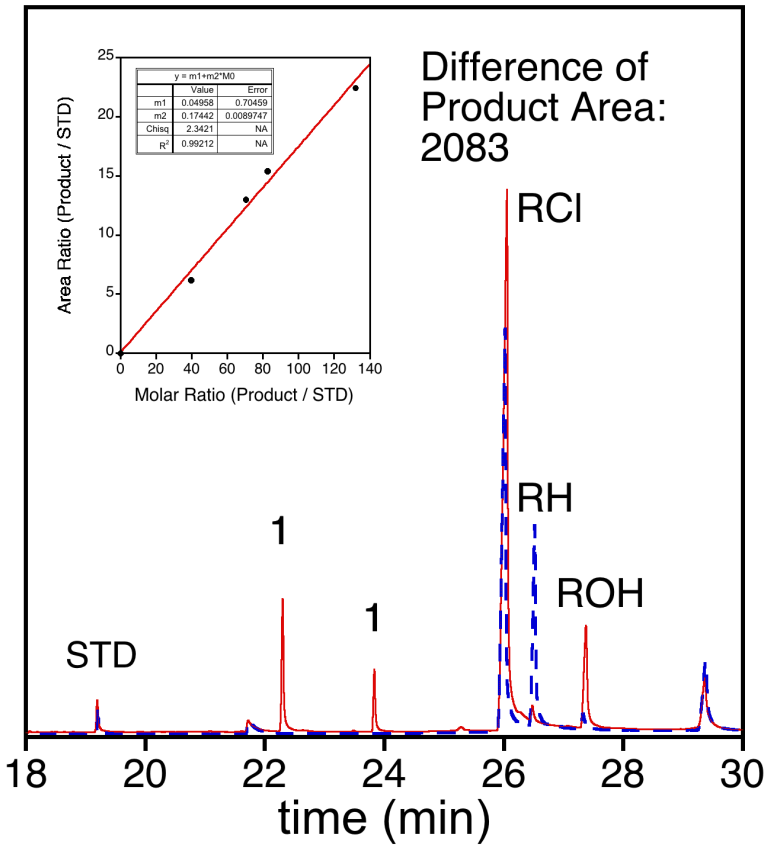

Figure S23. GC-FID quantification of (p-MeO-C_6H_4)$_3$CCl in $C_6H_5CH_3$: 2 µL injection of (p-MeO-C_6H_4)$_3$C• (18 mM, 0.51 mL) (blue, dashed line), showing residual (p-MeO-C_6H_4)$_3$CCl at R_T = 26 min; 2 µL injection of **1** (5.4 mM, 0.51 mL) with (p-MeO-C_6H_4)$_3$C• (3.34 equiv, 18 mM) (solid, red line), showing an increase in the peak at 26 min. Inset: Calibration curve of (p-MeO-C_6H_4)$_3$CCl at R_T = 26 min referenced to an internal standard eicosane at R_T = 18.6 min.

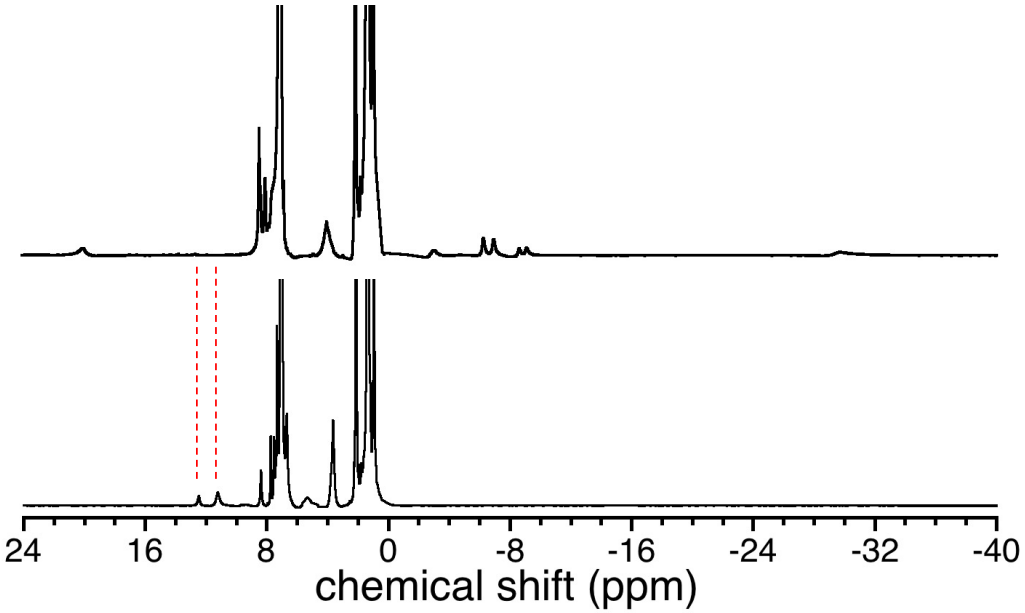

Figure S24. ^{1}H NMR spectra (400 MHz, $C_6D_5CD_3$, 23 °C) of **4** (top), and **4** with (p-MeO-C_6H_4)$_3$C• (bottom). Appearance of the peaks highlighted by red, dashed lines in the reaction mixture are characteristic of Fe^{III}(ttppc).[3]

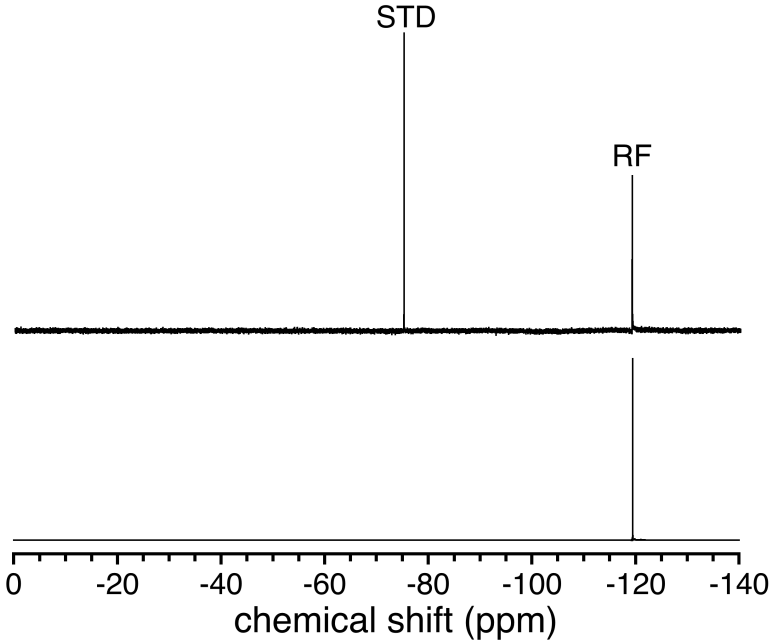

Figure S25. ^{19}F {^{1}H} NMR (300 MHz, $C_6D_5CD_3$, 23 °C) of **4** + (p-MeO-C_6H_4)$_3$C• with $CF_3C(O)OC_2H_5$ added as an internal standard (STD) (top), and the fluorinated product, (p-MeO-C_6H_4)$_3$CF (RF) (bottom).

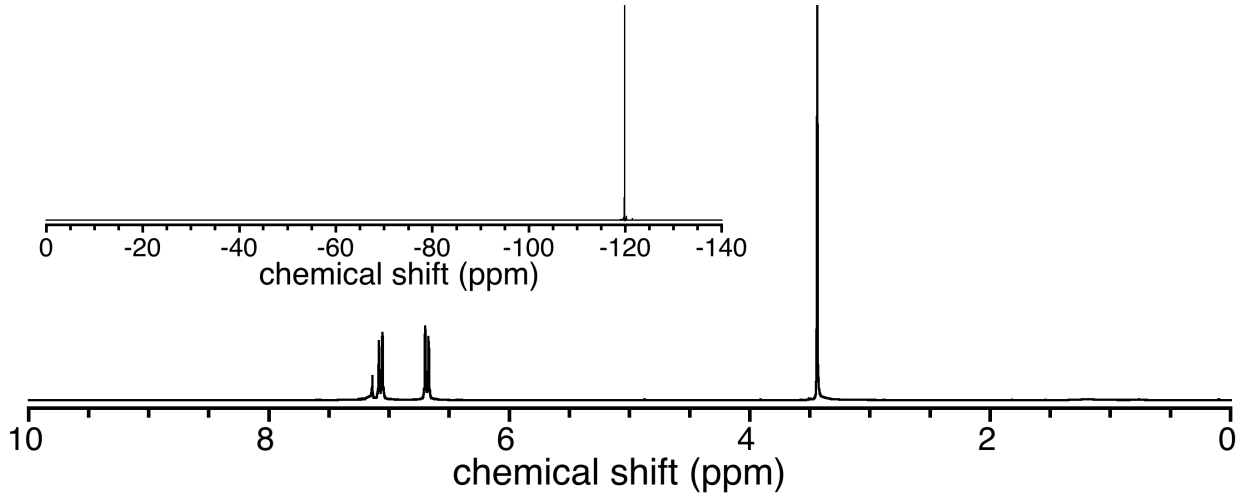

Figure S26. ^{1}H NMR (400 MHz) of (p-MeO-C_6H_4)$_3$CF in C_6D_6 at 23 °C. Inset: ^{19}F {^{1}H} NMR (300 MHz) in C_6D_6 at 23 °C.

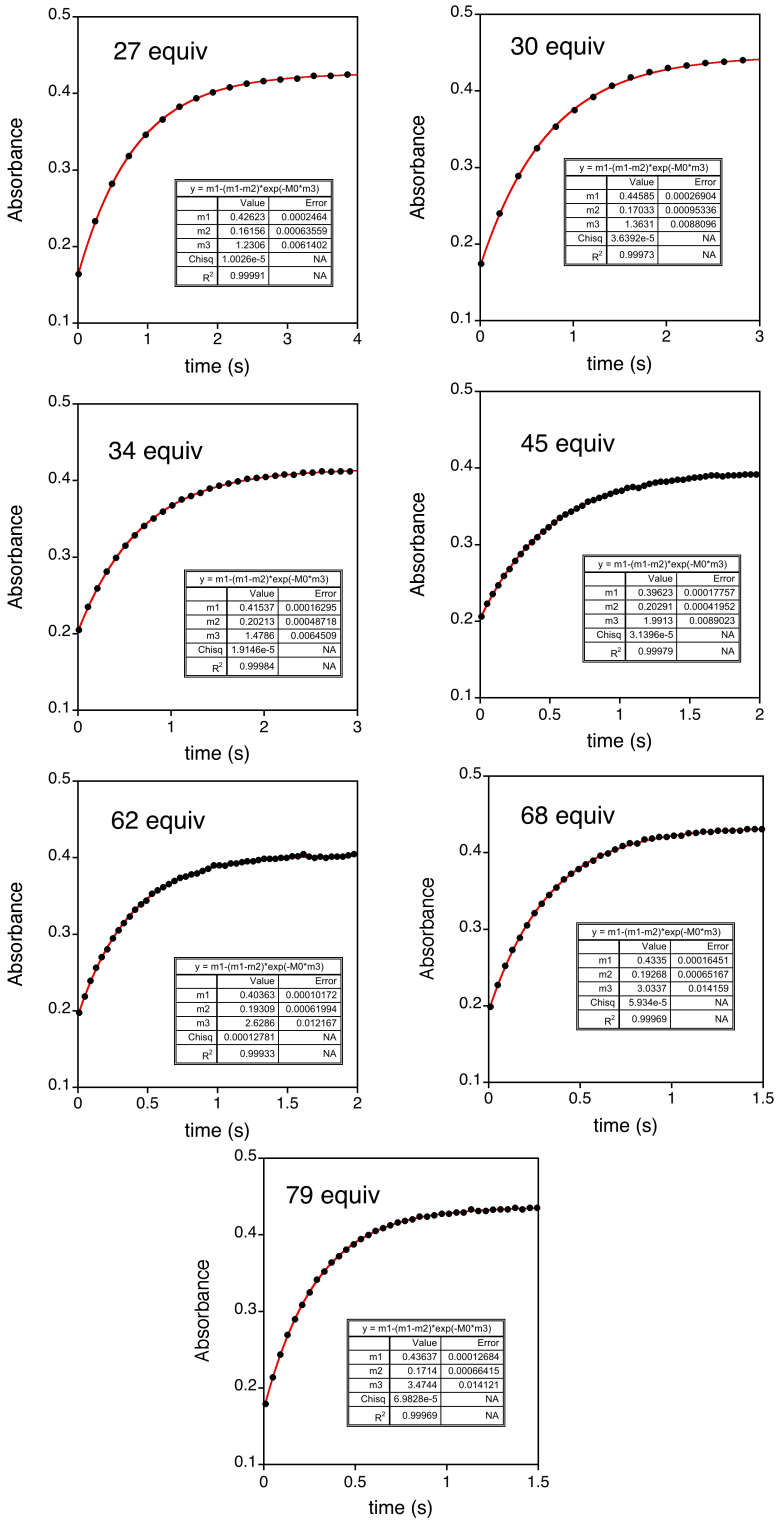

Figure S27. Kinetic study of **1** (32 μM) and (p-MeO-C_6H_4)$_3$C• (27 – 79 equiv) in $C_6H_5CH_3$ at 23 °C. Plots of changes in absorbance vs time (s) for the formation of Fe^{III}(ttppc) (573 nm) (black circles), fit to a single exponential expression (red line).

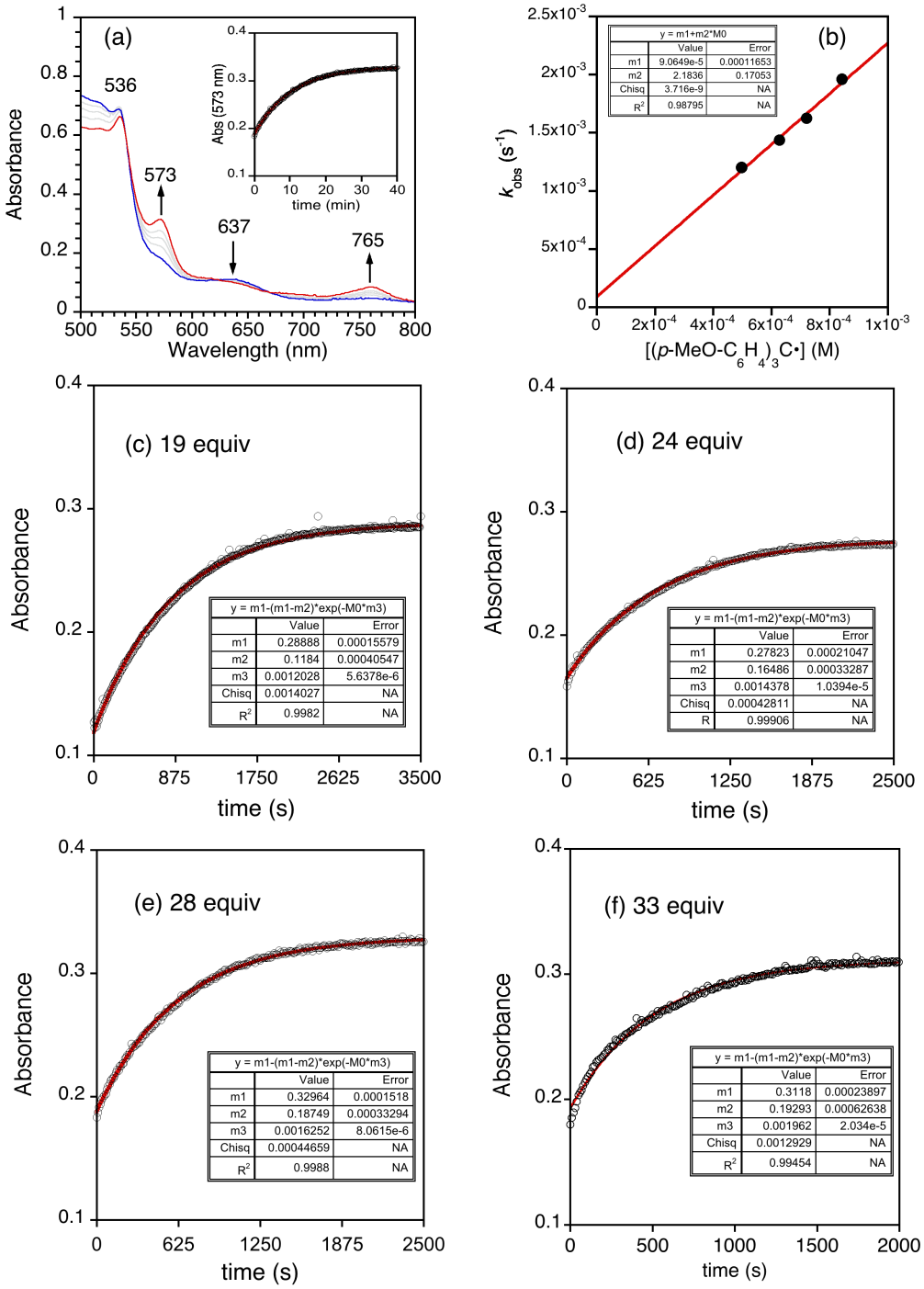

Figure S28. Kinetic study of **1** (25.8 μM) and $(p\text{-MeO-C}_6\text{H}_4)_3\text{C}\bullet$ (19 – 33 equiv) in $C_6H_5CH_3$ at -60 °C. (a) UV−vis time-resolved spectra of the addition of $(p\text{-MeO-C}_6\text{H}_4)_3\text{C}\bullet$ (28 equiv) to **1** (blue line) to form Fe^{III}(ttppc) (red line) in $C_6H_5CH_3$. Inset: Change in absorbance versus time (min) for the formation of Fe^{III}(ttppc) (573 nm) (black dots) fit to a single exponential expression (red line). (b) Plot of k_{obs} versus $[(p\text{-MeO-C}_6\text{H}_4)_3\text{C}\bullet]$ with best-fit line. (c)-(f) Plots of absorbance versus time (s) for the formation of Fe^{III}(ttppc) (573 nm), fit to a single exponential expression.

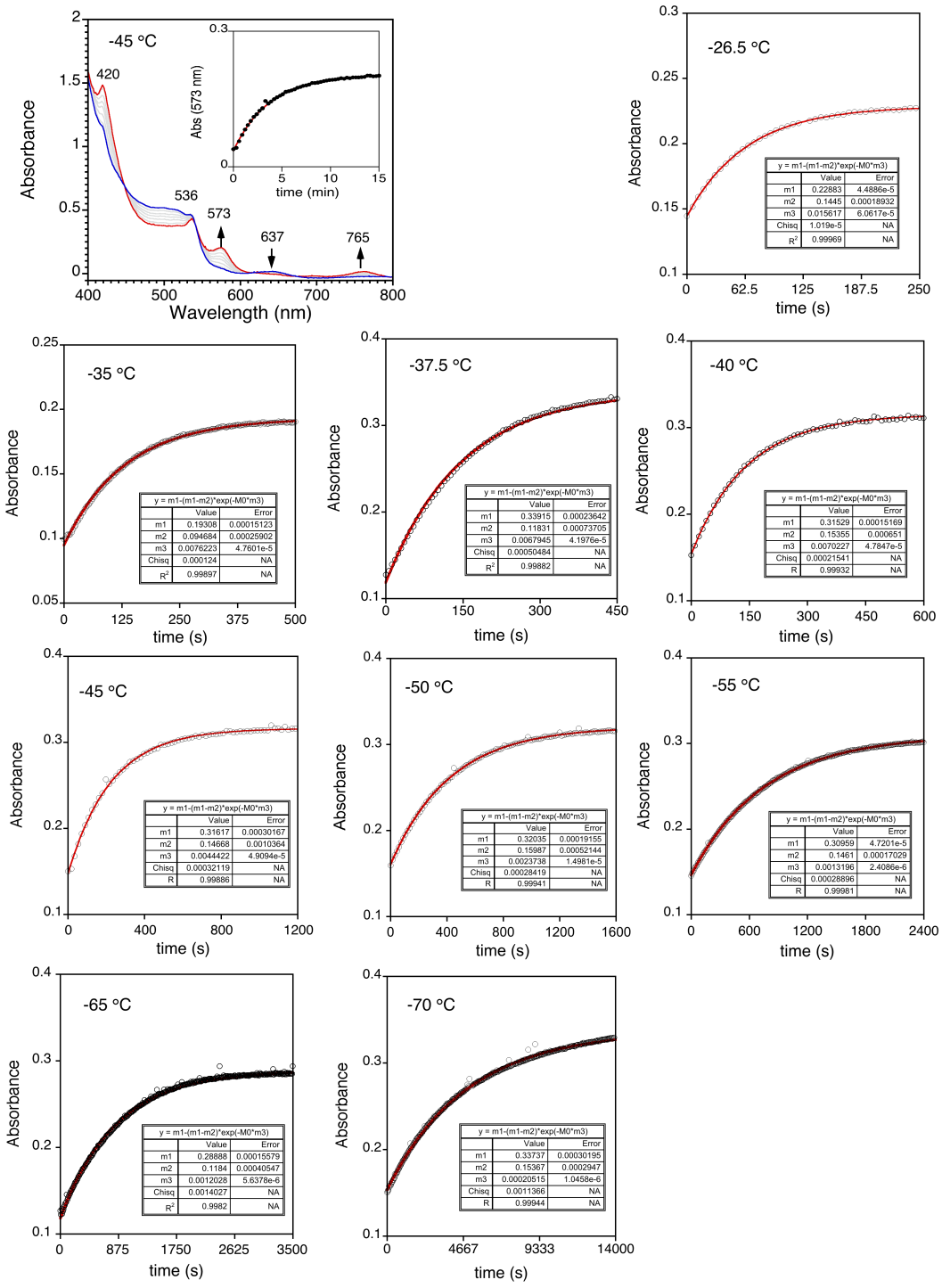

Figure S29. Temperature–dependent study of **1** and (p-MeO-C_6H_4)$_3$C• in $C_6H_5CH_3$. (top left) UV–vis time-resolved spectra of the addition of (p-MeO-C_6H_4)$_3$C• to **1** (blue line) to form Fe^{III}(ttppc) (red line) in $C_6H_5CH_3$ at -45 °C. Inset: changes in absorbance vs time (min) for the formation of Fe^{III}(ttppc) (573 nm) (black circles), fit to a single exponential expression (red line). Plots of changes in absorbance vs time (s) at different temperatures (-26.5 to -70 °C) showing the formation of Fe^{III}(ttppc) (573 nm), fit to a single exponential expression.

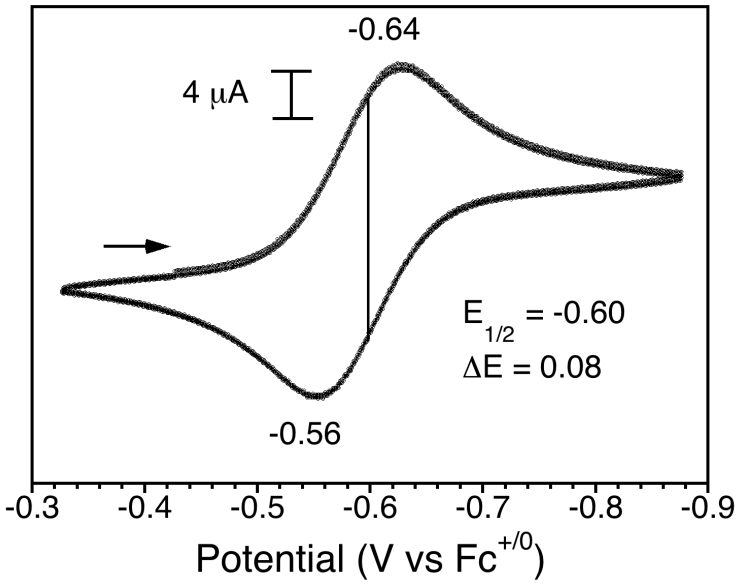

Figure S30. Cyclic voltammogram of $[(p\text{-MeO-}C_6H_4)_3C]^+(BF_4)^-$ (8 mM) in PhCN. The solution contains Bu_4N^+ PF_6^- (0.25 M) supporting electrolyte, with a scan rate of 100 mV/s.

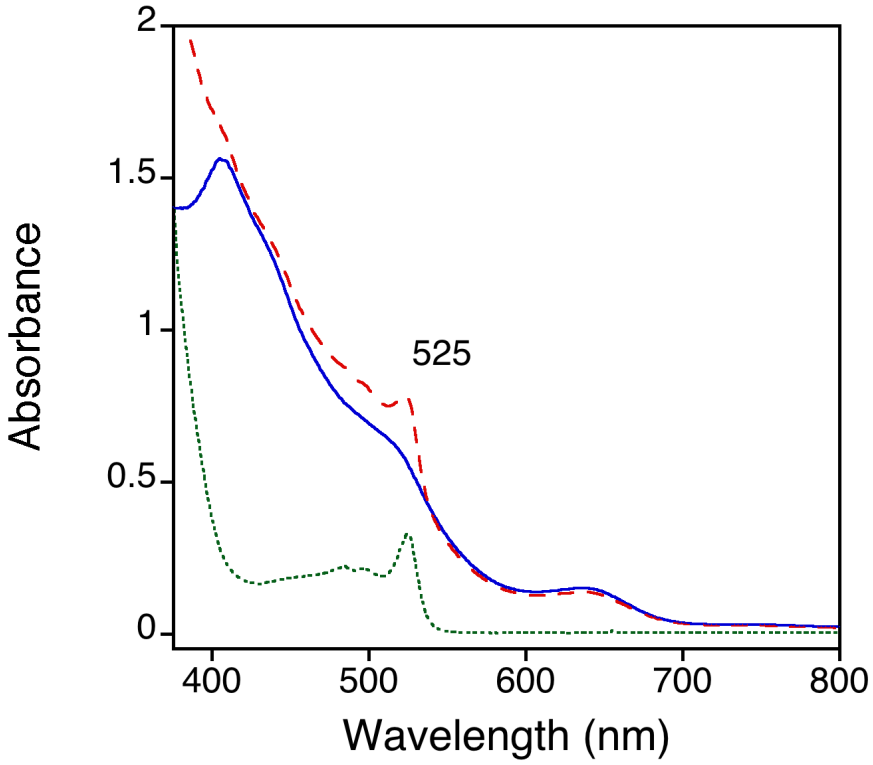

Figure S31. Overlay of UV-vis spectra of $(p\text{-tert-butyl-}C_6H_4)_3C\bullet$ (0.44 mM, green, dotted line), **1** (46 μM, t = 0, blue, solid line), and mixture of **1** and $(p\text{-tert-butyl-}C_6H_4)_3C\bullet$ (7 equiv, red, dashed line) after 100 min in $C_6H_5CH_3$ at 23 °C. No reaction is observed.

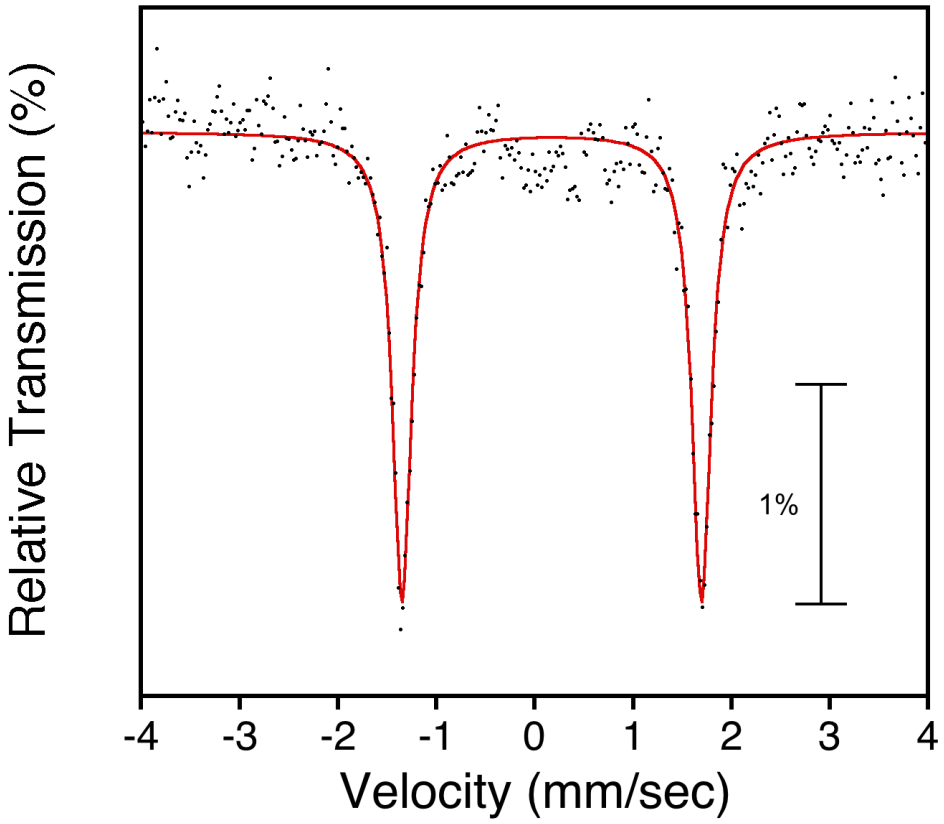

Figure S32. Zero-Field ^{57}Fe Mössbauer spectrum ($C_6H_5CH_3$, 80 K) of reaction mixture of **1** (1 mM) with (*p*-tert-butyl-$C_6H_4)_3C$• (20 equiv). Experimental data = black circles, best fit = red line with parameters $\delta = 0.18$ mm s^{-1}; $|\Delta E_Q| = 3.01$ mm s^{-1}.

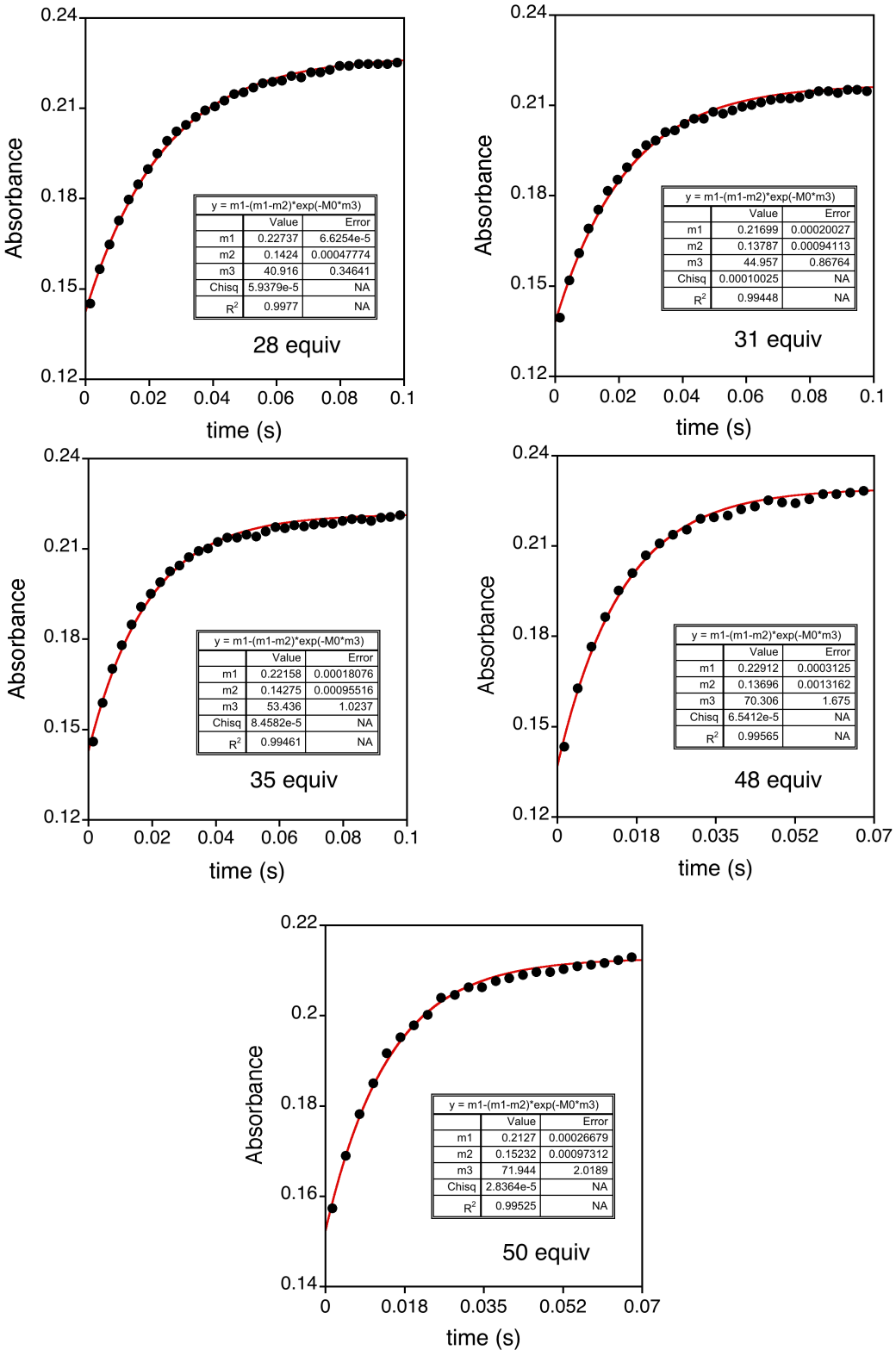

Figure S33. Kinetic study of **4** (12.5 μM) and (*p*-MeO-C_6H_4)$_3$C• (28 − 50 equiv) in $C_6H_5CH_3$ at 23 °C. Plots of changes in absorbance vs time (s) for the formation of Fe^{III}(ttppc) (573 nm) (black dots), fit to a single exponential expression (red line).

Density Functional Theory Calculations

Geometry optimizations were treated with spin-unrestricted Kohn-Sham method using the BP86 functional. Scalar relativistic effects were taken into account at the ZORA level. The basis set def2-tzvp was used on all atoms. The RIJCOSX approximation was implemented with a def2-tzvp/J auxiliary basis using a series of grids (Grid5 and FinalGrid6), and the iron atom's radial integration accuracy was increased using the "SpecialGridIntAcc" command (value 7). Dispersion effects were accounted for using keyword "D3BJ." Structures were optimized using tight self-consistent field (SCF) convergence, with the very slow convergence procedure, including a simulated conductor-like screening model "COSMO." In order to signal that the converge of the SCF was close to a minimum value, the DIIS solver was manually adjusted by using the keywords "lshift = 0.4, Damp fac = 0.9, ErrOff = 0.05, Min = 0.1 and Max = 0.99." Frequency calculations followed the same input parameters as the geometry optimizations, without any modification to SCF solver. The frequency calculation for Fe(F)(ttppc) did not converge in the initial attempt. Thus the geometry for Fe(F)(ttppc) complex was re-optimized without the former manual modifications to the SCF solver, and the criteria for convergence was increased using the keyword "TightOpt." Frequency calculations were run on the re-optimized geometry at the same level of theory, and this time, with no imaginary frequencies observed.

Fe(F)(ttppc) – Optimized Structure Coordinates:

Fe	-4.67052	5.99294	16.01176
F	-3.22872	5.18110	15.28731
C	-4.76604	8.25549	14.34484
C	-5.12511	8.70939	13.04158
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C	-5.90275	7.71080	12.46464
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C	-7.50562	3.33206	14.55076
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H	-7.66396	1.83185	16.16617
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C	-7.49364	3.56840	10.16797
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H	-1.12818	5.67989	18.41013
N	-5.33059	7.01609	14.55127
N	-6.07170	4.72531	15.67971
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N	-3.97536	7.70209	16.44455

Fe(Cl)(ttppc) – Optimized Structure Coordinates:

Fe	-4.53495	5.94540	15.96640
Cl	-2.70063	5.04133	15.15995
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C	-6.53127	4.43128	14.38363
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C	-5.63691	3.32698	17.67785
C	-4.79092	4.22958	18.33673
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H	-2.97646	5.46213	20.82878
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H	-11.24535	3.24590	5.07308
C	-11.43857	3.92264	7.11962
H	-12.52201	4.03969	7.06478
C	-10.77195	4.21419	8.31077
H	-11.34346	4.54208	9.18031
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C	-5.86317	1.64909	11.63214
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C	-4.47790	3.57906	12.07018
H	-4.32845	4.65833	12.07912
C	-6.04836	2.10055	18.41288
C	-5.12350	1.05507	18.62721
C	-5.52534	-0.07441	19.35095
H	-4.79862	-0.86844	19.52801
C	-6.83167	-0.20443	19.84569
C	-7.74244	0.83550	19.60348
H	-8.76844	0.75104	19.96415
C	-7.36859	1.98909	18.90465
C	-3.73485	1.14651	18.10792
C	-3.47437	1.47918	16.76735
H	-4.30039	1.64314	16.07580
C	-2.16390	1.61023	16.30983
H	-1.98633	1.89004	15.27151
C	-1.08959	1.40310	17.17936
H	-0.06478	1.51791	16.82328
C	-1.33617	1.05047	18.51000
H	-0.50411	0.88910	19.19741
C	-2.64826	0.92111	18.96945
H	-2.83727	0.67387	20.01562
C	-7.24115	-1.41063	20.60032
C	-6.71723	-2.67615	20.27731
H	-6.01832	-2.77406	19.44530
C	-7.10402	-3.81300	20.98886
H	-6.69280	-4.78629	20.71646
C	-8.02165	-3.70843	22.03941
H	-8.32347	-4.59689	22.59583
C	-8.54953	-2.45631	22.37127

H	-9.25963	-2.36251	23.19440
C	-8.16399	-1.31958	21.65885
H	-8.56531	-0.34525	21.94171
C	-8.36685	3.06287	18.65870
C	-9.59242	2.74433	18.05089
H	-9.80458	1.70631	17.78879
C	-10.51642	3.74382	17.73939
H	-11.45518	3.47979	17.25002
C	-10.23120	5.07948	18.03723
H	-10.94855	5.86242	17.78716
C	-9.02489	5.40387	18.66509
H	-8.79728	6.44091	18.91230
C	-8.10175	4.40593	18.97798
H	-7.16789	4.67445	19.47207
C	-2.36543	7.96166	19.83742
C	-3.05970	8.24787	21.03762
C	-2.36002	8.78564	22.12394
H	-2.90431	8.98931	23.04699
C	-0.98772	9.06717	22.04962
C	-0.31725	8.78383	20.85131
H	0.74985	8.99347	20.76806
C	-0.97905	8.22799	19.74900
C	-4.51425	7.97620	21.17293
C	-5.43958	8.42722	20.21653
H	-5.09615	9.02867	19.37509
C	-6.79370	8.11307	20.33473
H	-7.49647	8.47433	19.58233
C	-7.24817	7.34485	21.41129
H	-8.30496	7.08860	21.49682
C	-6.33978	6.91048	22.38097
H	-6.68435	6.31064	23.22469
C	-4.98545	7.22829	22.26457
H	-4.27532	6.86231	23.00808
C	-0.26647	9.64391	23.20650
C	-0.90225	10.55402	24.07132
H	-1.93184	10.85617	23.87384
C	-0.22209	11.09853	25.16179
H	-0.73046	11.80955	25.81491
C	1.10753	10.74318	25.41166
H	1.63892	11.16815	26.26435
C	1.75094	9.83883	24.56027
H	2.78525	9.54853	24.75132
C	1.07156	9.29552	23.46875
H	1.57709	8.57394	22.82527
C	-0.20575	7.92688	18.51737
C	0.65379	8.89762	17.97608

H	0.73725	9.87070	18.46323
C	1.36936	8.64305	16.80447
H	2.02103	9.41429	16.39050
C	1.23928	7.41091	16.15581
H	1.79062	7.21481	15.23487
C	0.39577	6.43387	16.69305
H	0.27819	5.47209	16.19322
C	-0.31595	6.68727	17.86489
H	-0.97004	5.91582	18.27030
N	-5.19191	6.94291	14.49571
N	-5.85804	4.61475	15.58657
N	-4.39683	5.45259	17.80996
N	-3.92619	7.67662	16.42794

[Fe(OTf)(ttppc)(AgOTf)] – XRD Structure Coordinates:

Fe	15.65423	8.45242	3.94341
C	18.13114	11.57439	5.86946
F	17.09782	11.68099	6.70828
F	18.02767	12.53575	4.94997
F	19.27248	11.77479	6.54230
S	18.16694	9.93334	5.10121
O	16.78547	9.99584	4.49197
O	18.25794	9.01643	6.18746
O	19.24136	10.00106	4.19995
C	17.32801	6.28356	4.40956
C	17.79070	5.33724	5.37365
H	18.51816	4.73495	5.27113
C	16.99106	5.46262	6.46629
H	17.05517	4.95507	7.26682
C	16.02992	6.50192	6.19560
C	14.95909	6.97148	6.92584
C	14.10238	7.99697	6.42538
C	12.93083	8.49019	7.07379
H	12.62348	8.24075	7.93740
C	12.33006	9.38221	6.23613
H	11.53726	9.87510	6.41242
C	13.11810	9.43806	5.03897
C	12.83887	10.17767	3.89203
C	13.58503	10.11802	2.70379
C	13.24284	10.73191	1.45524
H	12.50925	11.31375	1.29481
C	14.18148	10.31817	0.52742
H	14.21100	10.56016	-0.39079
C	15.09457	9.46244	1.20453
C	16.18824	8.76908	0.59819

C	16.96887	7.86518	1.31370
C	18.04772	7.01401	0.90786
H	18.44100	6.98254	0.04357
C	18.41057	6.25417	1.98693
H	19.09155	5.59204	2.00882
C	17.57441	6.64449	3.06930
C	14.55522	6.28118	8.19029
C	13.97188	4.99705	8.11350
C	13.50365	4.39724	9.28720
H	13.11454	3.53181	9.23715
C	13.58704	5.02392	10.52139
C	14.19975	6.26738	10.57879
H	14.28194	6.70101	11.41994
C	14.69825	6.89940	9.44387
C	13.80606	4.25568	6.83432
C	13.23279	4.81815	5.69301
H	12.96137	5.72846	5.70090
C	13.05774	4.05471	4.54354
H	12.68041	4.45141	3.76743
C	13.42649	2.72359	4.52105
H	13.29067	2.20292	3.73807
C	13.99141	2.15722	5.63871
H	14.25293	1.24402	5.62485
C	14.18400	2.91201	6.78662
H	14.57959	2.50970	7.55110
C	12.98070	4.43208	11.75094
C	11.87100	3.60149	11.66736
H	11.53704	3.34696	10.81570
C	11.24579	3.14057	12.82477
H	10.48576	2.57378	12.75167
C	11.70737	3.48787	14.05587
H	11.26271	3.18217	14.83747
C	12.81757	4.28314	14.16135
H	13.15306	4.51689	15.01918
C	13.45534	4.74932	13.01984
H	14.22836	5.29520	13.10647
C	15.37377	8.21615	9.63409
C	14.78574	9.17675	10.46109
H	13.92781	9.01405	10.83490
C	15.43895	10.36295	10.74109
H	15.03360	10.99990	11.31694
C	16.66356	10.62233	10.19544
H	17.11476	11.43285	10.39935
C	17.24004	9.70021	9.34614
H	18.07819	9.89055	8.94234
C	16.60067	8.49394	9.07643

H	17.01312	7.85803	8.50398
C	11.59622	11.01166	3.87555
C	10.33964	10.38090	3.80342
C	9.18667	11.15671	3.79081
H	8.34018	10.72551	3.77902
C	9.23712	12.55535	3.79508
C	10.49677	13.16591	3.83638
H	10.55249	14.11421	3.82963
C	11.66824	12.41805	3.88718
C	10.22154	8.89275	3.67505
C	10.78244	8.23561	2.58260
H	11.26075	8.73112	1.92827
C	10.64595	6.85785	2.44357
H	11.02809	6.41804	1.69268
C	9.96133	6.12703	3.38885
H	9.86902	5.18684	3.28833
C	9.40654	6.76273	4.48460
H	8.94187	6.25743	5.14162
C	9.52799	8.15046	4.62634
H	9.13587	8.58653	5.37396
C	7.99123	13.35851	3.69716
C	6.82153	12.94914	4.33626
H	6.83222	12.17365	4.88480
C	5.64519	13.66186	4.17959
H	4.85618	13.36773	4.62018
C	5.60446	14.79332	3.38943
H	4.79325	15.27501	3.27809
C	6.76571	15.21694	2.76312
H	6.75166	15.99753	2.22165
C	7.94507	14.51135	2.91960
H	8.73496	14.81836	2.49003
C	12.98059	13.12527	3.94070
C	13.31805	14.04235	2.93027
H	12.70325	14.21890	2.22787
C	14.55212	14.69536	2.95373
H	14.78292	15.29790	2.25644
C	15.44178	14.46567	3.99363
H	16.28586	14.90198	4.00715
C	15.08831	13.59424	5.01202
H	15.68436	13.45712	5.73937
C	13.87081	12.91827	4.98157
H	13.64984	12.31181	5.67860
C	16.44063	8.97185	-0.85376
C	16.32036	7.90777	-1.76336
C	16.58407	8.13283	-3.11467
H	16.53491	7.40270	-3.72044

C	16.91788	9.39526	-3.60505
C	17.00275	10.44938	-2.69720
H	17.19609	11.32293	-3.01642
C	16.81055	10.25001	-1.33347
C	15.91127	6.53705	-1.33600
C	14.77213	6.32329	-0.56135
H	14.22742	7.05957	-0.30885
C	14.42825	5.03628	-0.15532
H	13.64600	4.89652	0.36487
C	15.22620	3.95723	-0.50880
H	14.99532	3.08144	-0.22225
C	16.34880	4.15580	-1.27259
H	16.89380	3.41558	-1.51245
C	16.69402	5.43675	-1.69840
H	17.46567	5.56328	-2.23807
C	17.20402	9.60782	-5.04866
C	17.80398	8.59661	-5.79965
H	17.99523	7.75798	-5.39701
C	18.12286	8.81206	-7.13177
H	18.53316	8.11955	-7.63580
C	17.84944	10.02071	-7.73093
H	18.07772	10.16376	-8.64144
C	17.24644	11.02607	-7.00379
H	17.04604	11.85589	-7.42053
C	16.92790	10.82637	-5.66663
H	16.52118	11.52649	-5.16943
C	17.11556	11.36503	-0.40041
C	18.02859	11.19851	0.63465
H	18.44910	10.35508	0.75401
C	18.33921	12.24837	1.50217
H	18.96096	12.11410	2.20778
C	17.74046	13.48133	1.33173
H	17.94439	14.19405	1.92573
C	16.83912	13.68046	0.29260
H	16.43802	14.53262	0.16848
C	16.52220	12.62488	-0.57182
H	15.90208	12.76284	-1.27808
N	16.28862	6.98590	4.93891
N	14.20555	8.59381	5.18633
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N	16.72274	7.61417	2.63999
Ag	14.67467	12.72722	1.21539
C	11.02134	13.94600	-0.52800
F	10.78981	15.20330	-0.17393
F	10.01784	13.56040	-1.31195
F	10.96854	13.19285	0.57609

S	12.63815	13.78126	-1.36469
O	13.56739	14.26059	-0.35155
O	12.73455	12.37032	-1.62026
O	12.51379	14.63555	-2.51357

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