Supporting Information

for

"Six-coordinate iron(II) and cobalt(II) paraSHIFT agents for measuring temperature by magnetic resonance spectroscopy"

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Instrumentation

Varian Inova 500 MHz NMR spectrometer equipped with FTS Systems TC-84 Kinetics Air Jet Temperature Controller was used to collect ^{1}H NMR spectra. ^{13}C NMR spectra were acquired using a Varian Mercury 300 MHz NMR spectrometer operating at 75 MHz. A Thermo Scientific Orion 9826BN NMR micro pH electrode connected to a SympHony SB20 pH meter and the Orion 8115BNUWP Ross-ultra semi-micro pH electrode connected to a Titrino 702 pH meter were used for pH measurements. ThermoFinnigan LCQ Advantage IonTrap LC/MS equipped with a Surveyor HPLC system was used to collect mass spectral data.

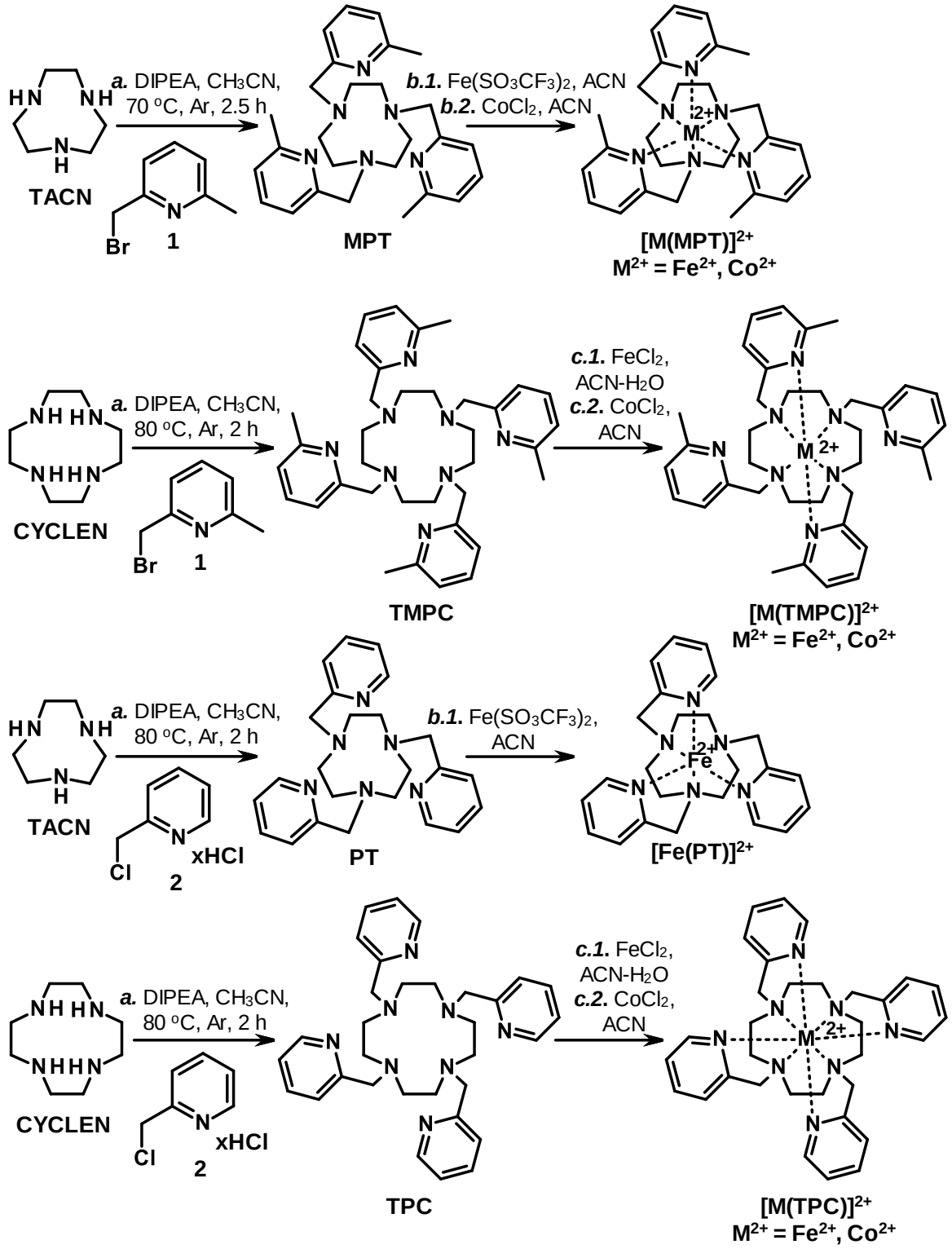
Materials

All solvents and reagents were reagent grade, and they were used as received without additional purification. 1,4,7-Triazacyclononane (TACN) was purchased from TCI America (Portland, OR). 1,4,7,10-Tetraazacyclododecane (CYCLEN) and Iron(II) trifluoromethanesulfonate (98%) were obtained from Strem Chemicals, Inc. (Newburyport, MA). *N*,*N*-Diisopropylethylamine (DIPEA), 3-(trimethylsilyl)propionic acid sodium salt (TMSP) and albumin from porcine serum were obtained from Sigma-Aldrich (St. Louis, MO). 2-Bromomethyl-6-methylpyridine (97%), 2-picolyl chloride hydrochloride, Cobalt(II) chloride hexahydrate (98%), Cobalt(II) nitrate hexahydrate (97%) and Iron(II) chloride tetrahydrate (98%) were received from Alfa Aesar (Ward Hill, MA). Basic alumina (50-200 μm) was purchased from Dynamic Adsorbents, Inc. (Norcross, GA).

1,4,7-Tris[(6-methyl-2-pyridyl)methyl]-1,4,7-triazacyclononane (MPT) was prepared using a similar procedure as described for TMPC synthesis. TACN (0.34 g, 2.62 mmol), 2-bromomethyl-6-methylpyridine (1.46 g, 7.86 mmol, 3.0 equiv.) and DIPEA (2.1 mL, 11.8 mmol, 4.5 equiv.) were stirred in 50 mL of acetonitrile at 70 ^{o}C for 2.5 hours (Scheme S1). After extraction with chloroform, the crude product was subjected to basic Al_2O_3 column chromatography using 1 to 10% of methanol in methylene chloride as the eluting solvent. Yield: 0.72 g, 1.62 mmol, 62%. ^{1}H NMR, 500 MHz ($CDCl_3$, ppm): δ = 7.49 t (3H, Ar), 7.31 d (3H, Ar), 6.95 d (3H, Ar), 3.77 s (6H, $3CH_2$), 2.85 s (12H, $6CH_2$), 2.47 s (9H, $3CH_3$). ^{13}C NMR, 75 MHz ($CDCl_3$, ppm): δ = 159.75, 157.20, 136.35, 121.08, 119.82, 64.79, 55.80, 24.32. ESI-MS (m/z): $[M+H^+]$, calculated: 445.3, found: 445.3 (100%).

1,4,7,10-Tetrakis(2-pyridylmethyl)-1,4,7,10-tetrazacyclododecane (TPC) was prepared using a similar procedure as described for TMPC synthesis. CYCLEN (0.20 g, 1.16 mmol), 2-picolyl chloride hydrochloride (0.76 g, 4.64 mmol, 4.0 equiv.) and DIPEA (2.0 mL, 11.6 mmol, 10 equiv.) were stirred in 30 mL of acetonitrile at 80 ^{o}C for 2 hours (Scheme S1). After extraction with chloroform, the crude product was subjected to basic Al_2O_3 column chromatography using 1 to 4% of methanol in methylene chloride as the eluting solvent. Yield: 0.47 g, 0.85 mmol, 73%. ^{1}H NMR, 500 MHz ($CDCl_3$, ppm): δ = 8.48 d (4H, Ar), 7.69 d (4H, Ar), 7.43 t (4H, Ar), 7.09 t (4H, Ar), 3.66 s (8H, $4CH_2$), 2.79 s (16H, $8CH_2$). ^{13}C NMR, 75 MHz ($CDCl_3$, ppm): δ = 160.07, 148.85, 136.15, 122.92, 121.67, 61.54, 53.34. ESI-MS (m/z): $[M+Na^+]^+$, calculated: 559.3, found: 559.4 (100%).

Reaction Schemes



Scheme S1. Synthesis of MPT, TMPC, PT, TPC ligands and $[M(MPT)]^{2+}$, $[M(TMPC)]^{2+}$, $[Fe(PT)]^{2+}$, $[M(TPC)]^{2+}$ complexes (M^{2+} = Fe^{2+}, Co^{2+}).

Overlap of crystal structures

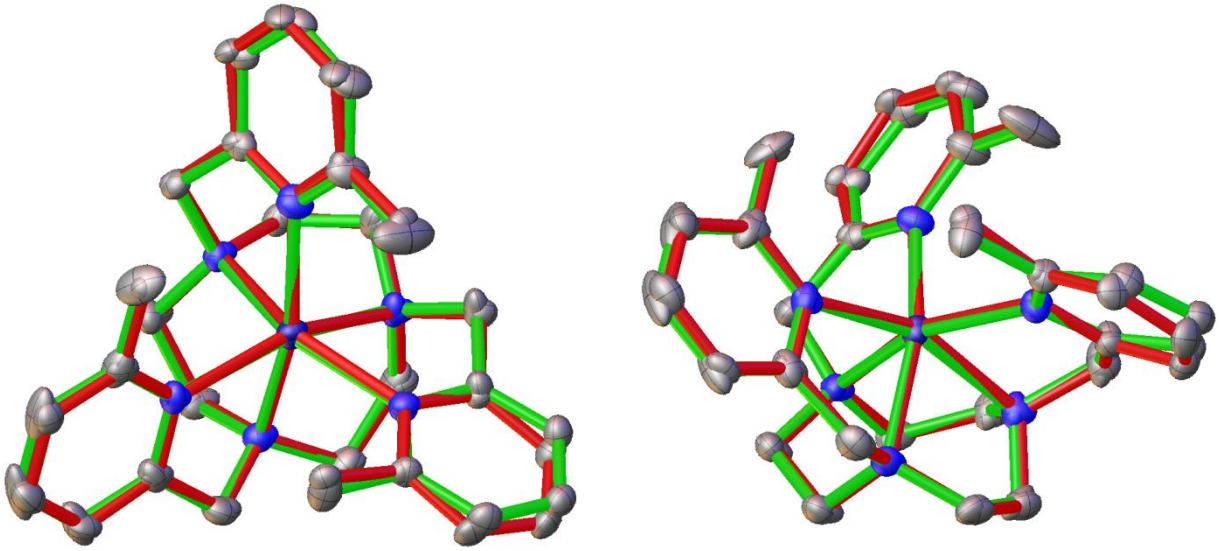


Figure S1. The overlay of the $[Fe4(MPT)]^{2+}$ (red) and $[Co(MPT)]^{2+}$ (green) crystal structures.

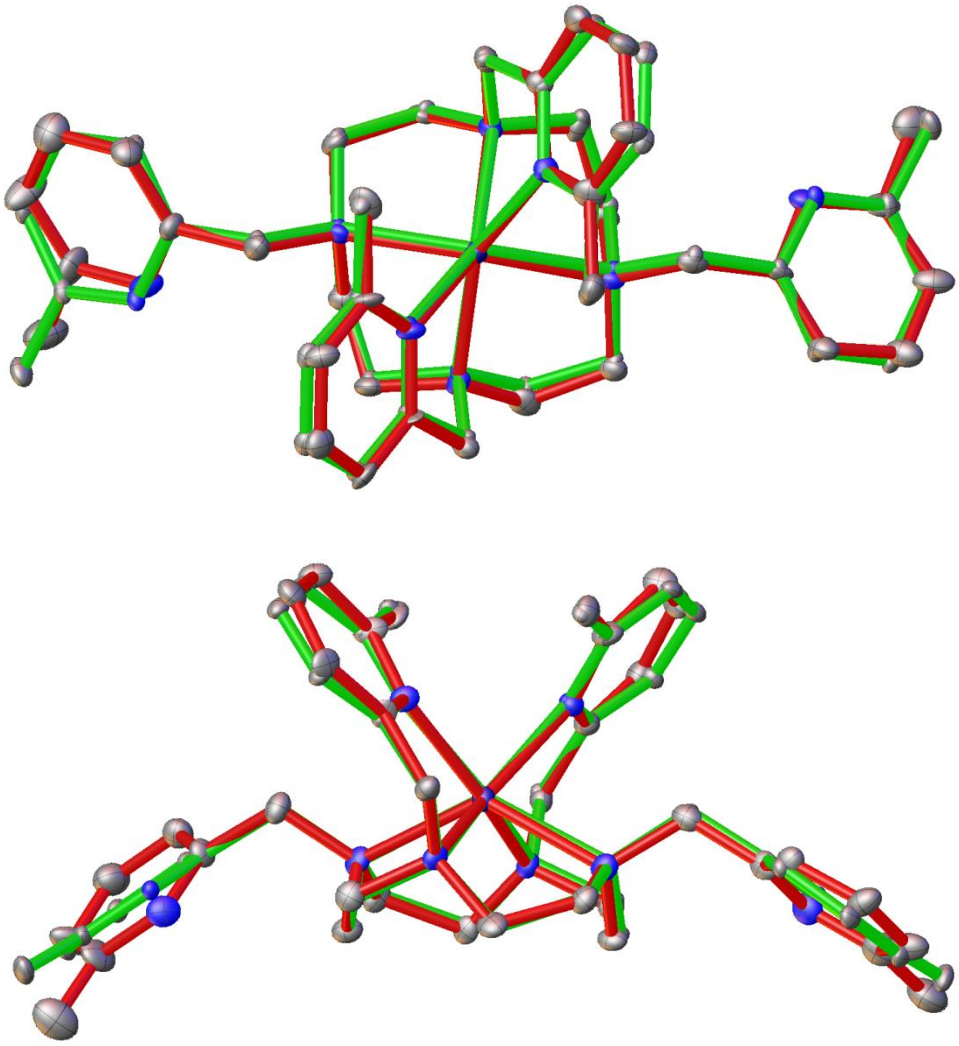


Figure S2. The overlay of the $[Fe(TMPC)]^{2+}$ (red) and $[Co(TMPC)]^{2+}$ (green) crystal structures.

^{1}H NMR data for $[Fe(MPT)]^{2+}$

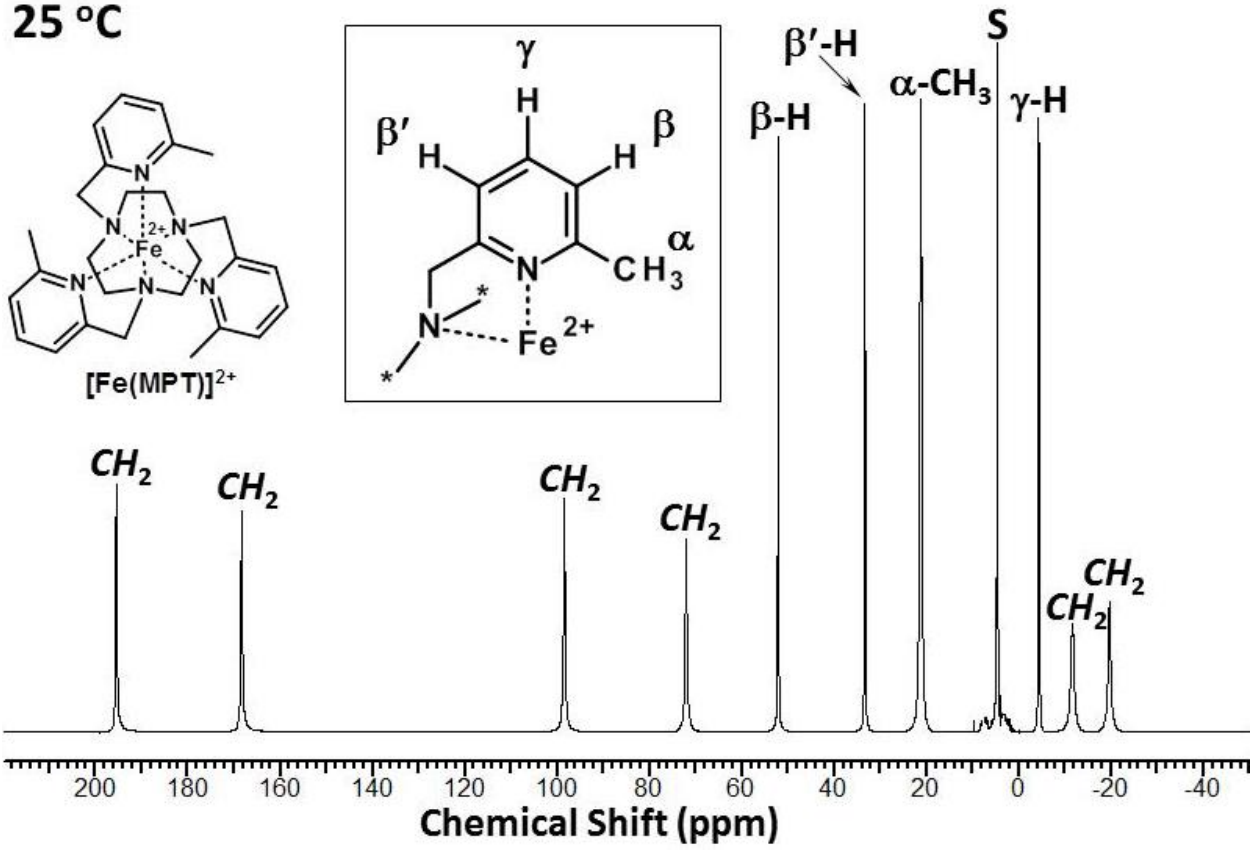


Figure S3. ^{1}H NMR spectrum of 36 mM $[Fe(MPT)]^{2+}$ at 25 °C in 100 mM NaCl, D_2O, pD 7.60. Aromatic protons and their ^{1}H NMR resonances are labeled with β, β′ and γ, while solvent peak is labeled with "s".

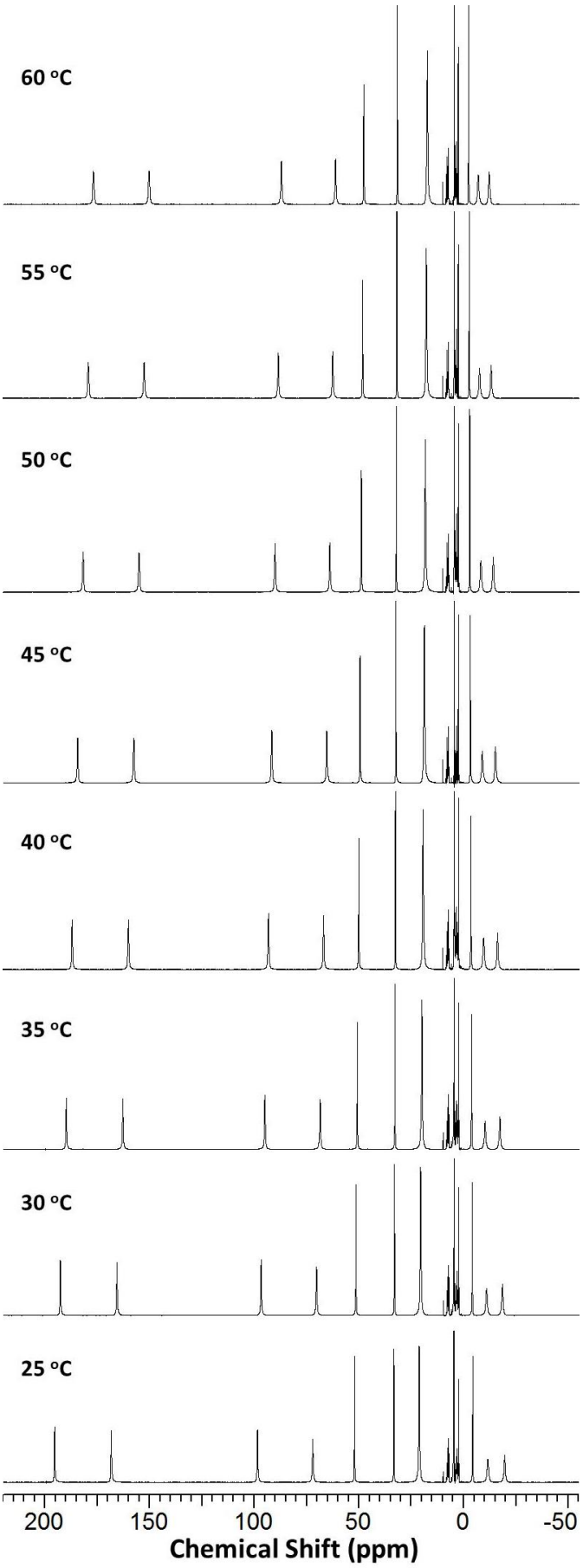


Figure S4. Variable temperature ^{1}H NMR spectra of $[Fe(MPT)]^{2+}$ at 25 to 60 °C in 100 mM NaCl, D_2O, pD 7.60.

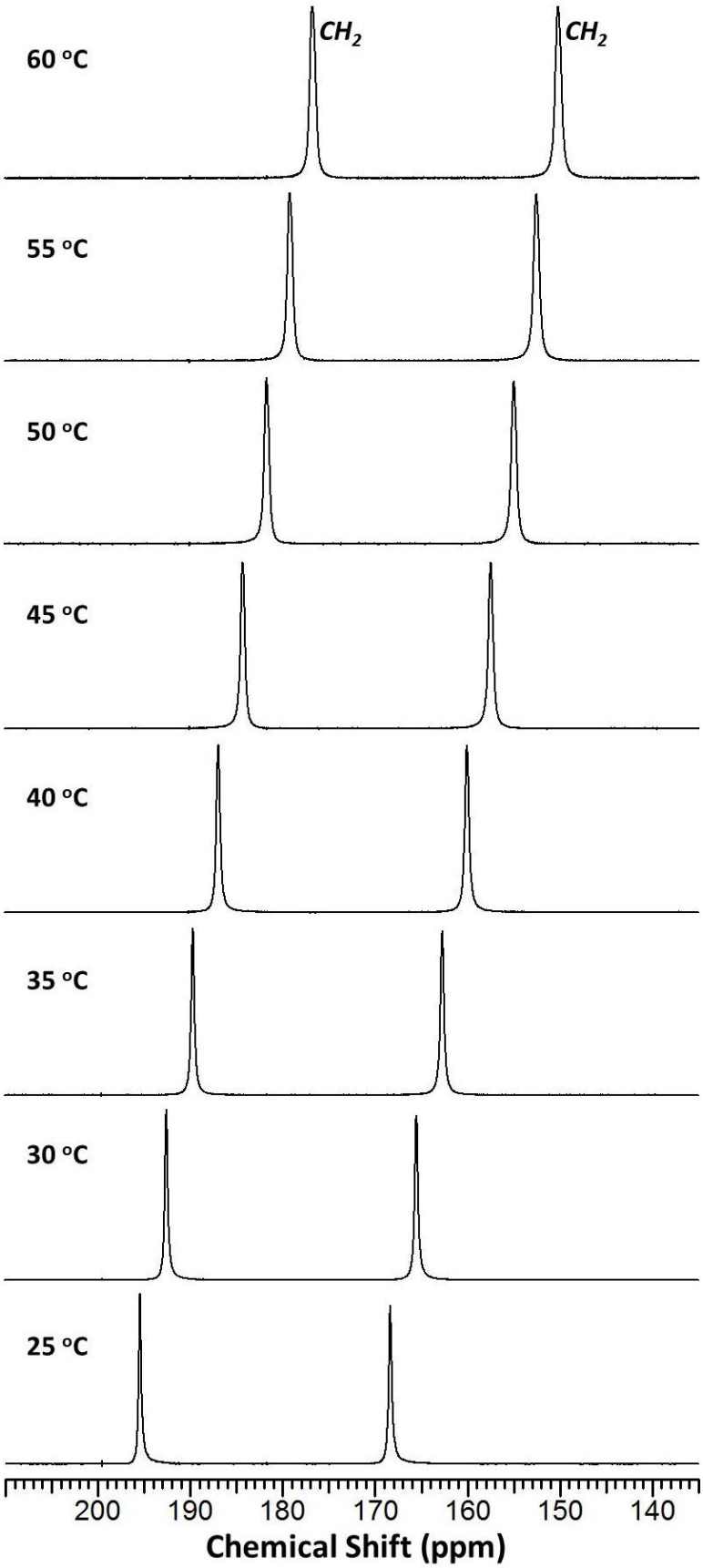


Figure S5. Expansion showing ^{1}H NMR resonances of two downfield highly-shifted CH_2 peaks of $[Fe(MPT)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.60.

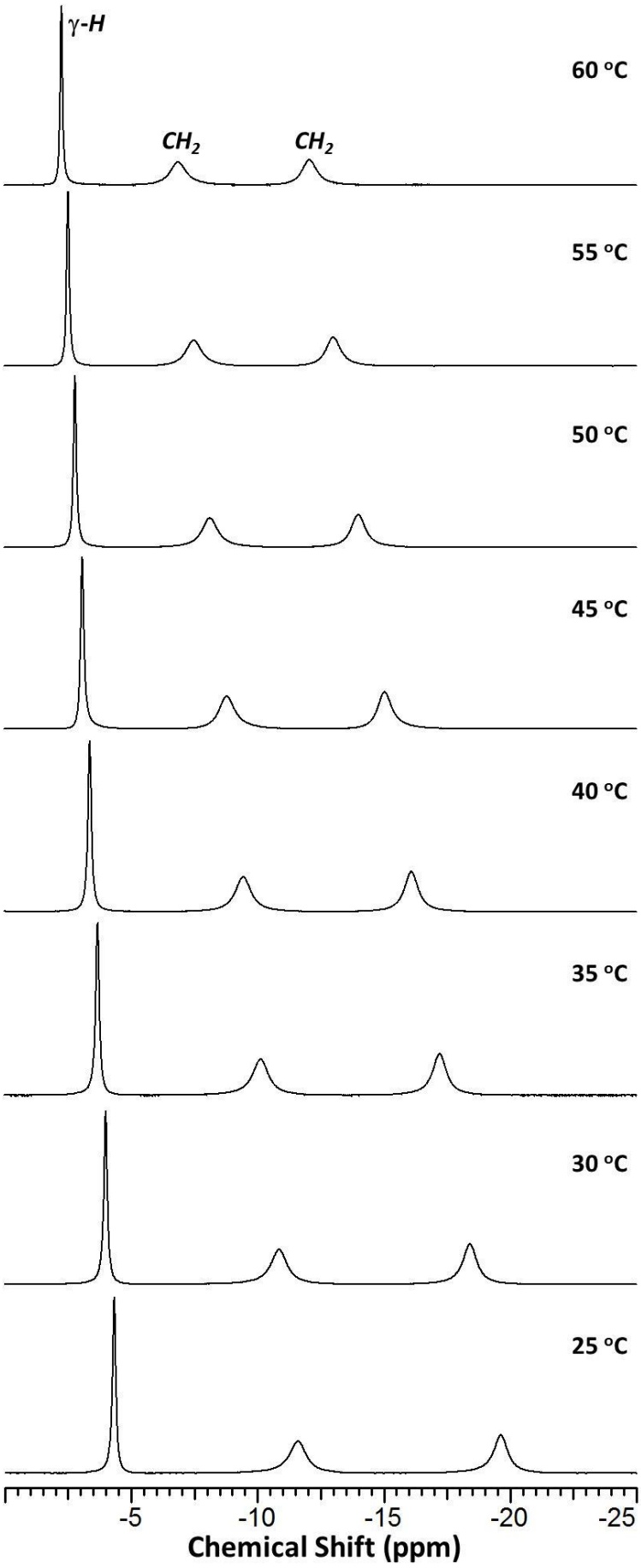


Figure S6. Expansion showing ^{1}H NMR resonances of some upfield shifted peaks of $[Fe(MPT)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.60.

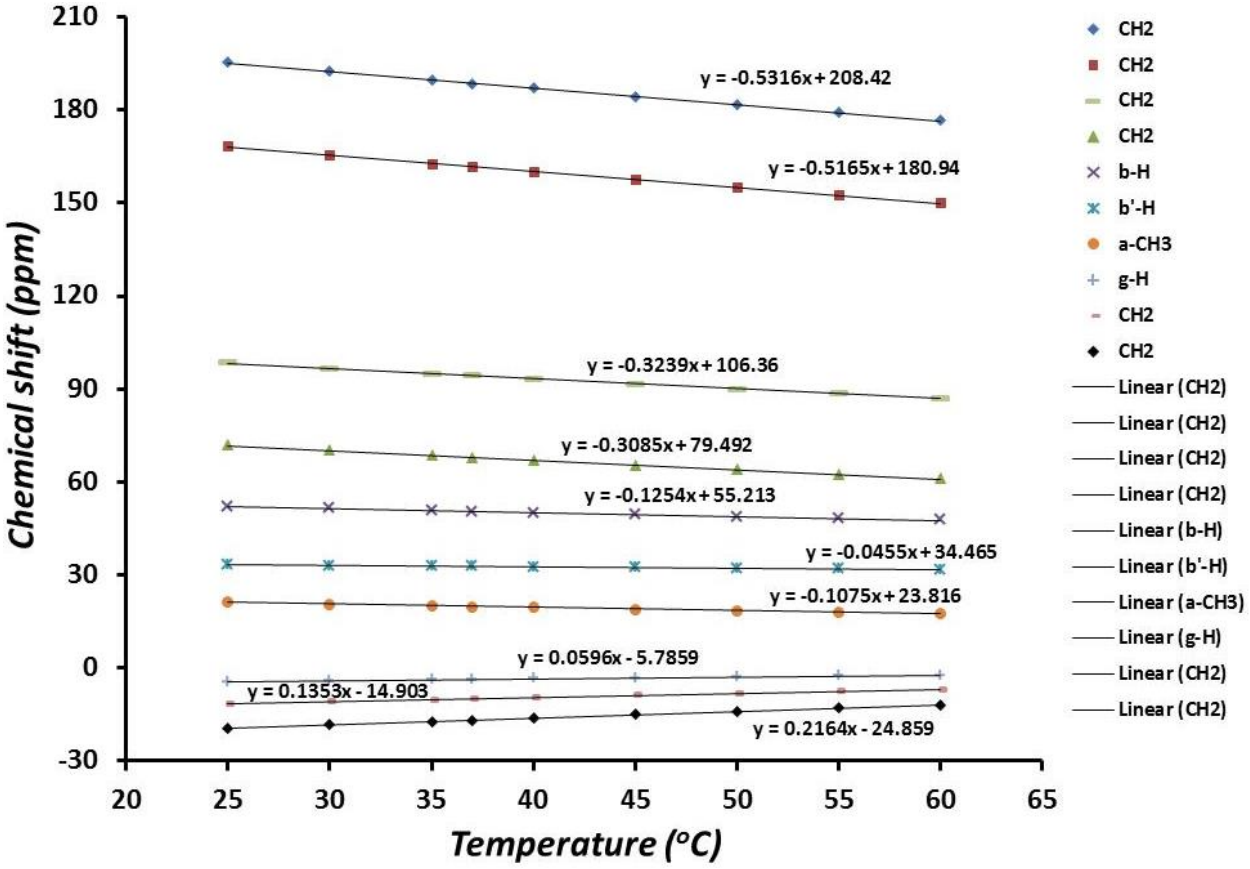


Figure S7. Linear fit of temperature-dependent paramagnetically-shifted ^{1}H NMR resonances of $[Fe(MPT)]^{2+}$ in the range of 25 to 60 ^{o}C. Solutions contained 100 mM NaCl, D_2O, pD 7.60.

Table S1. Chemical shift and peak width of ^{1}H NMR resonances of 36 mM $[Fe(MPT)]^{2+}$, 100 mM NaCl, D_2O, pD 7.60 as a function of temperature.

	Type of $[Fe(MPT)]^{2+}$ protons										
T (^{o}C)	***CH_2***	***CH_2***	***CH_2***	***CH_2***	***β-H***	***β′-H***	***α-CH_3***	**S**	***γ-H***	***CH_2***	***CH_2***
	Peak width in FWHM (*Hz*)										
25	149	175	179	213	75.1	70.7	207	8.80	73.4	358	307
30	173	193	187	211	81.3	69.8	211	7.64	78.3	350	302
35	193	209	196	211	86.6	66.1	217	6.89	80.1	345	298
37	207	223	203	215	89.7	64.3	220	7.03	80.1	344	300
40	226	241	214	221	93.8	61.4	225	7.30	78.9	347	303
45	263	276	231	232	100	56.3	232	7.43	74.5	348	309
50	294	308	247	243	104	52.3	237	7.54	67.8	351	316
55	326	338	263	255	107	50.5	237	8.21	60.8	353	321
60	353	362	277	263	108	50.1	229	9.33	54.7	359	330
T (^{o}C)	***^{1}H NMR Chemical shift (ppm)***										
25	*195.45*	*168.36*	*98.46*	*72.09*	*52.14*	*33.33*	*21.22*	*4.67*	*-4.34*	*-11.63*	*-19.65*
30	*192.56*	*165.53*	*96.70*	*70.31*	*51.47*	*33.10*	*20.62*	*4.67*	*-4.01*	*-10.87*	*-18.41*
35	*189.70*	*162.75*	*94.96*	*68.59*	*50.80*	*32.87*	*20.02*	*4.67*	*-3.68*	*-10.11*	*-17.21*
37	*188.60*	*161.68*	*94.29*	*67.94*	*50.54*	*32.78*	*19.79*	*4.67*	*-3.56*	*-9.85*	*-16.76*
40	*186.96*	*160.08*	*93.29*	*66.96*	*50.16*	*32.65*	*19.46*	*4.67*	*-3.37*	*-9.44*	*-16.09*
45	*184.29*	*157.50*	*91.67*	*65.43*	*49.53*	*32.41*	*18.92*	*4.67*	*-3.08*	*-8.77*	*-15.02*
50	*181.74*	*154.99*	*90.09*	*63.96*	*48.92*	*32.19*	*18.41*	*4.67*	*-2.79*	*-8.10*	*-13.97*
55	*179.23*	*152.60*	*88.59*	*62.58*	*48.32*	*31.96*	*17.92*	*4.67*	*-2.51*	*-7.49*	*-12.99*
60	*176.82*	*150.25*	*87.11*	*61.26*	*47.75*	*31.74*	*17.45*	*4.67*	*-2.25*	*-6.87*	*-12.05*
	CT (ppm/^{o}C)										
	-0.53	-0.52	-0.32	-0.31	-0.13	-0.05	-0.11	N/A	0.06	0.14	0.22
T (^{o}C)	***|CT|/FWHM (1/^{o}C) ****										
37	1.28	1.17	0.79	0.72	0.73	0.39	0.25	N/A	0.38	0.20	0.37
T (^{o}C)	***T_1 / (St. Dev.) (ms) *****										
25	4.4	3.7	3.8	2.4	30	21	2.4	*ND*	63	1.1	1.2
	(0.1)	(0.2)	(0.1)	(0.1)	(1)	(2)	(0.1)	*ND*	(1.)	(0.1)	(0.2)

***** – Calculated for FWHM (Hz) measured at 37 ^{o}C.

****** – Measured at 25 ^{o}C.

S – Solvent peak.

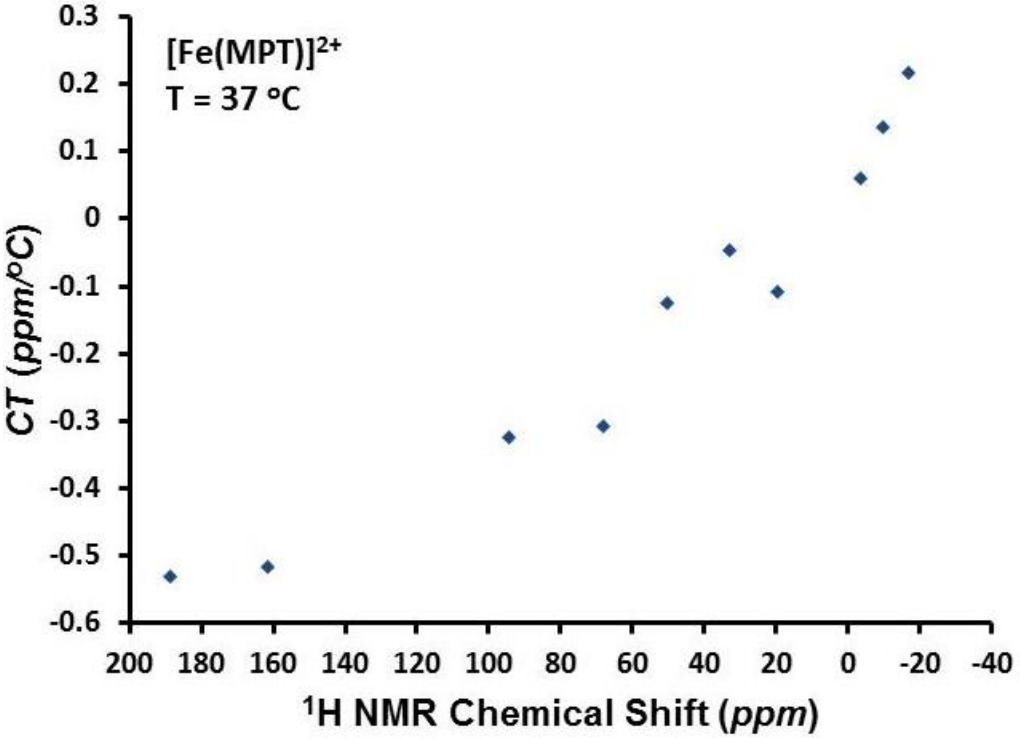


Figure S8. Dependence of *CT* values (ppm/^{o}C) of ^{1}H NMR resonances on their corresponding chemical shifts (37 ^{o}C) for $[Fe(MPT)]^{2+}$. ^{1}H NMR data was collected in 100 mM NaCl, D_2O, pD 7.60.

^{1}H NMR data for $[Fe(AMPT)]^{2+}$

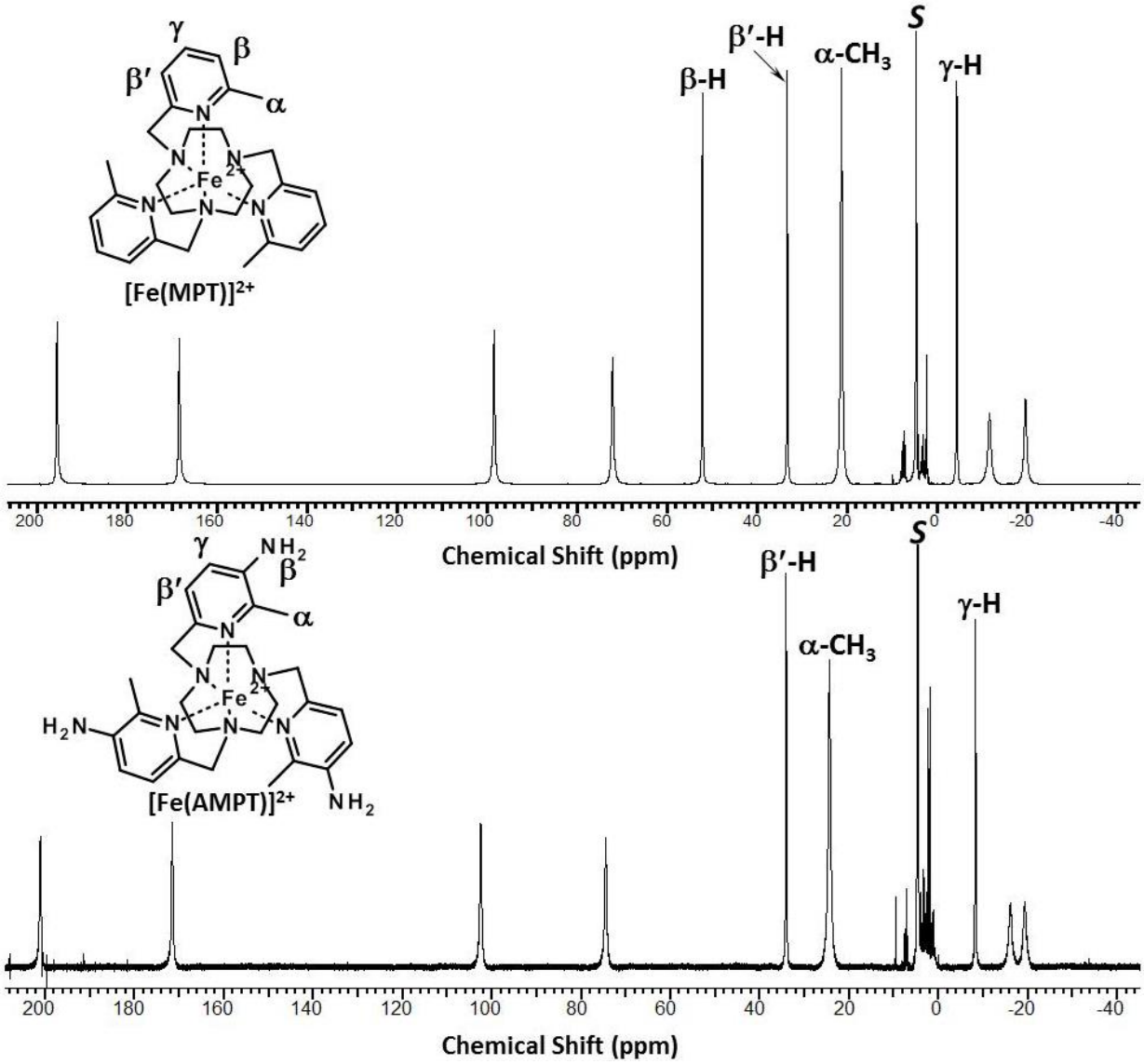


Figure S9. Comparison of ^{1}H NMR spectra of $[Fe(MPT)]^{2+}$ and $[Fe(AMPT)]^{2+}$ at 25 ^oC in 100 mM NaCl, D_2O, pD 7.00-7.20. Aromatic protons and their ^{1}H NMR resonances are labeled with β, β' and γ; while solvent peak is labeled with "s".

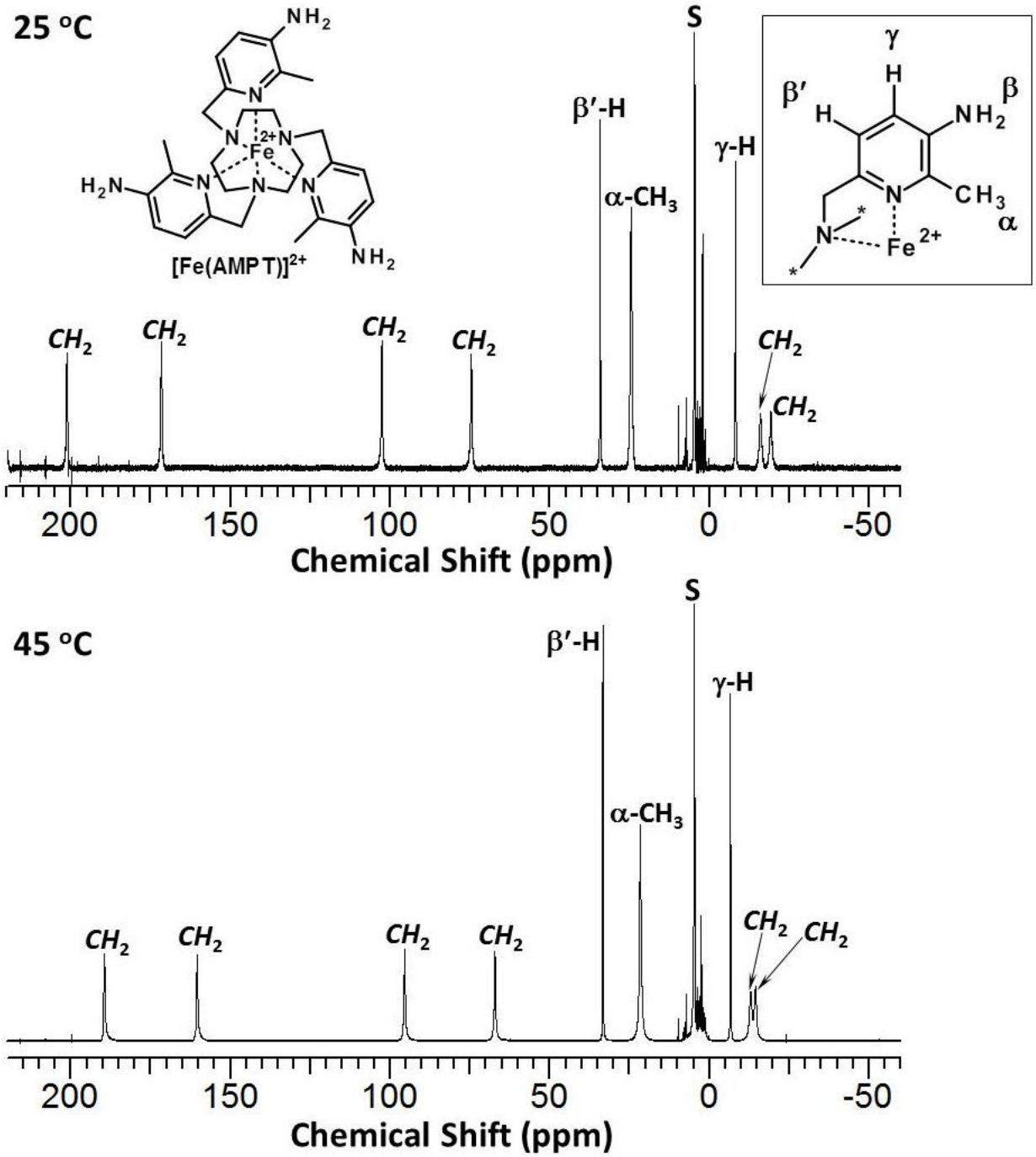


Figure S10. ^{1}H NMR spectrum of $[Fe(AMPT)]^{2+}$ at 25 ^{o}C and 45 ^{o}C n 100 mM NaCl, D_2O, pD 7.00. Aromatic protons, amine, methyl and their ^{1}H NMR resonances are labeled with α, β, β' and γ; while solvent peak is labeled with "s".

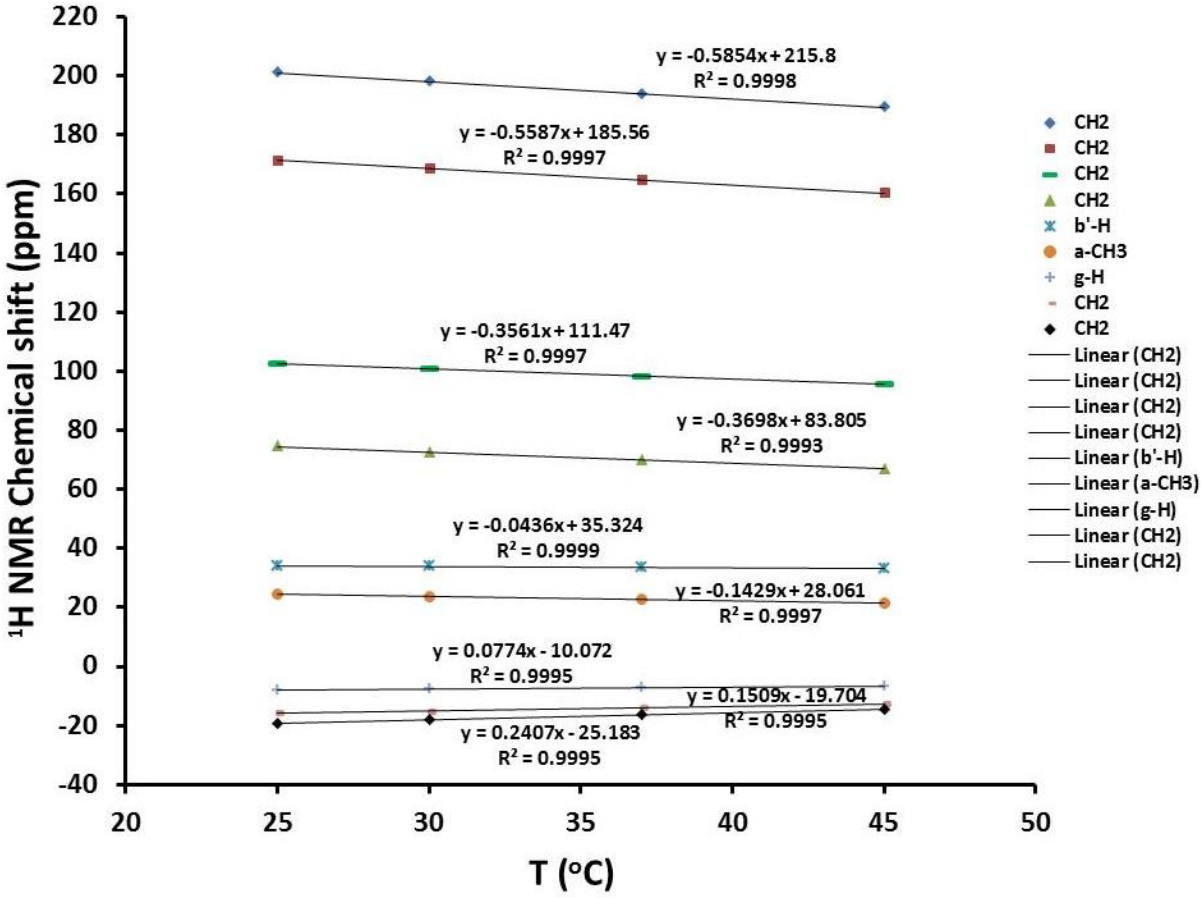


Figure S11. Linear fit of temperature-dependent paramagnetically-shifted ^{1}H NMR resonances of $[Fe(AMPT)]^{2+}$ in the range of 25 to 45 ^{o}C. All samples contained 100 mM NaCl, D_2O, pD 7.00.

Table S2. Properties of temperature-dependent ^{1}H NMR resonances of $[Fe(AMPT)]^{2+}$, 100 mM NaCl, D_2O, pD 7.00.

***T* (^{o}*C*)**	***Type of [Fe(AMPT)]$^{2+}$ protons***									
	CH_2	***CH_2***	***CH_2***	***CH_2***	***β′-H***	***α-CH_3***	**S**	***γ-H***	***CH_2***	***CH_2***
	Peak width in FWHM (*Hz*)									
25	190	200	209	233	76.7	288	1.81	83.4	402	397
30	180	202	209	224	70.9	287	1.67	80.0	395	383
37	196	213	227	225	60.9	287	1.62	70.9	406	373
45	197	221	216	218	46.7	279	1.43	55.0	416	368
***T* (^{o}*C*)**	***^{1}H NMR Chemical shift (ppm)***									
25	*201.23*	*171.67*	*102.62*	*74.64*	*34.23*	*24.51*	*4.75*	*-8.15*	*-15.96*	*-19.21*
30	*198.19*	*168.74*	*100.75*	*72.65*	*34.02*	*23.76*	*4.75*	*-7.74*	*-15.16*	*-17.93*
37	*194.08*	*164.82*	*98.24*	*70.04*	*33.71*	*22.75*	*4.75*	*-7.19*	*-14.09*	*-16.23*
45	*189.51*	*160.48*	*95.49*	*67.23*	*33.36*	*21.65*	*4.75*	*-6.60*	*-12.94*	*-14.39*
	CT (ppm/^{o}C)									
	-0.59	-0.56	-0.36	-0.37	-0.04	-0.14	N/A	0.08	0.15	0.24
***T* (^{o}*C*)**	***|CT|/FWHM (1/^{o}C) ****									
37	1.51	1.43	0.92	0.94	0.10	0.36	N/A	0.20	0.38	0.61

***** – Calculated for FWHM (Hz) measured at 37 ^{o}C.

S – Solvent peak.

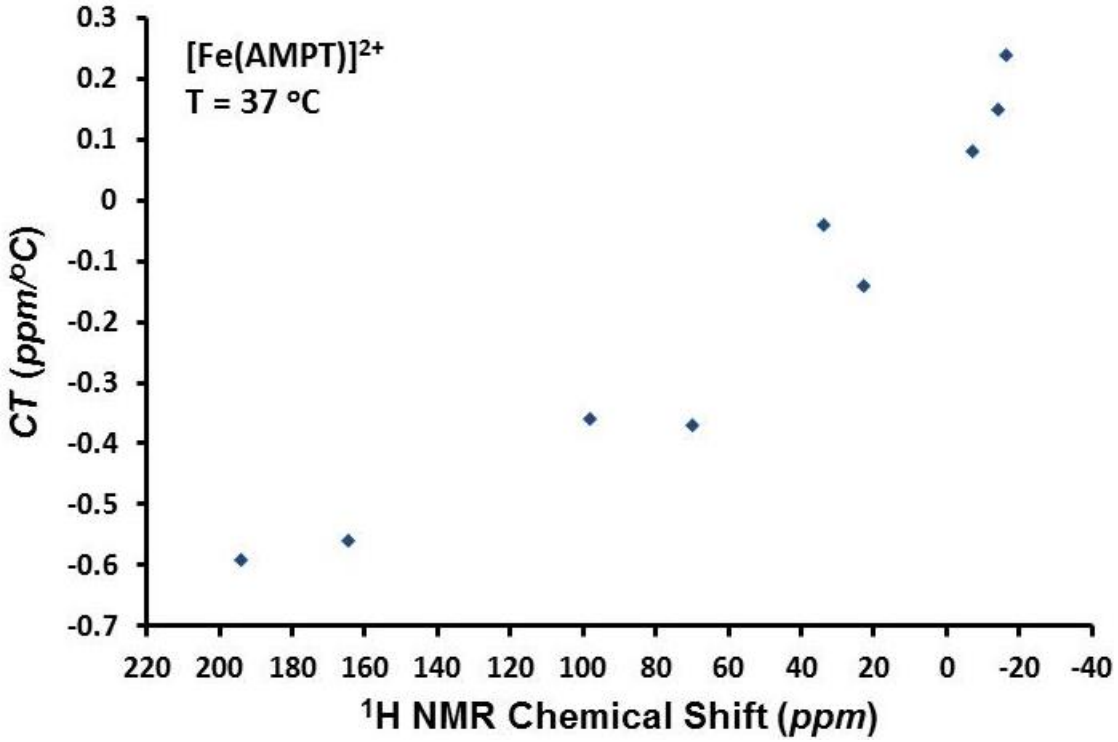


Figure S12. Dependence of *CT* values (ppm/^{o}C) of ^{1}H NMR resonances on their corresponding chemical shifts (37 ^{o}C) for $[Fe(AMPT)]^{2+}$. Samples contained 100 mM NaCl, D_2O, pD 7.00.

^{1}H NMR data for $[Co(MPT)]^{2+}$

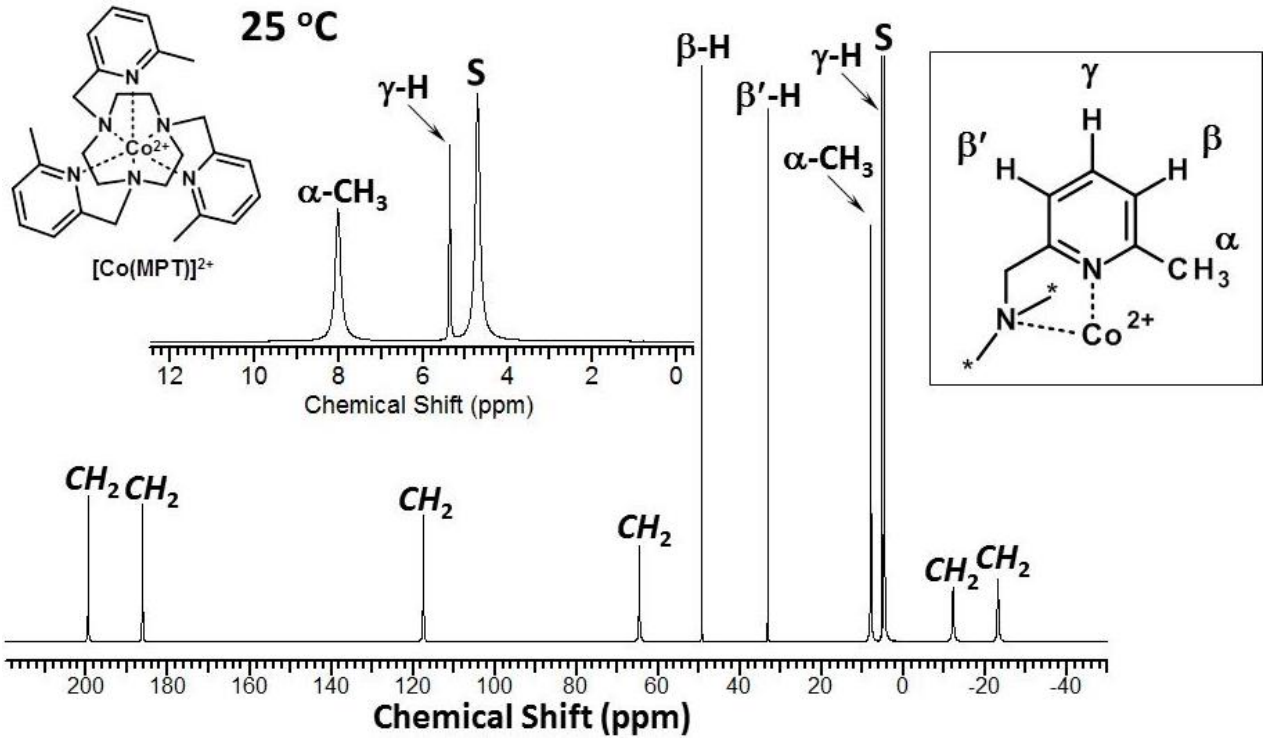


Figure S13. ^{1}H NMR spectrum of 98 mM $[Co(MPT)]^{2+}$ at 25 °C in 100 mM NaCl, D_2O, pD 7.30. Insert shows diamagnetic region. Aromatic protons and their ^{1}H NMR resonances are labeled with β, β′ and γ; while solvent peak is labeled with "s".

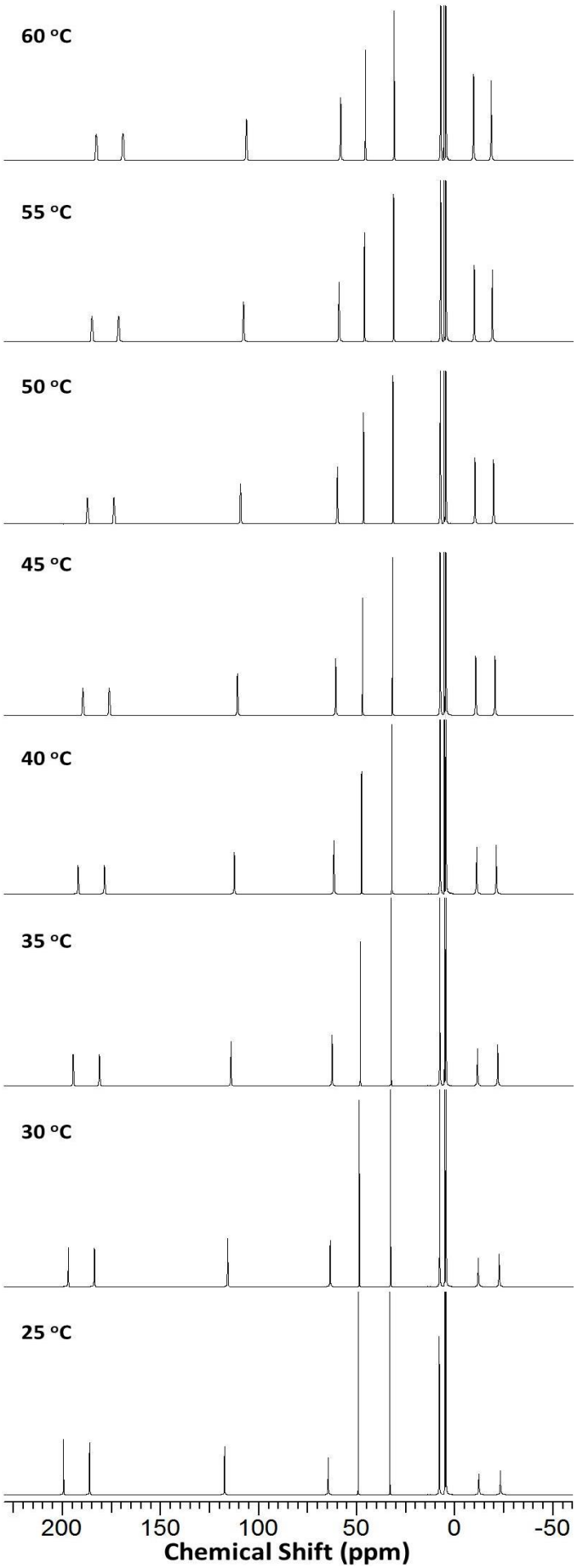


Figure S14. Variable temperature ^{1}H NMR spectra of $[Co(MPT)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.30.

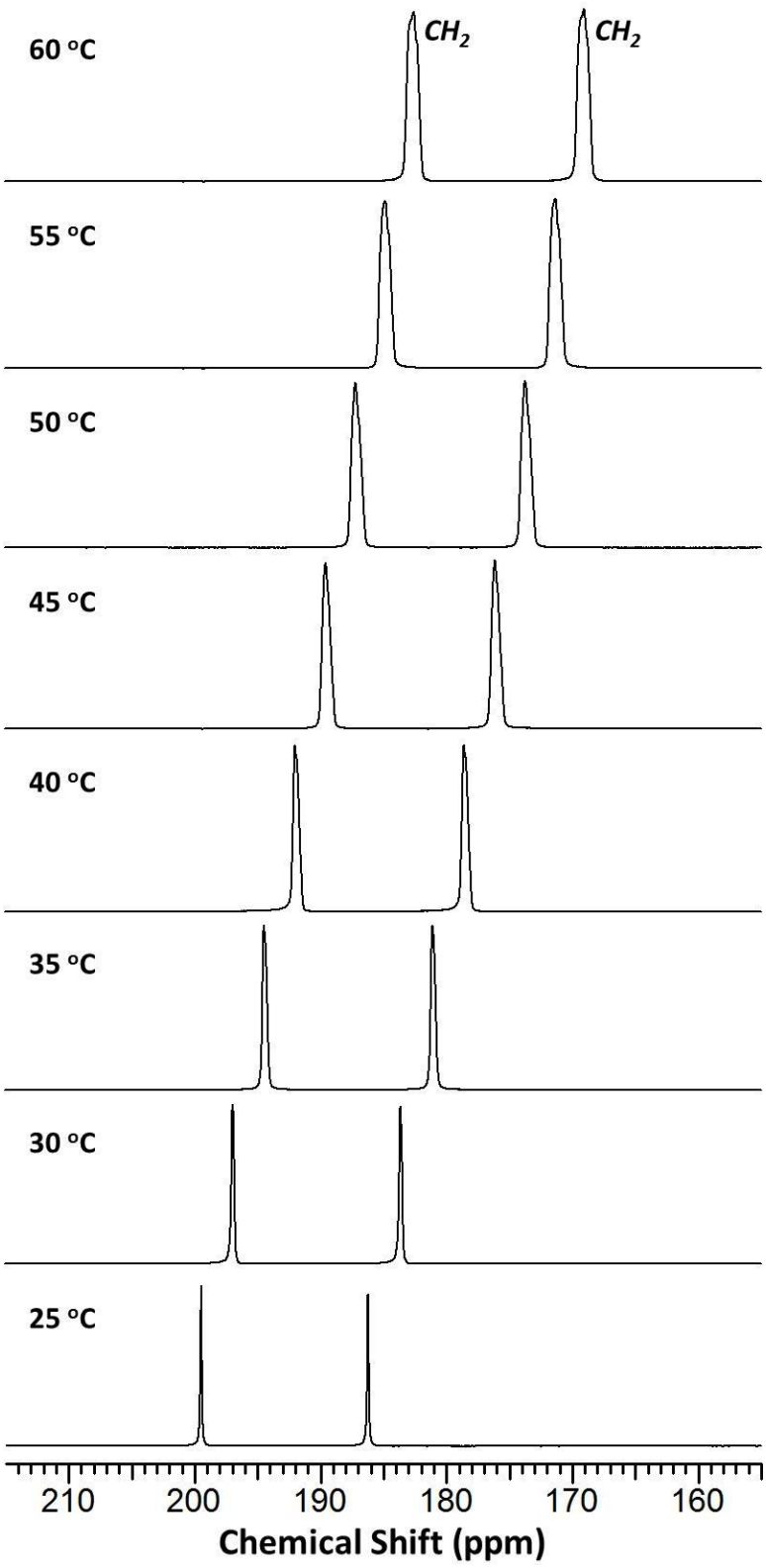


Figure S15. Expansion showing ^{1}H NMR resonances of two downfield highly-shifted CH_2 peaks of $[Co(MPT)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.30.

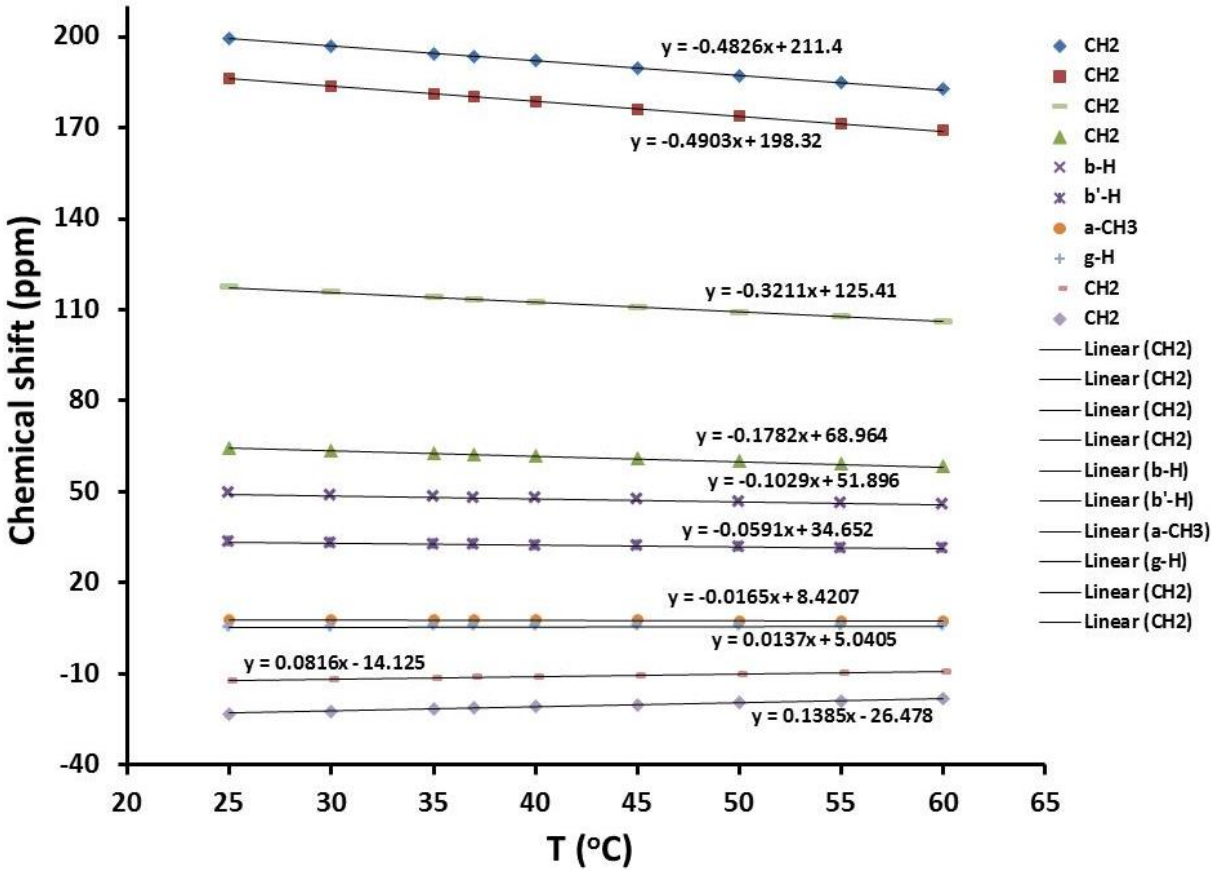


Figure S16. Linear fit of temperature-dependent paramagnetically-shifted ^{1}H NMR resonances of $[Co(MPT)]^{2+}$ in the range of 25 to 60 ^{o}C. All samples contained 100 mM NaCl, D_2O, pD 7.30.

Table S3. Chemical shift and peak width of ^{1}H NMR resonances of 98 mM $[Co(MPT)]^{2+}$, 100 mM NaCl, D_2O, pD 7.30 as a function of temperature.

T (^{o}*C*)	*Type of* $[Co(MPT)]^{2+}$ *protons*										
	CH_2	CH_2	CH_2	CH_2	β-*H*	β′-*H*	α-CH_3	γ-*H*	S	CH_2	CH_2
	Peak width in FWHM (*Hz*)										
25	52.4	58.3	72.1	98.5	16.5	17.2	66.5	15.0	57.4	157	149
30	62.3	67.6	71.3	90.8	18.2	17.8	60.8	15.6	42.6	142	134
35	71.3	75.9	71.6	85.7	19.8	18.2	56.4	15.4	32.6	130	123
37	74.2	78.6	71.8	83.9	20.3	18.4	54.9	15.5	29.2	126	119
40	83.3	87.7	75.5	82.5	22.2	19.3	53.0	15.8	25.1	121	114
45	102	106	84.2	82.2	26.4	21.4	50.7	16.4	20.1	113	107
50	119	123	93.6	83.1	30.4	23.7	49.2	17.1	16.4	107	102
55	134	137	102	85.3	34.7	26.4	48.5	18.2	13.8	103	98.8
60	150	152	111	88.2	38.8	29.1	48.8	19.6	12.0	98.8	96.4
***T* (^{o}*C*)**	***^{1}H NMR Chemical shift (ppm)***										
25	*199.48*	*186.23*	*117.50*	*64.63*	*49.38*	*33.21*	*8.03*	*5.38*	*4.67*	*-12.12*	*-23.10*
30	*196.96*	*183.65*	*115.81*	*63.65*	*48.83*	*32.89*	*7.93*	*5.45*	*4.67*	*-11.69*	*-22.35*
35	*194.48*	*181.12*	*114.14*	*62.69*	*48.29*	*32.58*	*7.84*	*5.52*	*4.67*	*-11.26*	*-21.60*
37	*193.48*	*180.10*	*113.47*	*62.31*	*48.05*	*32.45*	*7.80*	*5.55*	*4.67*	*-11.09*	*-21.31*
40	*192.02*	*178.61*	*112.50*	*61.75*	*47.72*	*32.26*	*7.75*	*5.59*	*4.67*	*-10.84*	*-20.88*
45	*189.60*	*176.16*	*110.90*	*60.88*	*47.24*	*31.98*	*7.67*	*5.66*	*4.67*	*-10.43*	*-20.19*
50	*187.23*	*173.76*	*109.32*	*60.02*	*46.73*	*31.69*	*7.59*	*5.73*	*4.67*	*-10.03*	*-19.52*
55	*184.86*	*171.36*	*107.77*	*59.18*	*46.24*	*31.41*	*7.52*	*5.79*	*4.67*	*-9.64*	*-18.87*
60	*182.60*	*169.07*	*106.25*	*58.38*	*45.78*	*31.14*	*7.45*	*5.86*	*4.67*	*-9.27*	*-18.25*
	CT (ppm/^{o}C)										
	-0.48	-0.49	-0.32	-0.18	-0.1	-0.06	-0.017	0.014	*N/A*	0.08	0.14
***T* (^{o}*C*)**	***|CT|/FWHM (1/^{o}C) ****										
37	3.24	3.12	2.23	1.07	2.46	1.63	0.16	0.45	*N/A*	0.32	0.59
***T* (^{o}*C*)**	***T_1 / (St. Dev.) (ms) *****										
25	8.3	7.3	7.0	4.6	50	38	5.7	102	*ND*	2.2	2.3
	(0.2)	(0.2)	(0.1)	(0.1)	(1)	(1)	(0.1)	(3)	*ND*	(0.1)	(0.1)

***** – Calculated for FWHM (Hz) measured at 37 ^{o}C.

****** – Measured at 25 ^{o}C.

S – Solvent peak.

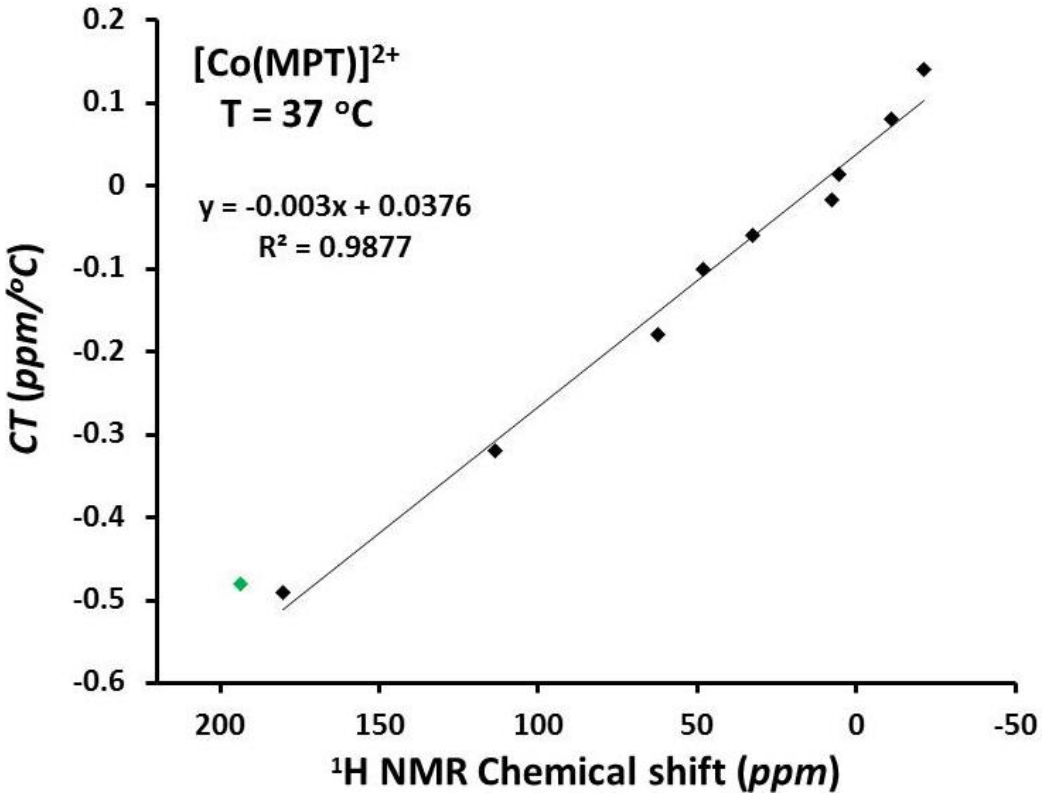


Figure S17. Dependence of CT values (ppm/^{o}C) of ^{1}H NMR resonances on their corresponding chemical shifts at 37 ^{o}C for $[Co(MPT)]^{2+}$. The proton resonance at δ = 193.48 ppm at 37 ^{o}C (green diamond) was omitted from the fitting process. Best-fit slope and intercept are -0.003 $^{o}C^{-1}$ and 0.0376 ppm/^{o}C, respectively. Samples contained 100 mM NaCl, D_2O, pD 7.30.

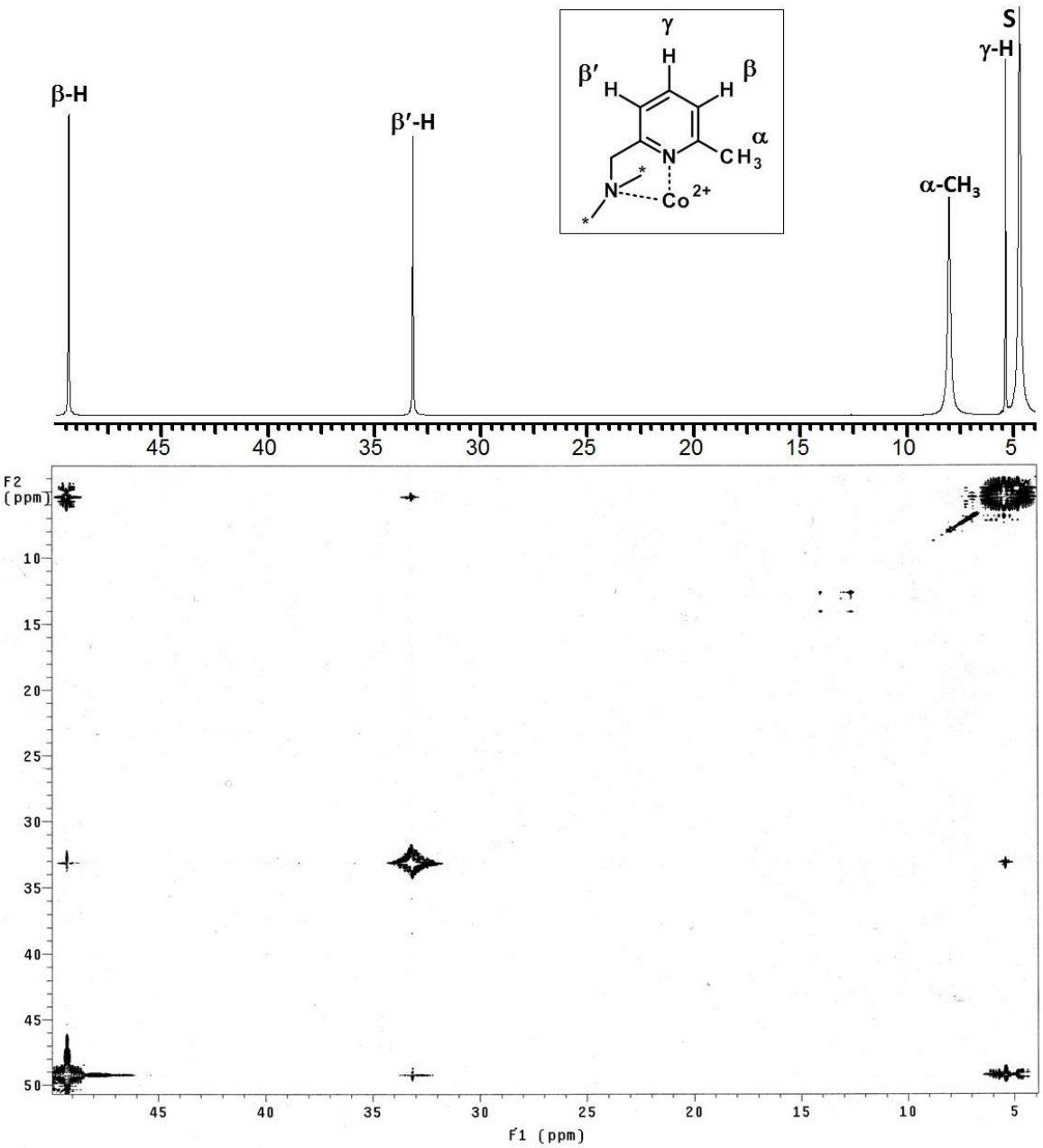


Figure S18. Two-dimensional ^{1}H-zTOCSY NMR spectrum (25 ^{o}C) obtained at 252 scans of 120 mM [Co(MPT)]Cl_2 in D_2O (pD 7.0) showing the cross-peaks that allowed the identification of the proton resonances produced by aromatic protons of 6-methyl-2-picolyl pendants.

^{1}H NMR data for $[Fe(PT)]^{2+}$

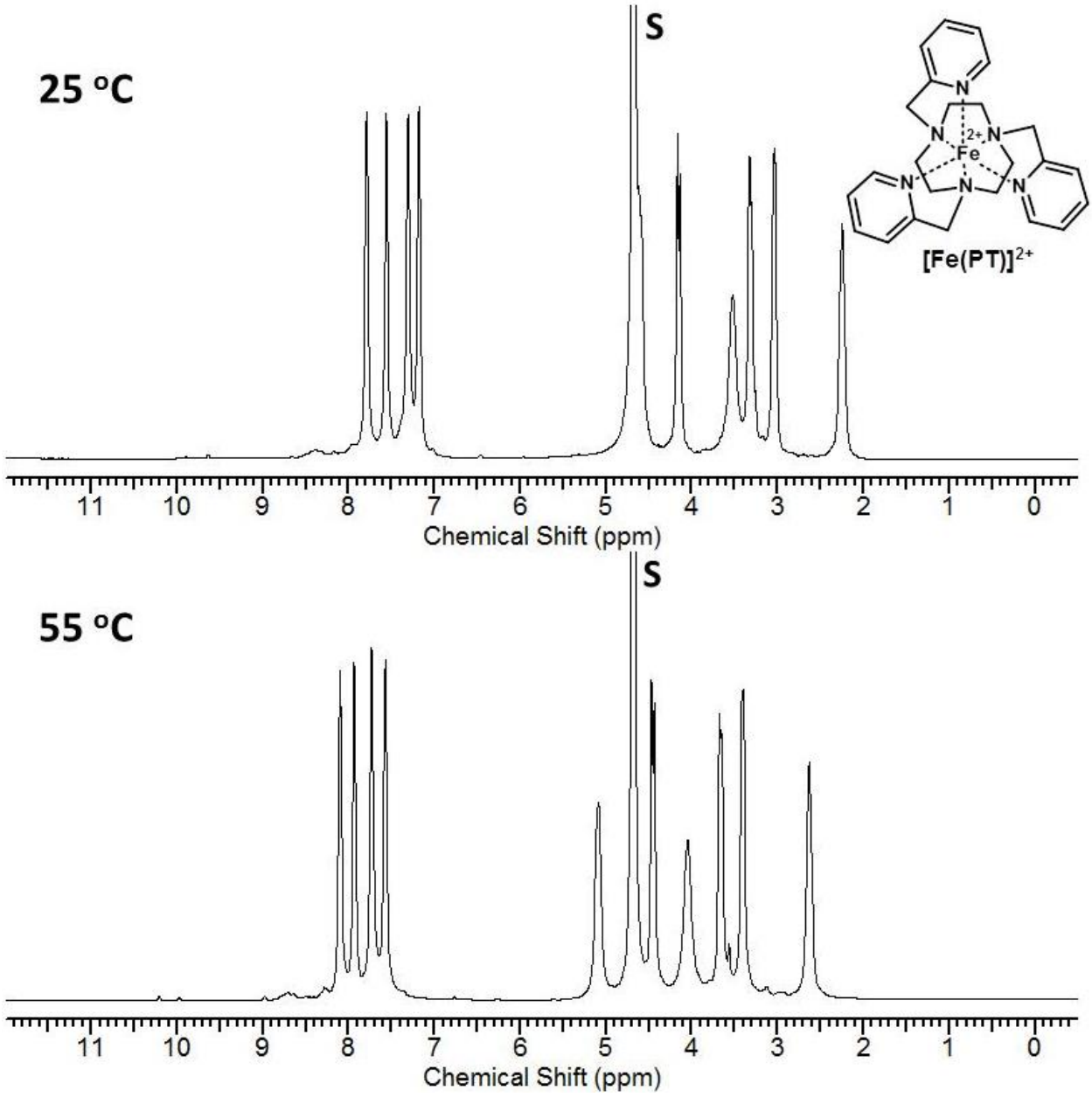


Figure S19. ^{1}H NMR spectra of $[Fe(PT)]^{2+}$ at 25 °C and 55 °C in D_2O, pD 6.70. Solvent peak is labeled with "s".

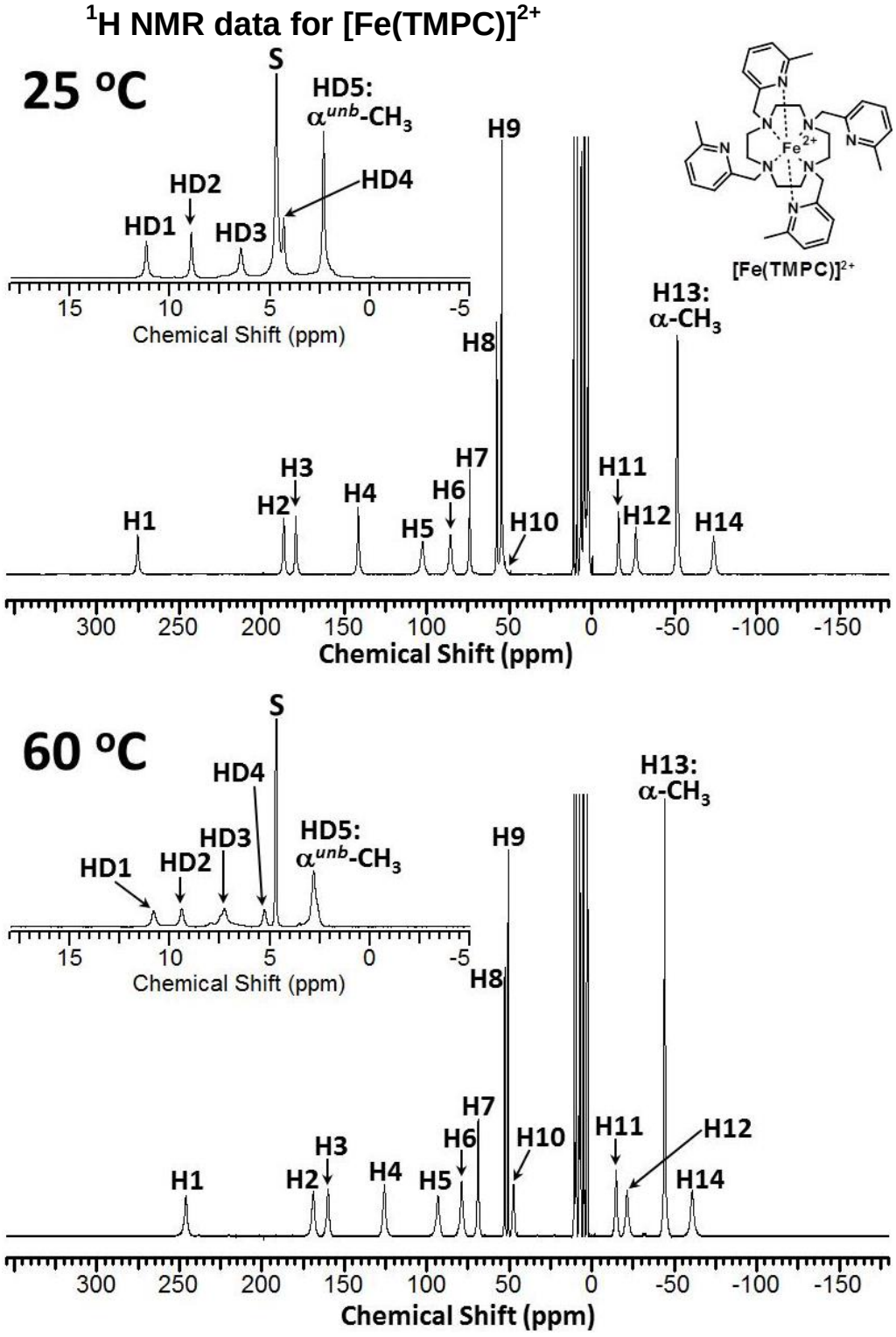


Figure S20. ^{1}H NMR spectra of $[Fe(TMPC)]^{2+}$ at 25 ^{o}C and 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.40. Proton resonances that display significant paramagnetic shifts are labeled **H1-H14**, while proton resonances that are not shifted from diamagnetic region are labeled **HD1-HD5**. Inserts show diamagnetic regions with solvent peaks labeled with "S".

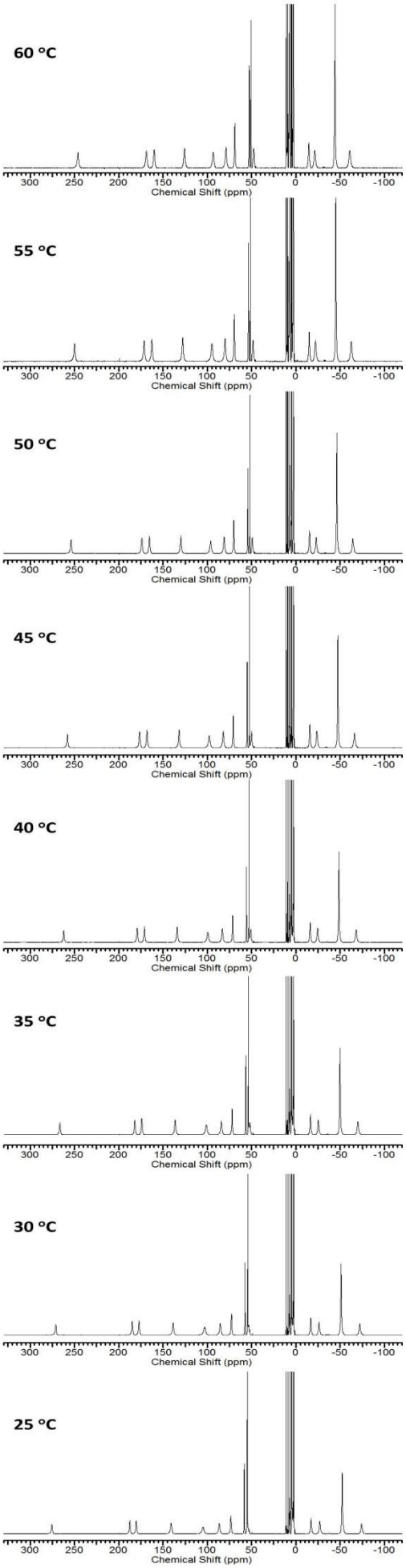


Figure S21. Variable temperature ^{1}H NMR spectra of $[Fe(TMPC)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.40.

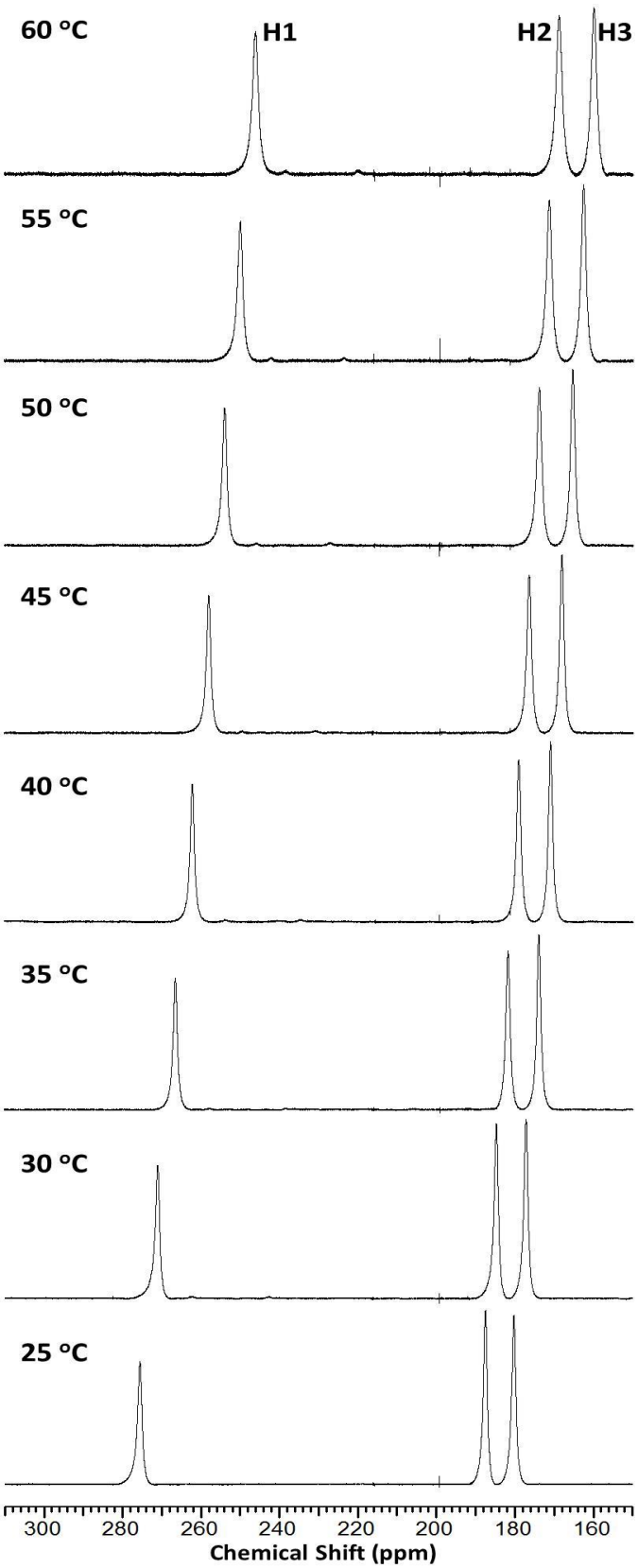


Figure S22. Expansion showing ^{1}H NMR resonances of some downfield highly-shifted peaks of $[Fe(TMPC)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.40.

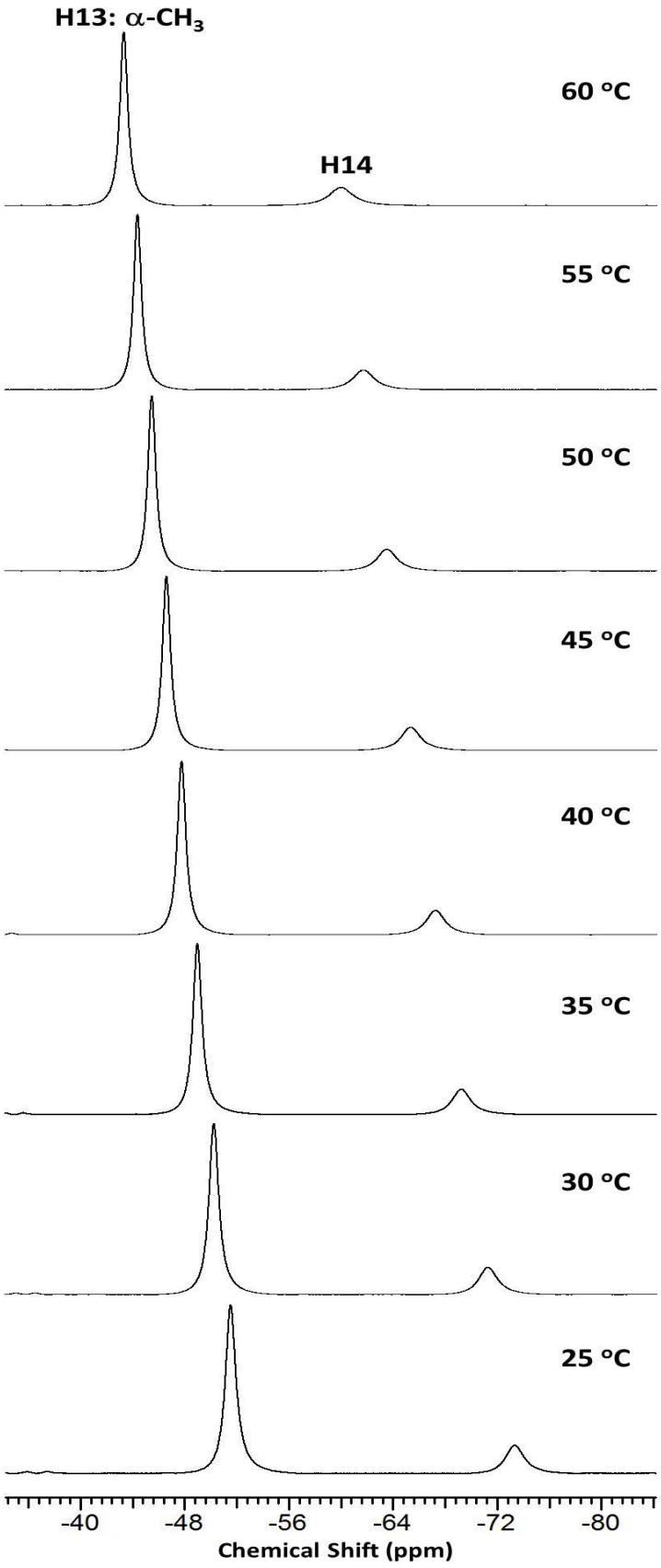


Figure S23. Expansion showing ^{1}H NMR resonances of some highly-shifted peaks, including proton resonances of α-CH_3 groups, of $[Fe(TMPC)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.40.

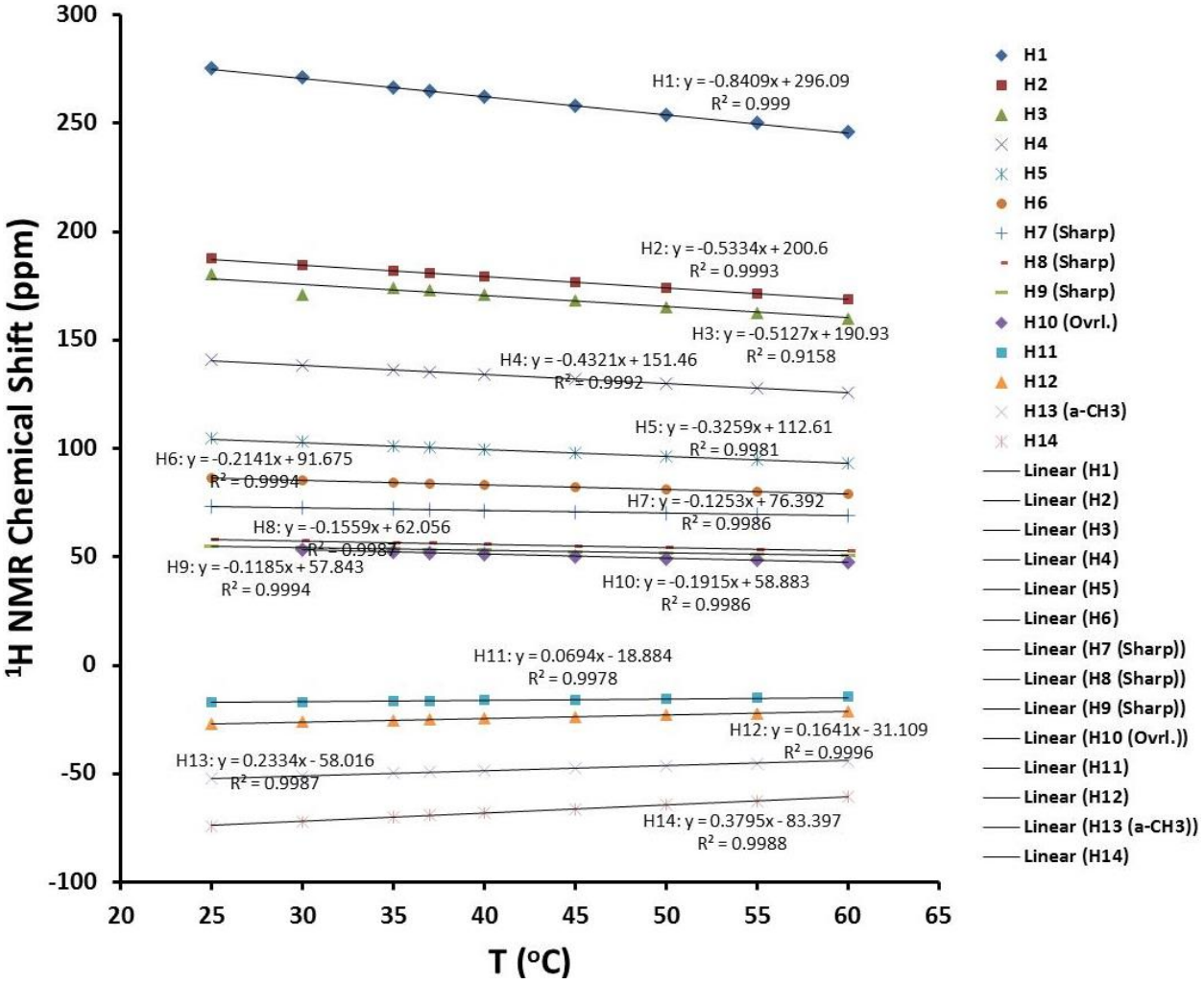


Figure S24. Linear fit of temperature-dependent paramagnetically-shifted ^{1}H NMR resonances of $[Fe(TMPC)]^{2+}$ in the range of 25 to 60 °C. Samples contained 100 mM NaCl, D_2O, pD 7.40.

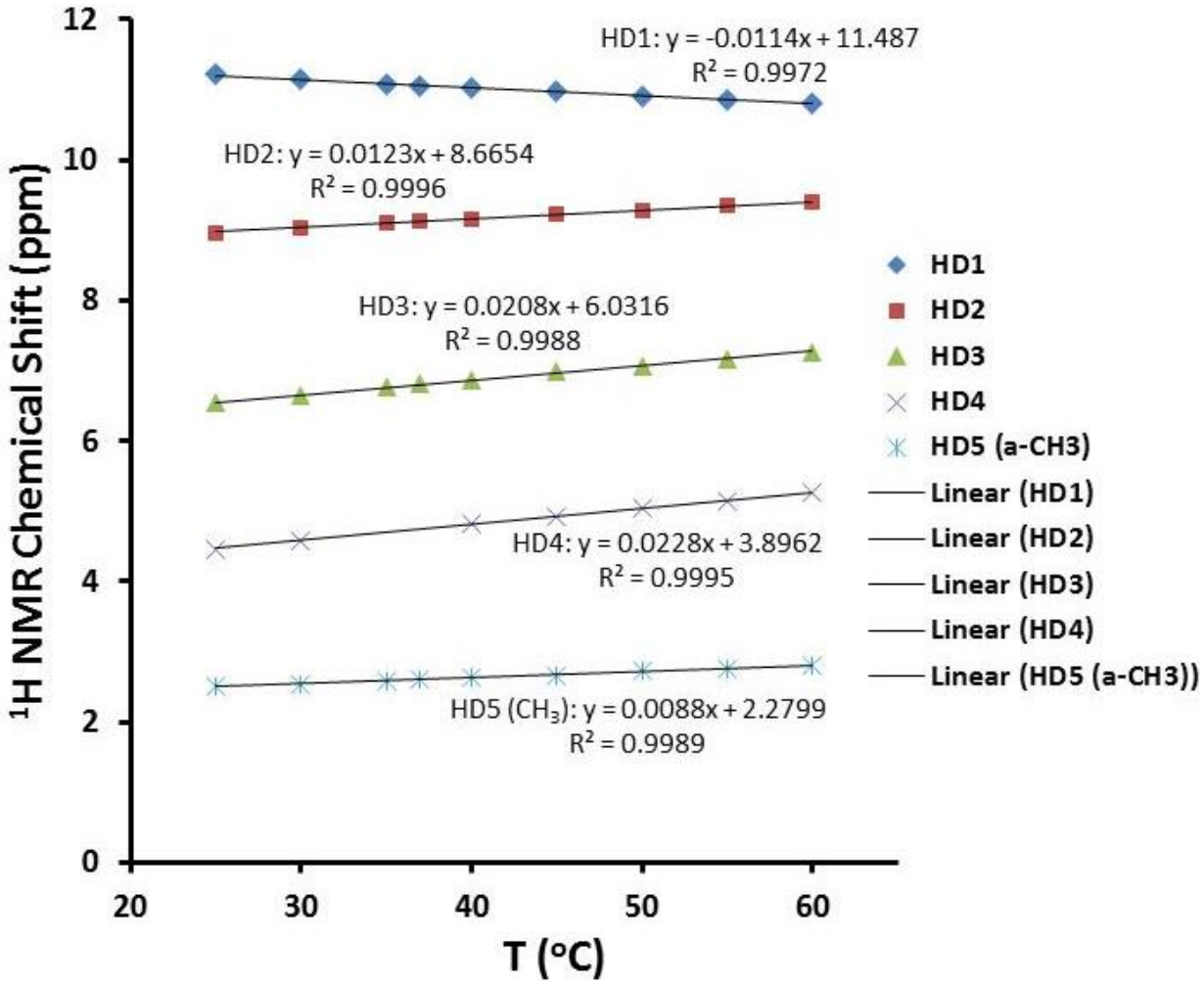


Figure S25. Linear fit of temperature-dependent ^{1}H NMR resonances in diamagnetic region of $[Fe(TMPC)]^{2+}$ spectra in the range of 25 to 60 ^{o}C. Sample contained 100 mM NaCl, D_2O, pD 7.40.

Table S4. Chemical shift and peak width of ^{1}H NMR resonances of $[Fe(TMPC)]^{2+}$, 100 mM NaCl, D_2O, pD 7.40, as a function of temperature.

	Labeled protons of $[Fe(TMPC)]^{2+}$																			
											Diamagnetic Region									
	H1	***H2***	***H3***	***H4***	***H5***	***H6***	***H7***	***H8***	***H9***	***H10****	***HD1***	***HD2***	***HD3***	***S***	***HD4***	***HD5: α-CH_3***	***H11***	***H12***	***H13: α-CH_3***	***H14***
T (^{o}C)	**Peak width in FWHM (*Hz*)**																			
25	576	514	572	682	1290	610	393	137	64.4	*Ovrlp.*	33.1	21.1	50.0	14.6	19.7	22.4	386	636	458	617
30	516	545	567	639	1090	561	360	143	67.0	*Ovrlp.*	33.4	22.2	48.4	13.8	N/A	24.1	358	596	425	578
35	509	578	573	624	1030	551	347	149	69.7	1450	37.1	26.1	51.3	16.6	N/A	28.5	356	593	399	588
37	501	585	568	598	971	531	340	152	71.3	951	38.5	27.5	52.3	15.4	N/A	29.8	348	580	389	579
40	507	610	575	587	941	528	336	156	75.2	802	41.0	30.4	54.6	15.7	N/A	32.7	346	571	378	580
45	558	679	627	621	955	556	346	167	85.0	752	47.5	37.1	61.1	16.8	37.6	40.9	360	590	369	633
50	581	700	629	641	863	533	341	175	99.1	728	59.5	49.2	75.3	20.3	50.2	54.1	347	552	358	621
55	670	770	674	719	840	545	350	176	120	861	84.4	73.8	107	44.0	72.5	80.2	350	554	350	661
60	766	840	745	804	829	550	355	195	145	799	104	93.6	141	47.3	92.1	124	335	525	357	703
T (^{o}C)	***^{1}H NMR Chemical shift (ppm)***																			
25	*275.55*	*187.51*	*180.22*	*140.87*	*104.68*	*86.42*	*73.34*	*58.26*	*54.93*	*Ovrlp.*	*11.21*	*8.97*	*6.54*	*4.68*	*4.46*	*2.50*	*-17.11*	*-27.06*	*-52.34*	*-74.14*
30	*271.04*	*184.70*	*171.14*	*138.59*	*102.95*	*85.30*	*72.67*	*57.41*	*54.31*	*53.22*	*11.15*	*9.03*	*6.65*	*4.68*	*4.58*	*2.54*	*-16.78*	*-26.19*	*-51.05*	*-72.09*
35	*266.49*	*181.84*	*174.01*	*136.26*	*101.11*	*84.12*	*71.97*	*56.56*	*53.68*	*52.20*	*11.08*	*9.10*	*6.76*	*4.68*	*Ovrlp.*	*2.59*	*-16.46*	*-25.34*	*-49.79*	*-70.05*
37	*264.70*	*180.72*	*172.75*	*135.33*	*100.42*	*83.70*	*71.72*	*56.23*	*53.43*	*51.78*	*11.06*	*9.12*	*6.81*	*4.68*	*Ovrlp*	*2.61*	*-16.35*	*-25.05*	*-49.30*	*-69.21*
40	*262.13*	*179.12*	*171.00*	*134.04*	*99.41*	*83.03*	*71.33*	*55.76*	*53.07*	*51.12*	*11.02*	*9.16*	*6.87*	*4.68*	*4.82*	*2.63*	*-16.13*	*-24.50*	*-48.59*	*-68.09*
45	*257.96*	*176.44*	*168.11*	*131.88*	*97.79*	*82.00*	*70.70*	*54.97*	*52.47*	*50.27*	*10.97*	*9.22*	*6.98*	*4.68*	*4.93*	*2.67*	*-15.79*	*-23.68*	*-47.42*	*-66.17*
50	*253.93*	*173.84*	*165.34*	*129.78*	*96.17*	*80.96*	*70.09*	*54.23*	*51.90*	*49.20*	*10.91*	*9.28*	*7.07*	*4.68*	*5.04*	*2.72*	*-15.46*	*-22.89*	*-46.30*	*-64.32*
55	*249.91*	*171.35*	*162.63*	*127.72*	*94.75*	*79.95*	*69.53*	*53.50*	*51.34*	*48.44*	*10.86*	*9.34*	*7.17*	*4.68*	*5.15*	*2.76*	*-15.08*	*-22.08*	*-45.20*	*-62.56*
60	*246.08*	*168.81*	*159.91*	*125.75*	*93.29*	*78.88*	*68.95*	*52.79*	*50.78*	*47.42*	*10.81*	*9.40*	*7.27*	*4.68*	*5.26*	*2.81*	*-14.65*	*-21.32*	*-44.15*	*-60.86*
	CT (ppm/^{o}C)																			
	-0.84	-0.53	-0.51	-0.43	-0.33	-0.21	-0.13	-0.16	-0.12	-0.19	-0.01	0.01	0.02	N/A	0.02	0.01	0.07	0.16	0.23	0.38
T (^{o}C)	***|CT|/FWHM (1/^{o}C) ****																			
37	0.84	0.45	0.45	0.36	0.17	0.20	0.19	0.53	0.84	0.10	0.13	0.18	0.19	N/A	N/A	0.17	0.10	0.14	0.30	0.33
T (^{o}C)	***T_1* / (St. Dev.) (ms) *****																			
25	0.83	1.6	1.1	3.8	0.46	0.53	1.9	4.9	9.8	N/A	18	50	9.6	224	54	42	1.2	0.81	1.1	0.56
	(0.01)	(0.0)	(0.0)	(0.2)	(0.01)	(0.02)	(0.0)	(0.0)	(0.1)	N/A	(0)	(0)	(0.0)	(16)	(1)	(1)	(0.0)	(0.01)	(0.0)	(0.01)

Table S4 Legend:
***** – Calculated for FWHM (Hz) measured at 37 ^{o}C.
****** – Measured at 25 ^{o}C.
S – Solvent peak.

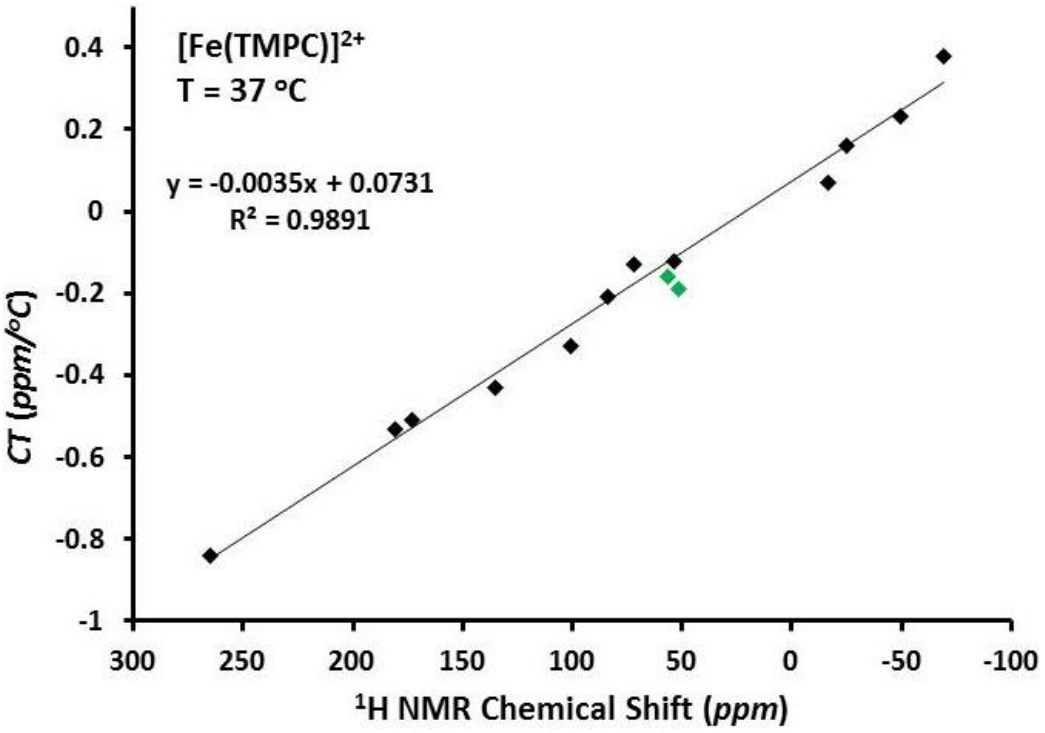


Figure S26. Dependence of *CT* values (ppm/^{o}C) of paramagnetically-shifted ^{1}H NMR resonances on their corresponding chemical shifts at 37 ^{o}C for $[Fe(TMPC)]^{2+}$. The proton resonances in diamagnetic region (0-10 ppm) are excluded from consideration. The proton resonances at δ = 51.78 and 56.23 ppm at 37 ^{o}C (green diamonds) were omitted from the fitting process. Best-fit slope and intercept are -0.0035 $^{o}C^{-1}$ and 0.0731 ppm/^{o}C, respectively. Samples contained 100 mM NaCl, D_2O, pD 7.40.

^{1}H NMR data for [Fe(TMPC)]$^{2+}$ in water

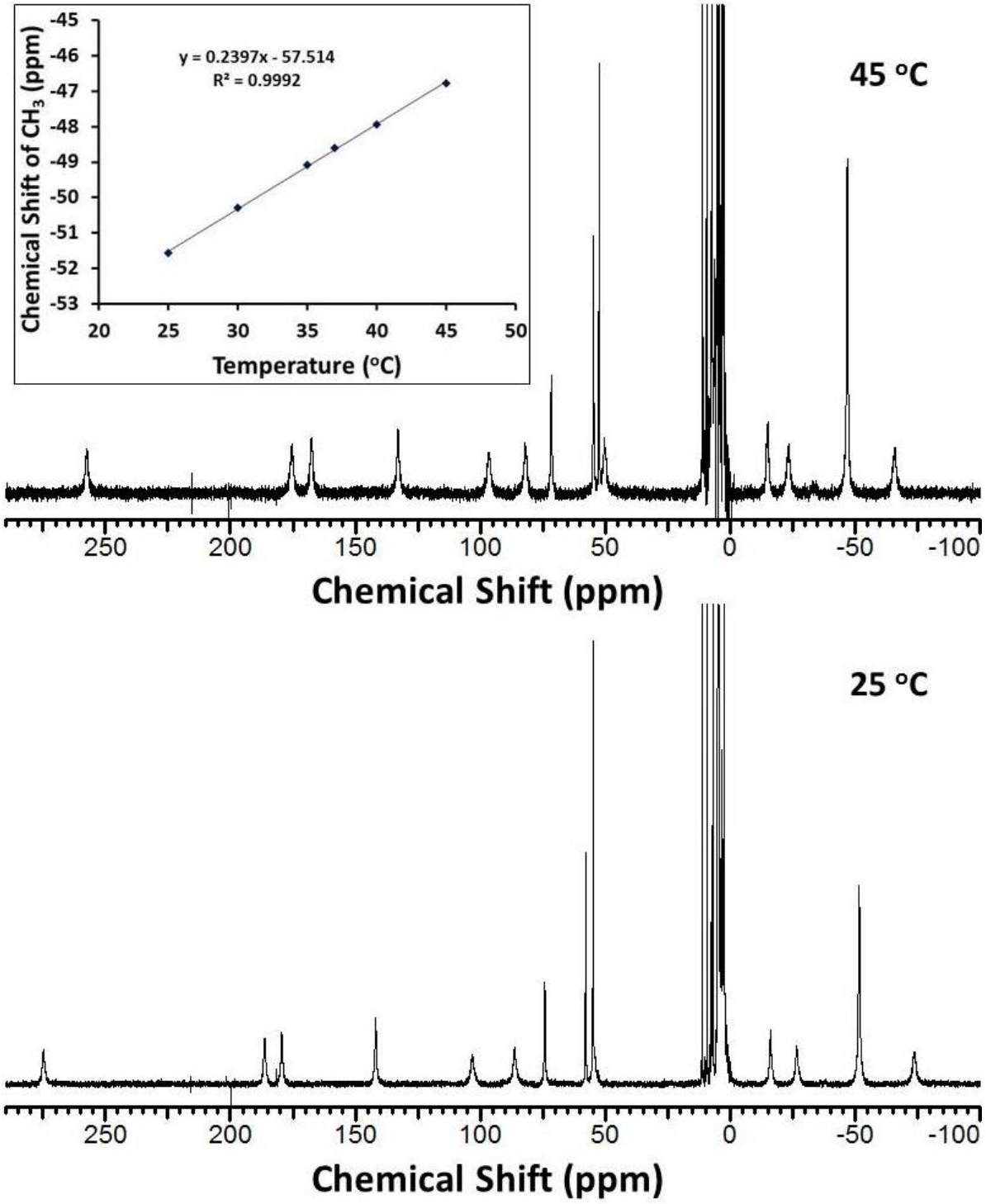


Figure S27. Variable temperature ^{1}H NMR spectra of [Fe(TMPC)]$^{2+}$ at 25 and 45 ^{o}C in 100 mM NaCl, H_2O, pH 7.40. Insert shows temperature dependence of α-CH_3 chemical shift of [Fe(MPT)]$^{2+}$, while the solid line presents linear fit of the data.

^{1}H NMR data for $[Co(TMPC)]^{2+}$

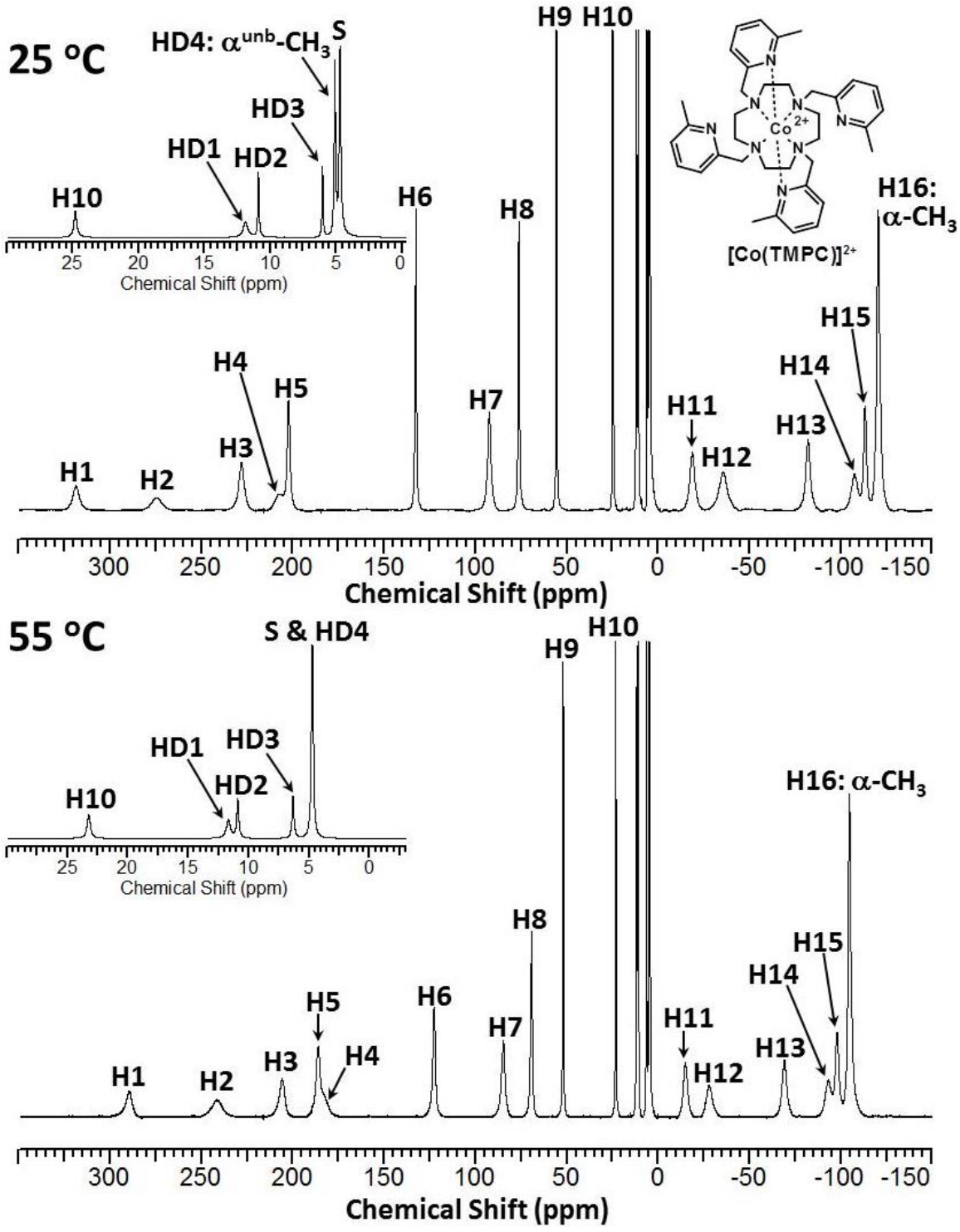


Figure S28. ^{1}H NMR spectra of $[Co(TMPC)]^{2+}$ at 25 °C and 55 °C in 100 mM NaCl, D_2O, pD 7.00. Proton resonances that display significant paramagnetic shifts are labeled **H1-H16**, while proton resonances that are not shifted from diamagnetic region are labeled **HD1-HD4**. Inserts show diamagnetic regions with solvent peaks labeled with "S".

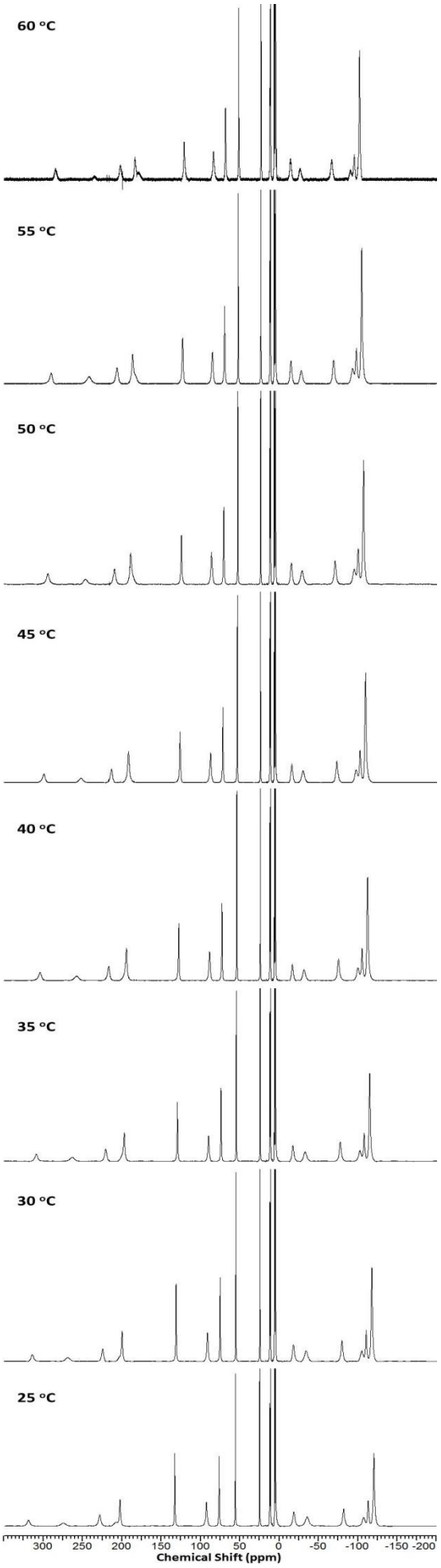


Figure S29. Variable temperature ^{1}H NMR spectra of $[Co(TMPC)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.00.

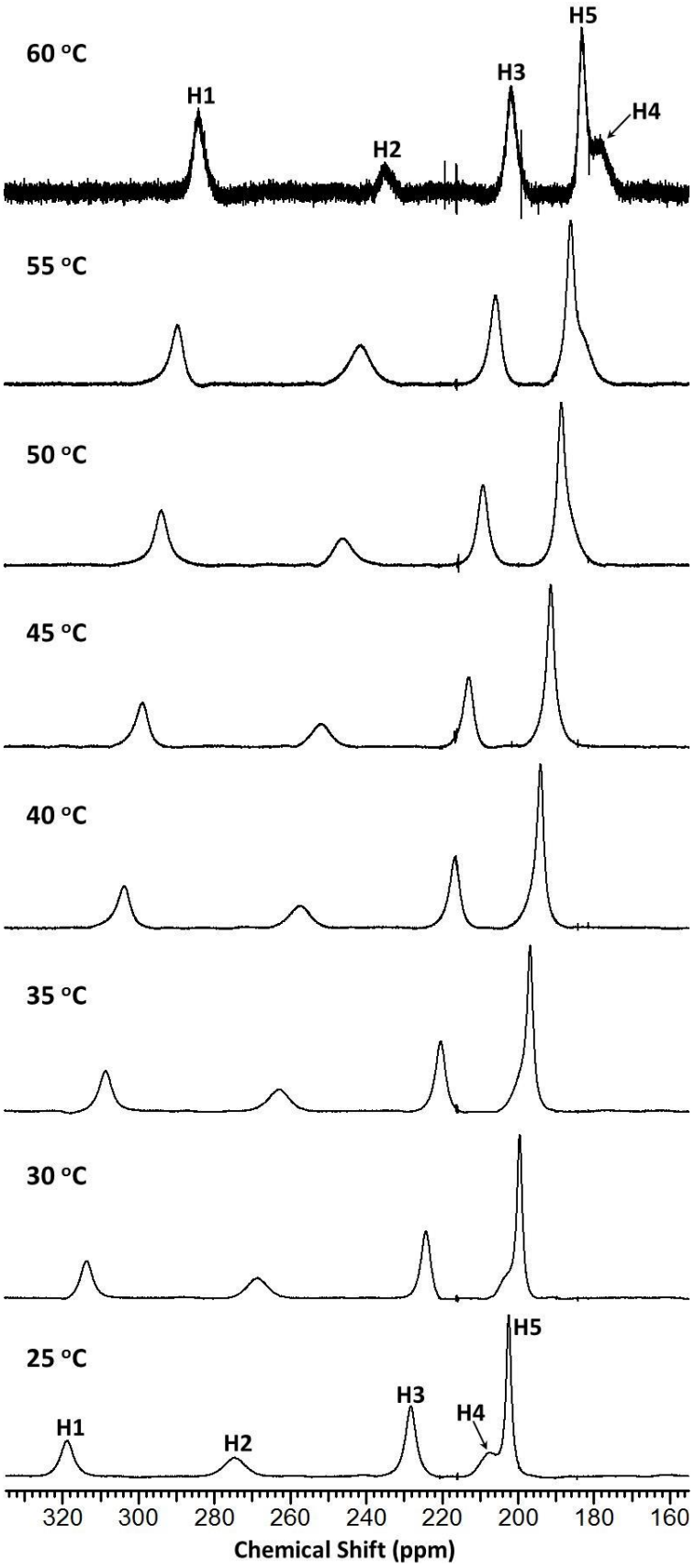


Figure S30. Expansion showing ^{1}H NMR resonances of some downfield highly-shifted peaks of $[Co(TMPC)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.00.

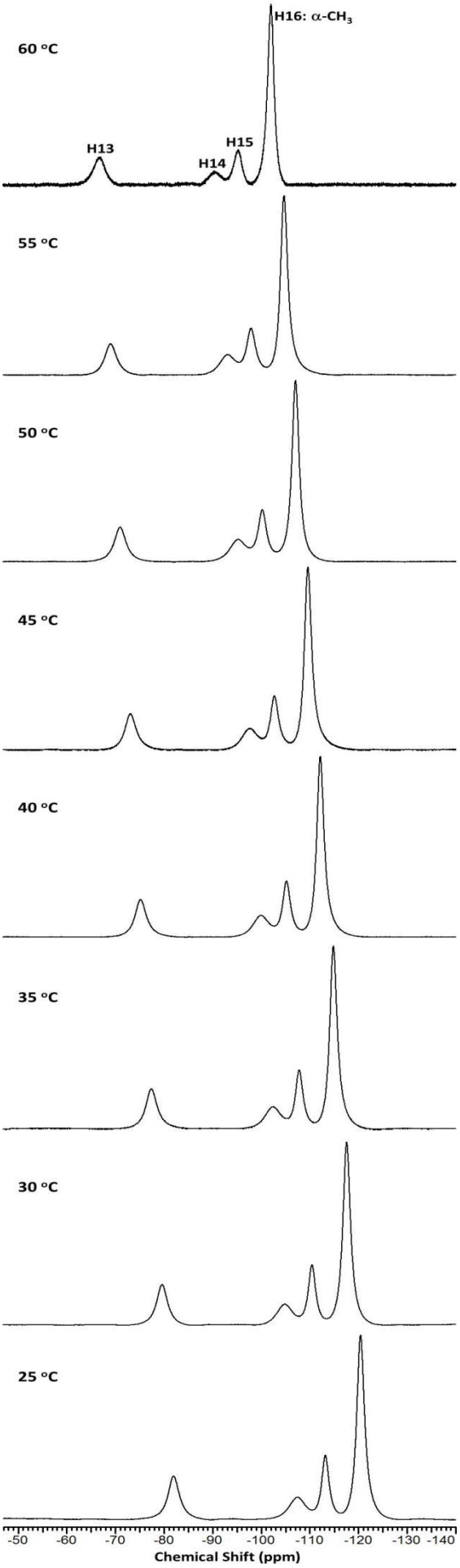


Figure S31. Expansion showing ^{1}H NMR resonances of some highly-shifted peaks, including proton resonances of α-CH_3 groups, of $[Co(TMPC)]^{2+}$ at 25 to 60 ^{o}C in 100 mM NaCl, D_2O, pD 7.00.

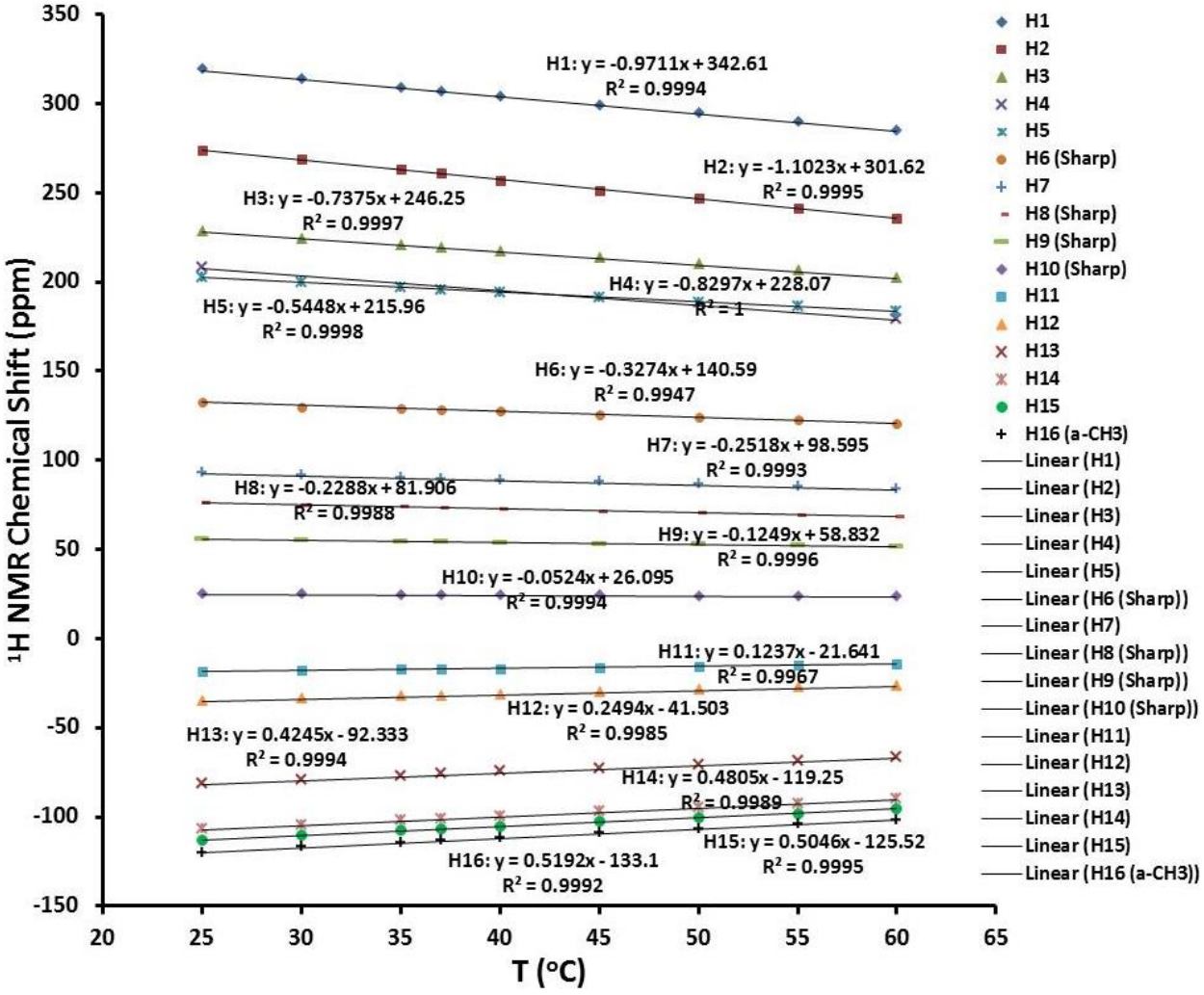


Figure S32. Linear fit of temperature-dependent paramagnetically-shifted ^{1}H NMR resonances of $[Co(TMPC)]^{2+}$ in the range of 25 to 60 ^{o}C. Samples contained 100 mM NaCl, D_2O, pD 7.00.

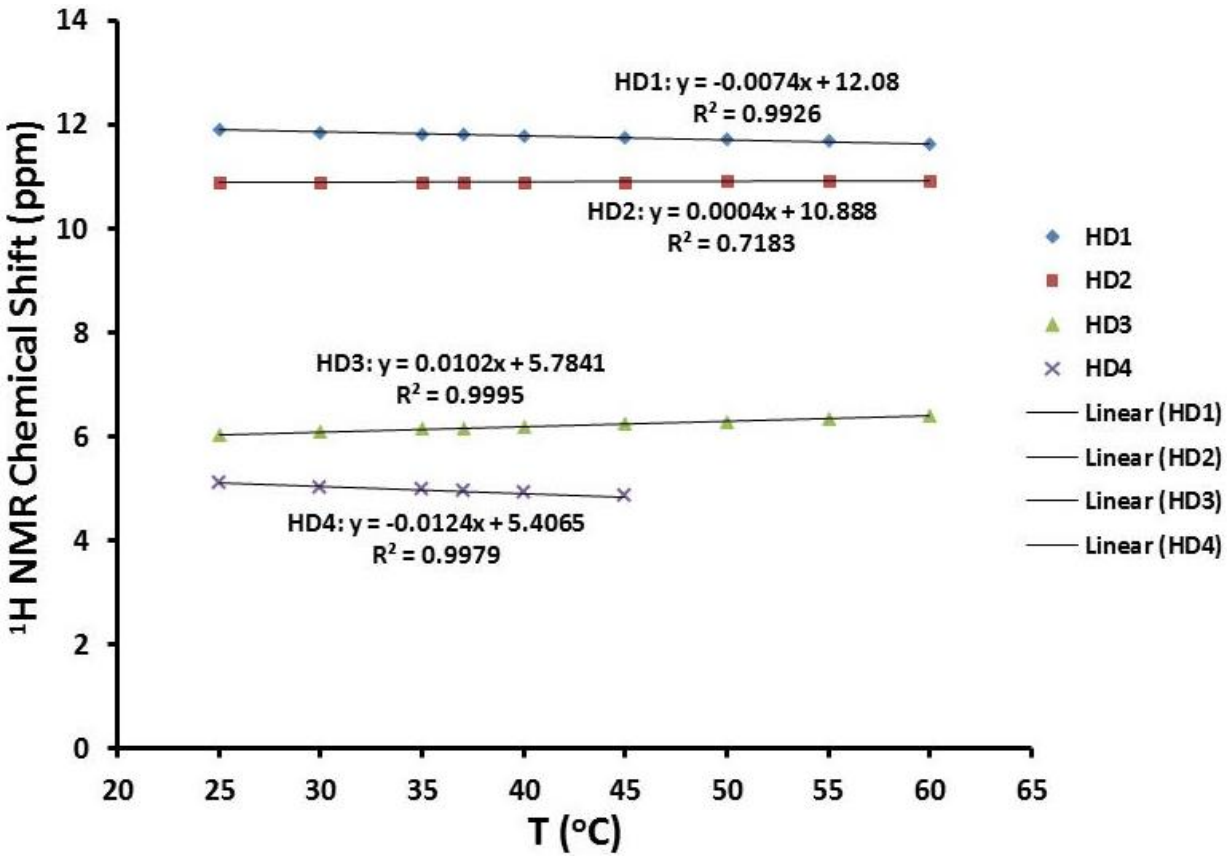


Figure S33. Linear fit of temperature-dependent ^{1}H NMR resonances in diamagnetic region of $[Co(TMPC)]^{2+}$ spectra in the range of 25 to 60 ^{o}C. Samples contained in 100 mM NaCl, D_2O, pD 7.00.

Table S5. Chemical shift and peak width of ^{1}H NMR resonances of $[Co(TMPC)]^{2+}$, 100 mM NaCl, D_2O, pD 7.00, as a function of temperature.

	Labeled protons of $[Co(TMPC)]^{2+}$																				
	H1	***H2***	***H3***	***H4$^{\perp}$***	***H5$^{\perp}$***	***H6***	***H7***	***H8***	***H9***	***H10***	***Diamagnetic Region***					***H11***	***H12***	***H13***	***H14***	***H15***	***H16: α-CH_3***
											HD1	***HD2***	***HD3***	***HD4: α-CH_3***	***S***						
T (^{o}C)	**Peak width in FWHM (*Hz*)**																				
25	1800	2450	1640	4930	787	323	967	347	163	118	204	44.5	40.3	52.2	70.7	1540	2830	1380	1930	855	909
30	1830	2100	1550	Overl.	846	363	943	347	160	117	190	44.1	40.3	53.1	55.2	1490	2800	1350	1870	874	882
35	1950	2350	1440	Overl.	956	424	928	358	160	117	182	45.9	41.7	55.8	44.0	1420	2450	1330	1980	914	873
37	2090	2510	1380	Overl.	1030	456	917	367	161	117	180	47.3	42.9	58.1	40.4	1420	2620	1320	1910	906	871
40	1920	2760	1450	Overl.	1100	499	918	381	164	119	179	50.5	45.9	45.6	36.2	1380	2410	1310	1950	936	872
45	2010	3130	1370	Overl.	1190	584	917	408	174	125	181	58.7	53.7	Overl.	31.2	1340	2240	1310	2020	967	865
50	1900	3070	1460	Overl.	1250	684	950	448	190	136	188	71.8	65.9	Overl.	27.3	1310	2140	1330	2010	1020	870
55	1800	2700	1420	Overl.	1360	773	990	476	208	153	206	92.7	86.0	Overl.	23.0	1290	2130	1360	Overl.	1140	859
60	Broad	Broad	Broad	1420	1060	811	831	447	214	173	236	125	113	Overl.	12.8	952	1560	938	Overl.	1270	802
T (^{o}C)	***^{1}H NMR Chemical shift (ppm)***																				
25	*318.76*	*274.12*	*228.06*	*207.33*	*202.37*	*132.69*	*92.43*	*76.35*	*55.76*	*24.81*	*11.89*	*10.90*	*6.04*	*5.10*	*4.71*	*-18.67*	*-35.38*	*-81.86*	*-107.30*	*-113.14*	*-120.45*
30	*313.33*	*268.69*	*224.11*	*N/A*	*199.74*	*130.10*	*91.05*	*75.07*	*55.09*	*24.52*	*11.85*	*10.90*	*6.09*	*5.03*	*4.71*	*-17.97*	*-34.05*	*-79.69*	*-104.97*	*-110.40*	*-117.55*
35	*308.42*	*263.02*	*220.28*	*N/A*	*196.79*	*129.25*	*89.71*	*73.84*	*54.44*	*24.25*	*11.82*	*10.90*	*6.14*	*4.97*	*4.72*	*-17.24*	*-32.57*	*-77.43*	*-102.26*	*-107.73*	*-114.81*
37	*306.53*	*260.93*	*218.85*	*N/A*	*195.71*	*128.58*	*89.23*	*73.37*	*54.18*	*24.14*	*11.81*	*10.90*	*6.16*	*4.94*	*4.72*	*-16.94*	*-32.40*	*-76.57*	*-101.44*	*-106.76*	*-113.73*
40	*303.63*	*257.31*	*216.65*	*N/A*	*194.10*	*127.58*	*88.44*	*72.64*	*53.80*	*23.98*	*11.79*	*10.90*	*6.19*	*4.91*	*4.72*	*-16.68*	*-31.49*	*-75.18*	*-100.01*	*-105.23*	*-112.15*
45	*298.63*	*251.42*	*213.00*	*N/A*	*191.42*	*125.94*	*87.19*	*71.54*	*53.18*	*23.73*	*11.75*	*10.90*	*6.24*	*4.85*	*4.72*	*-16.00*	*-30.18*	*-73.15*	*-97.43*	*-102.69*	*-109.59*
50	*294.42*	*246.95*	*209.48*	*N/A*	*188.79*	*124.34*	*86.03*	*70.44*	*52.59*	*23.47*	*11.71*	*10.91*	*6.29*	*N/A*	*4.72*	*-15.44*	*-29.01*	*-71.06*	*-95.28*	*-100.32*	*-107.13*
55	*289.46*	*241.11*	*205.89*	*N/A*	*186.07*	*122.61*	*84.85*	*69.38*	*51.99*	*23.23*	*11.68*	*10.91*	*6.34*	*N/A*	*4.72*	*-14.94*	*-27.76*	*-68.97*	*-93.21*	*-97.86*	*-104.66*
60	*284.21*	*235.44*	*201.94*	*178.29*	*183.23*	*120.77*	*83.49*	*68.28*	*51.35*	*22.95*	*11.62*	*10.91*	*6.40*	*N/A*	*4.72*	*-14.24*	*-26.66*	*-67.05*	*-90.22*	*-95.33*	*-102.11*
	CT (ppm/^{o}C)																				
	-0.97	-1.10	-0.74	-0.83	-0.55	-0.33	-0.25	-0.23	-0.13	-0.05	-0.01	0.4E-3	0.01	-0.01	N/A	0.12	0.25	0.43	0.48	0.51	0.52
T (^{o}C)	***|CT|/FWHM (1/^{o}C) ****																				
37	0.23	0.22	0.27	N/A	0.27	0.36	0.14	0.31	0.40	0.21	0.03	4.2E-3	0.12	0.09	N/A	0.04	0.05	0.16	0.13	0.28	0.30
T (^{o}C)	***T_1* / (St. Dev.) (ms) *****																				
25	0.14	N/A	0.21	N/A	0.51	2.5	0.36	1.0	2.5	3.6	2.2	14	19	17	84	0.19	N/A	0.28	0.14	0.48	0.37
	(0.03)	N/A	(0.01)	N/A	(0.01)	(0.0)	(0.01)	(0.0)	(0.2)	(0.1)	(0.0)	(0)	(0)	(0)	(0)	(0.03)	N/A	(0.01)	(0.02)	(0.01)	(0.01)

Table S5 Legend:
***** – Calculated for FWHM (Hz) measured at 37 ^{o}C.
****** – Measured at 25 ^{o}C.
$^{\perp}$ – ^{1}H NMR resonances H4 and H5 switch order at 60 ^{o}C.
S – Solvent peak.

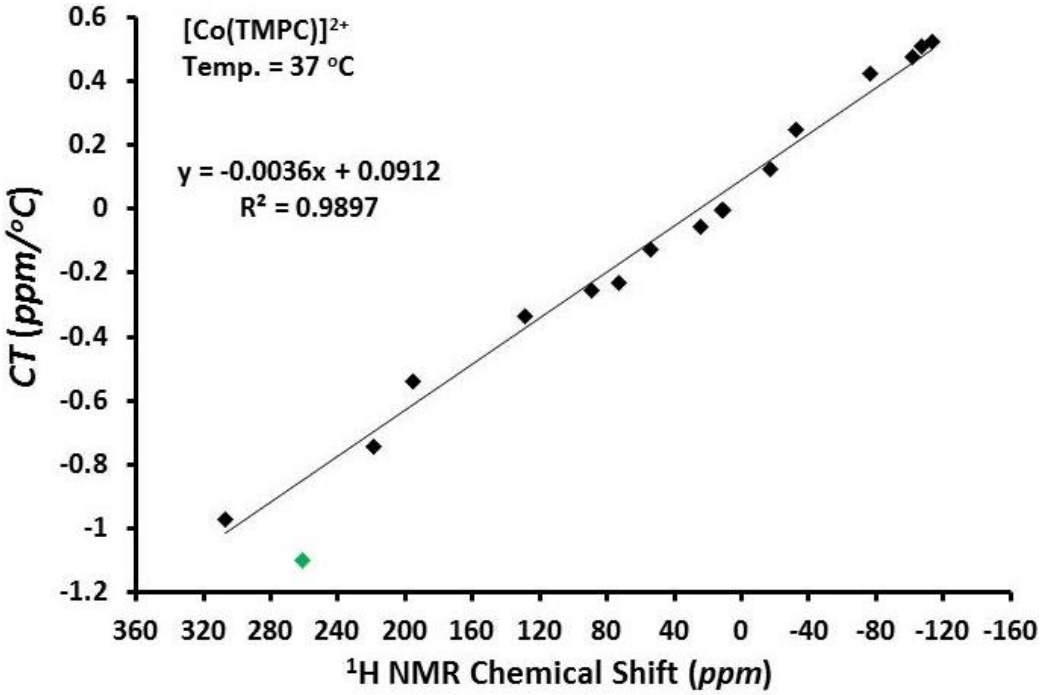


Figure S34. Dependence of *CT* values (ppm/^{o}C) of paramagnetically-shifted ^{1}H NMR resonances on their corresponding chemical shifts at 37 ^{o}C for $[Co(TMPC)]^{2+}$. The proton resonances in diamagnetic region (0-10 ppm) are excluded from consideration. The proton resonance at δ = 260.93 ppm at 37 ^{o}C (green diamond) was omitted from the fitting process. Best-fit slope and intercept are -0.0036 $^{o}C^{-1}$ and 0.0912 ppm/^{o}C, respectively. Samples contained 100 mM NaCl, D_2O, pD 7.00.

Table S6. Longitudinal relaxation times (T_1) of hyperfine-shifted proton resonances

Proton type	$[Co(MPT)]^{2+}$									
	CH_2	CH_2	CH_2	CH_2	β-H	β′-H	α-CH_3	γ-H	CH_2	CH_2
δ (ppm)	199.48	186.23	117.50	64.63	49.38	33.21	8.03	5.38	-12.12	-23.10
T_1 (St. Dev.) (ms)	8.3 (0.2)	7.3 (0.2)	7.0 (0.1)	4.6 (0.1)	50 (1)	38 (1)	5.7 (0.1)	102 (3)	2.2 (0.1)	2.3 (0.1)
Proton type	$[Fe(MPT)]^{2+}$									
	CH_2	CH_2	CH_2	CH_2	β-H	β′-H	α-CH_3	γ-H	CH_2	CH_2
δ (ppm)	195.45	168.36	98.46	72.09	52.14	33.33	21.22	-4.34	-11.63	-19.65
T_1 (St. Dev.) (ms)	4.4 (0.1)	3.7 (0.2)	3.8 (0.1)	2.4 (0.1)	30 (1)	21 (2)	2.4 (0.1)	63 (1)	1.1 (0.1)	1.2 (0.2)

	$[Fe(TMPC)]^{2+}$													
δ (ppm)	275.55	187.51	180.22	140.87	104.68	86.42	73.34	58.26	54.93	53.7*	-17.11	-27.06	-52.34	-74.14
T_1 (St. Dev.) (ms)	0.83 (0.01)	1.6 (0.0)	1.1 (0.0)	3.8 (0.2)	0.46 (0.01)	0.53 (0.02)	1.9 (0.0)	4.9 (0.0)	9.8 (0.1)	N/A	1.2 (0.0)	0.81 (0.01)	1.1 (0.0)	0.56 (0.01)

	$[Co(TMPC)]^{2+}$															
δ (ppm)	318.76	274.12	228.06	207.33	202.37	132.69	92.43	76.35	55.76	24.81	-18.67	-35.38	-81.86	-107.30	-113.14	-120.45
T_1 (St. Dev.) (ms)	0.14 (0.03)	N/A	0.21 (0.01)	N/A	0.51 (0.01)	2.5 (0.0)	0.36 (0.01)	1.0 (0.0)	2.5 (0.2)	3.6 (0.1)	0.19 (0.03)	N/A	0.28 (0.01)	0.14 (0.02)	0.48 (0.01)	0.37 (0.01)

Chemical shifts of proton resonances, δ (ppm), and longitudinal relaxation times, T_1 (ms), are obtained at 25 ^{o}C.

N/A – Data is not reported due to line broadening or overlap of proton resonances.

* – The peak is broadened at 25 ^{o}C.

^{1}H NMR data for $[Fe(TPC)]^{2+}$

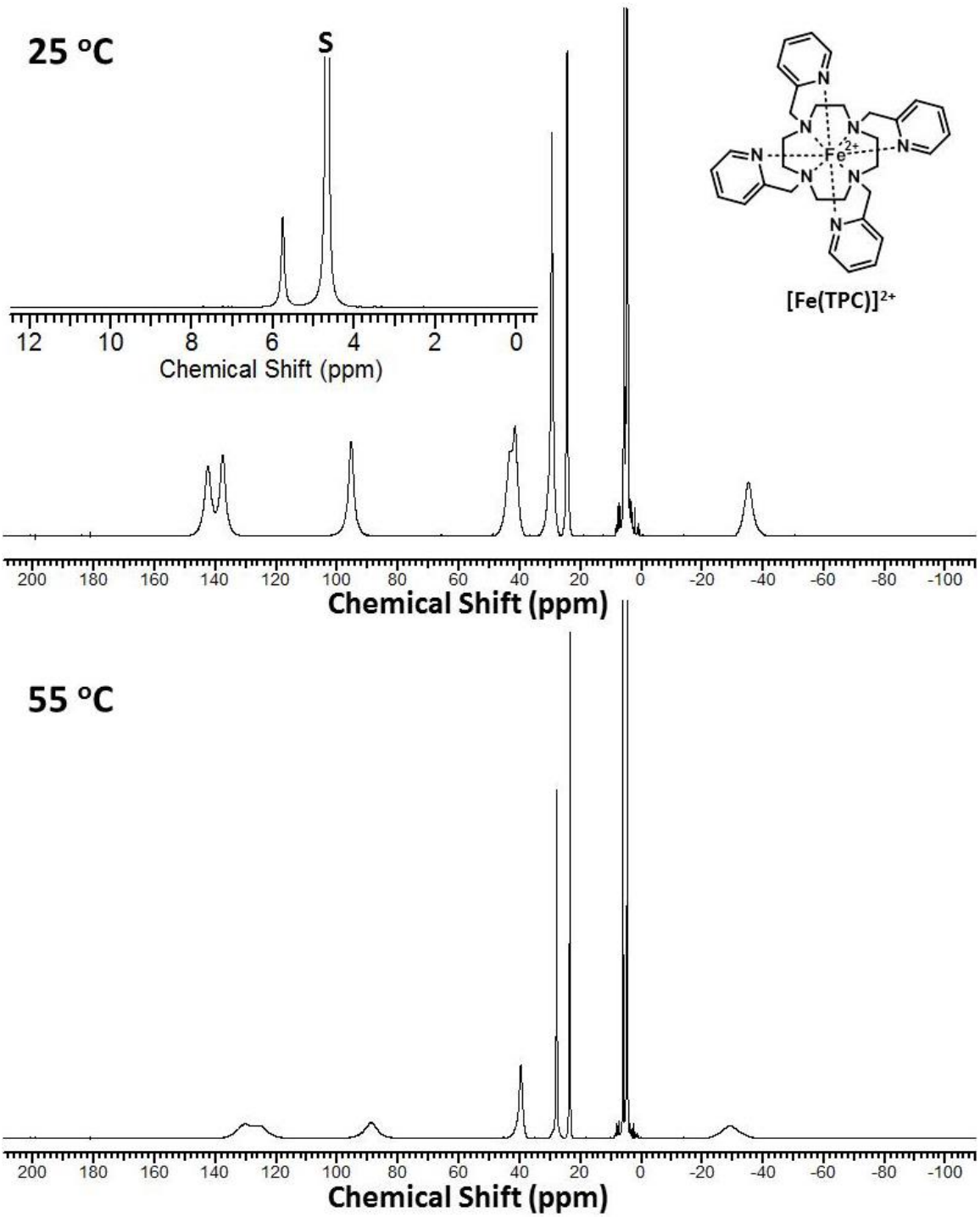


Figure S35. ^{1}H NMR spectra of $[Fe(TPC)]^{2+}$ at 25 ^{o}C and 55 ^{o}C in 100 mM NaCl, D_2O, pD 7.00. Insert shows diamagnetic region with solvent peak labeled with "S".

^{1}H NMR data for $[Co(TPC)]^{2+}$

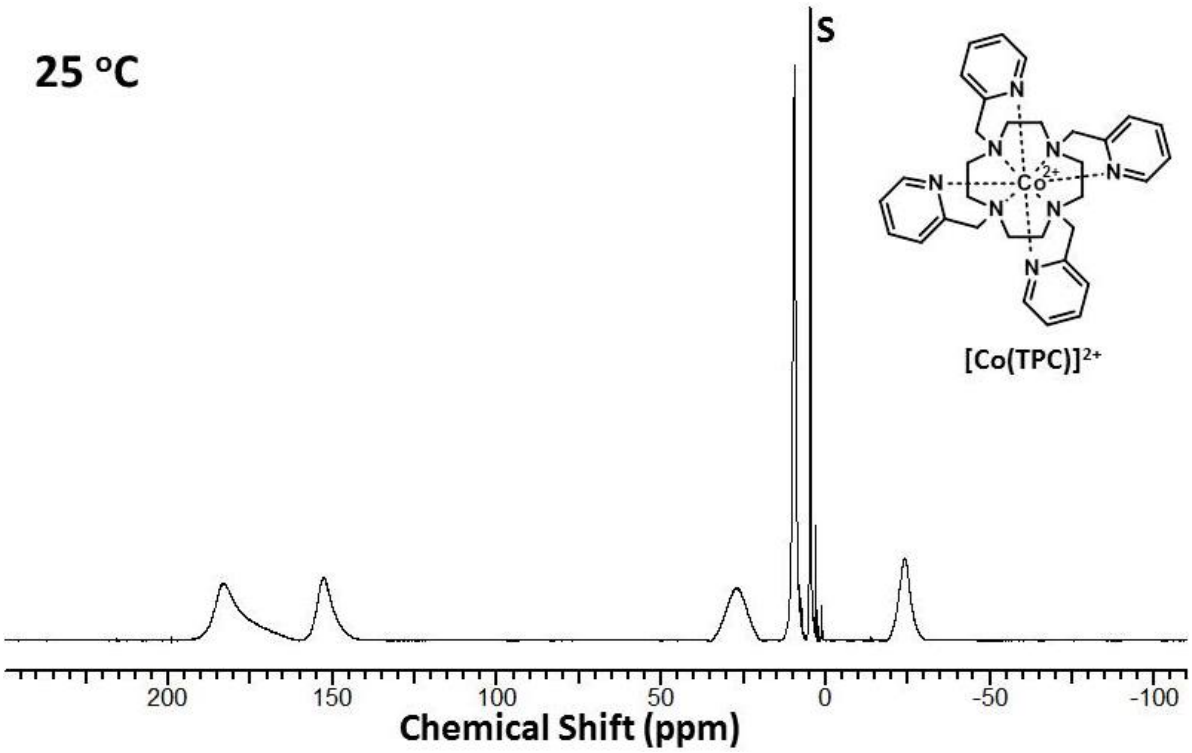


Figure S36. ^{1}H NMR spectrum of $[Co(TPC)]^{2+}$ at 25 ^{o}C in 100 mM NaCl, D_2O, pD 6.90. Solvent peak labeled with "S".

pH dependence of ^{1}H NMR resonances of $[Fe(TMPC)]^{2+}$

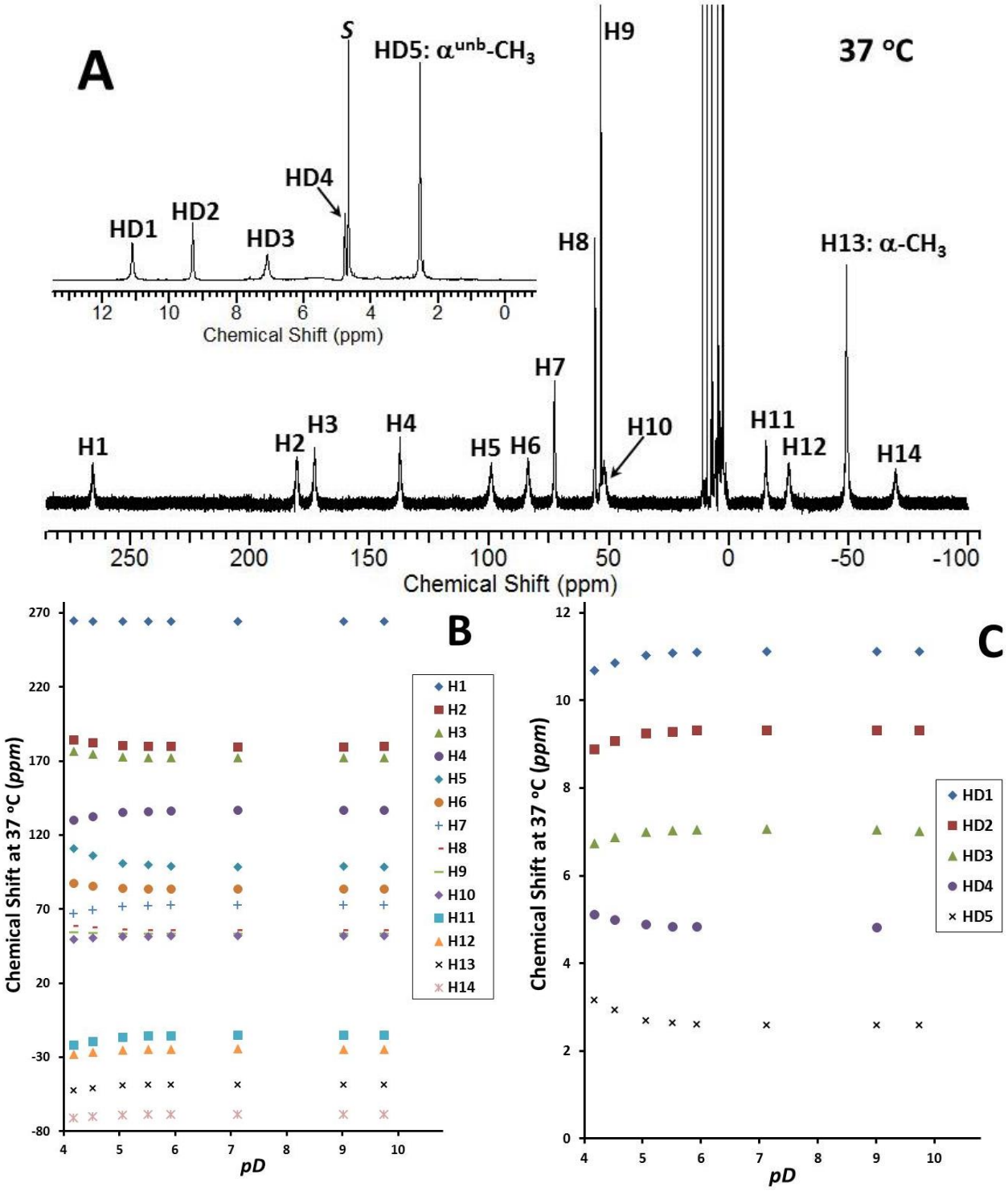


Figure S37. A) ^{1}H NMR spectrum of $[Fe(TMPC)]^{2+}$ in D_2O (100 mM NaCl, pD 7.2) with labeled protons, where insert shows expanded diamagnetic region, and a pD dependence of B) highly paramagnetically shifted proton resonances, and C) proton resonances in diamagnetic region of 20 mM $[Fe(TMPC)]^{2+}$ in D_2O solution containing 100 mM NaCl at 37 ^{o}C.

Acid dissociation studies

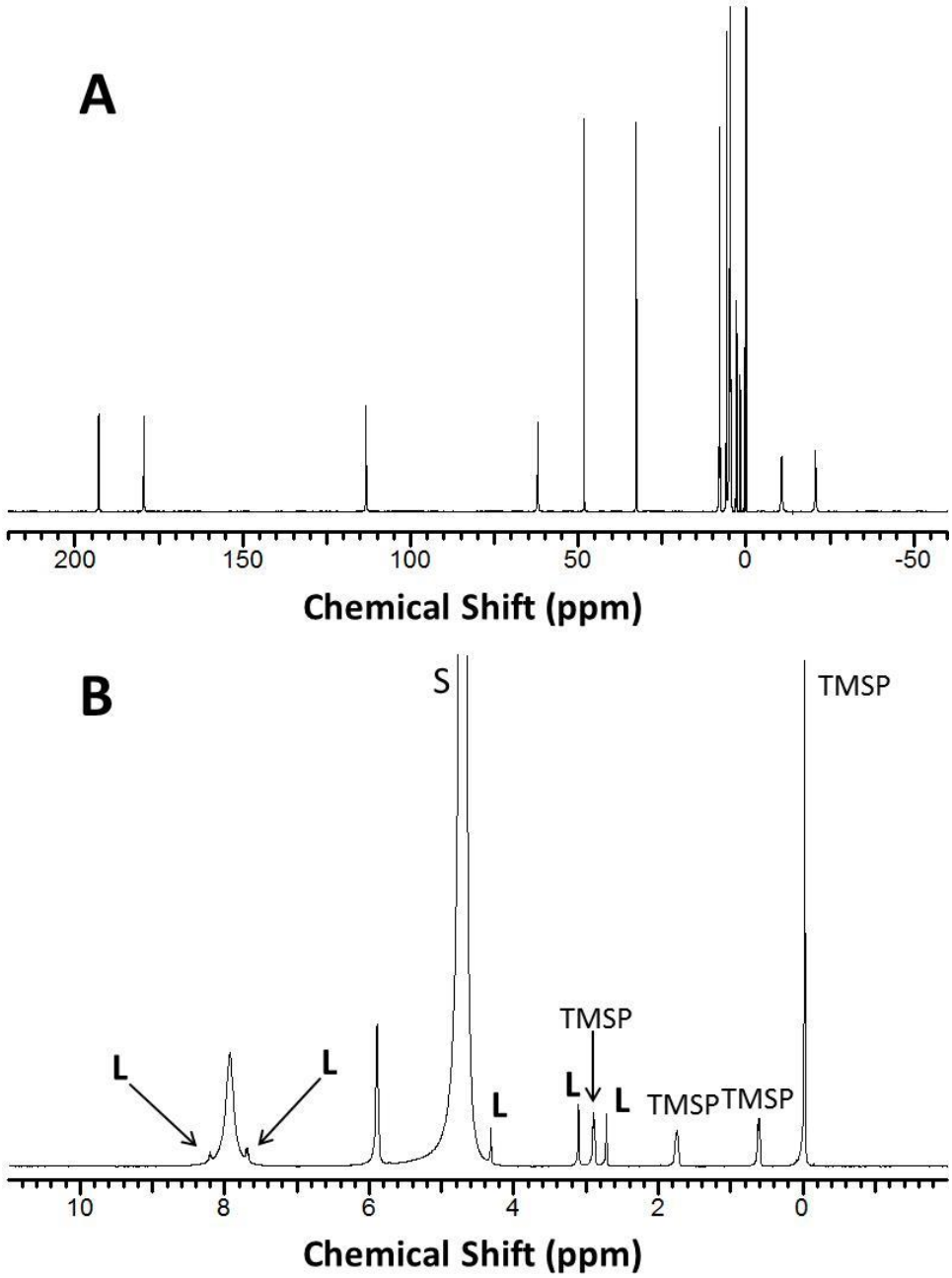


Figure S38. A) ^{1}H NMR (37 ^{o}C) of $[Co(MPT)]^{2+}$ after incubation at pD 3.0(1) at 37 ^{o}C for 48 h. B) Expended diamagnetic region showing TMSP proton resonances and proton resonances of a free MPT ligand (L) produced due to the complex dissociation.

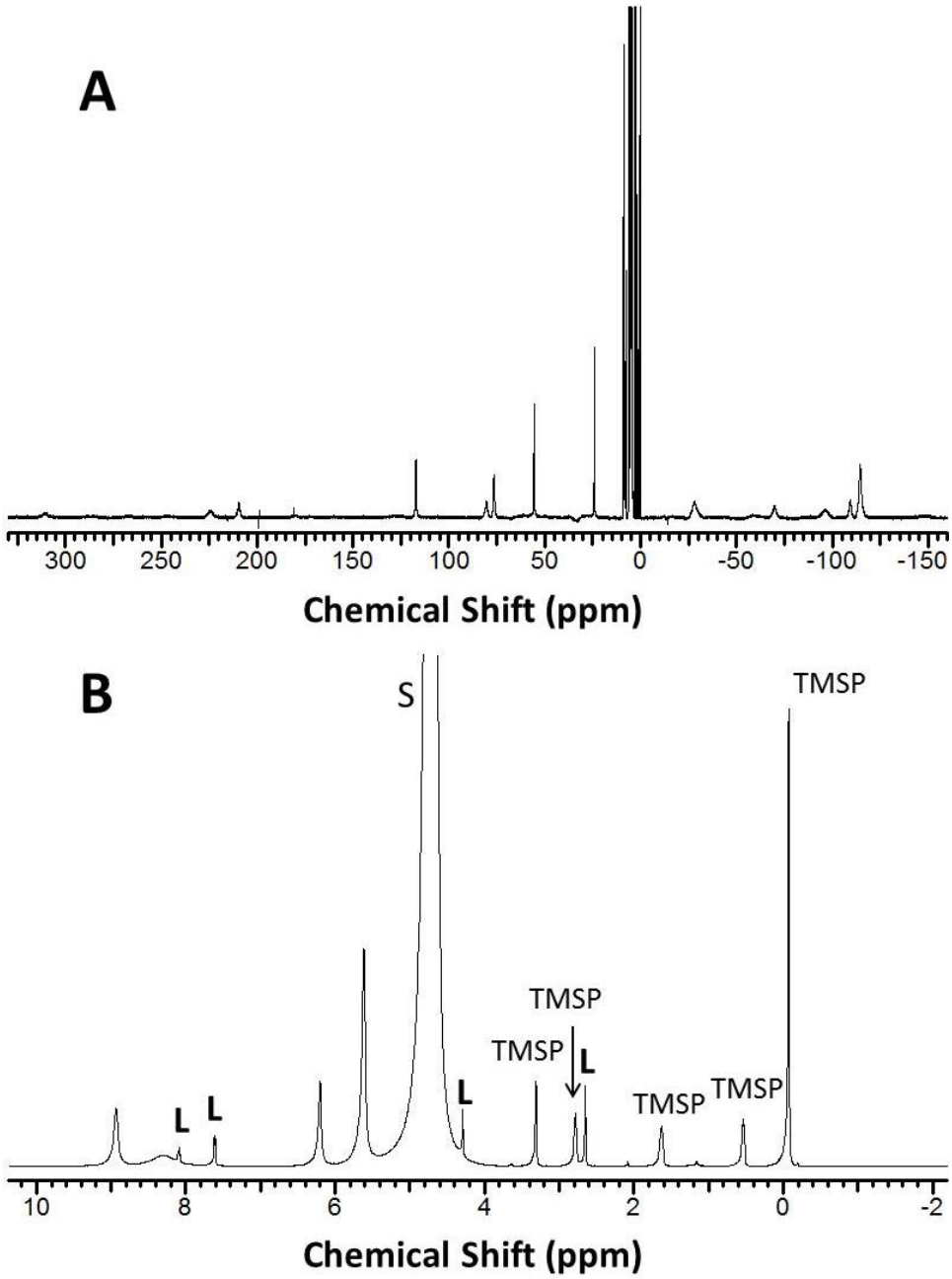


Figure S39. A) ^{1}H NMR (37 ^{o}C) of $[Co(TMPC)]^{2+}$ after incubation at pD 3.0(1) at 37 ^{o}C for 48 h. B) Expended diamagnetic region showing TMSP proton resonances and proton resonances of a free TMPC ligand (L) produced due to the complex dissociation.

^{1}H NMR temperature dependence of [Fe(TMPC)]$^{2+}$ in serum albumin

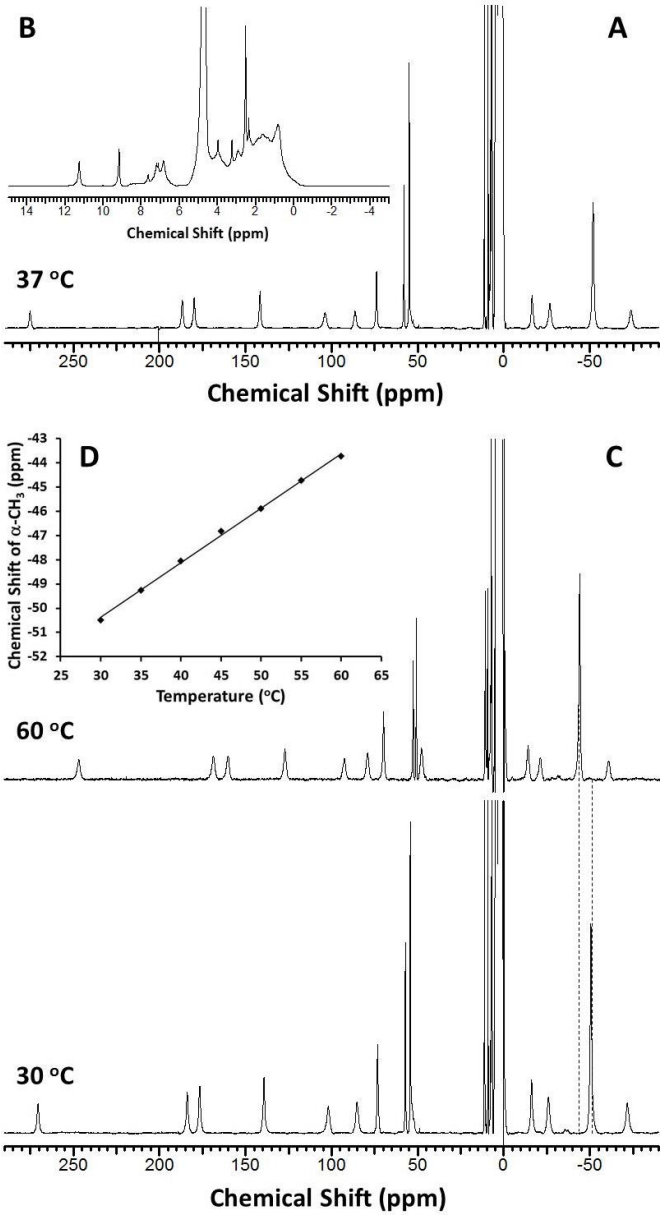


Figure S40. ^{1}H NMR spectra of 10 mM [Fe(TMPC)]$^{2+}$ in serum albumin (35 mg/mL) in D_2O, pD 7.4, at variable temperature. A) Spectrum was collected in 3 min using 128 transients and 0.4 s delay time at 37 ^oC. Insert B shows diamagnetic region complicated by the resonances of serum albumin. C) Spectra were collected at 30 and 60 ^oC, and the dotted grid line demonstrates a temperature dependent shift of the α-CH_3 resonance. Each spectrum (C) was collected in 12 s using 128 transients and 40 ms delay time. Insert D shows a temperature dependence of α-CH_3 resonance. Solid line represents a linear fit with CT = 0.23 ppm/^oC.

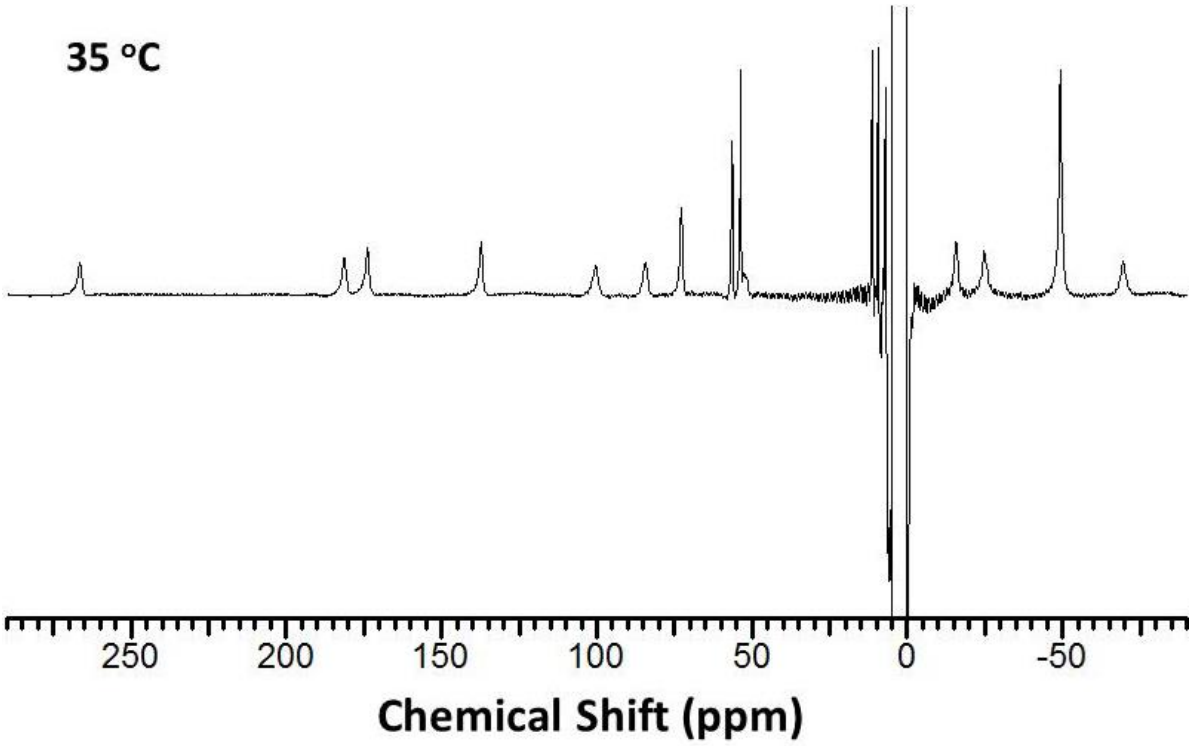


Figure S41. ^{1}H NMR spectra of 10 mM $[Fe(TMPC)]^{2+}$ in serum albumin (35 mg/mL) in D_2O, pD 7.4, collected in 4 s using 128 transients and 10 ms delay time at 35 ^{o}C.

Appendix 1. ^{1}H and ^{13}C NMR spectra of TMPC, MPT and TPC ligands

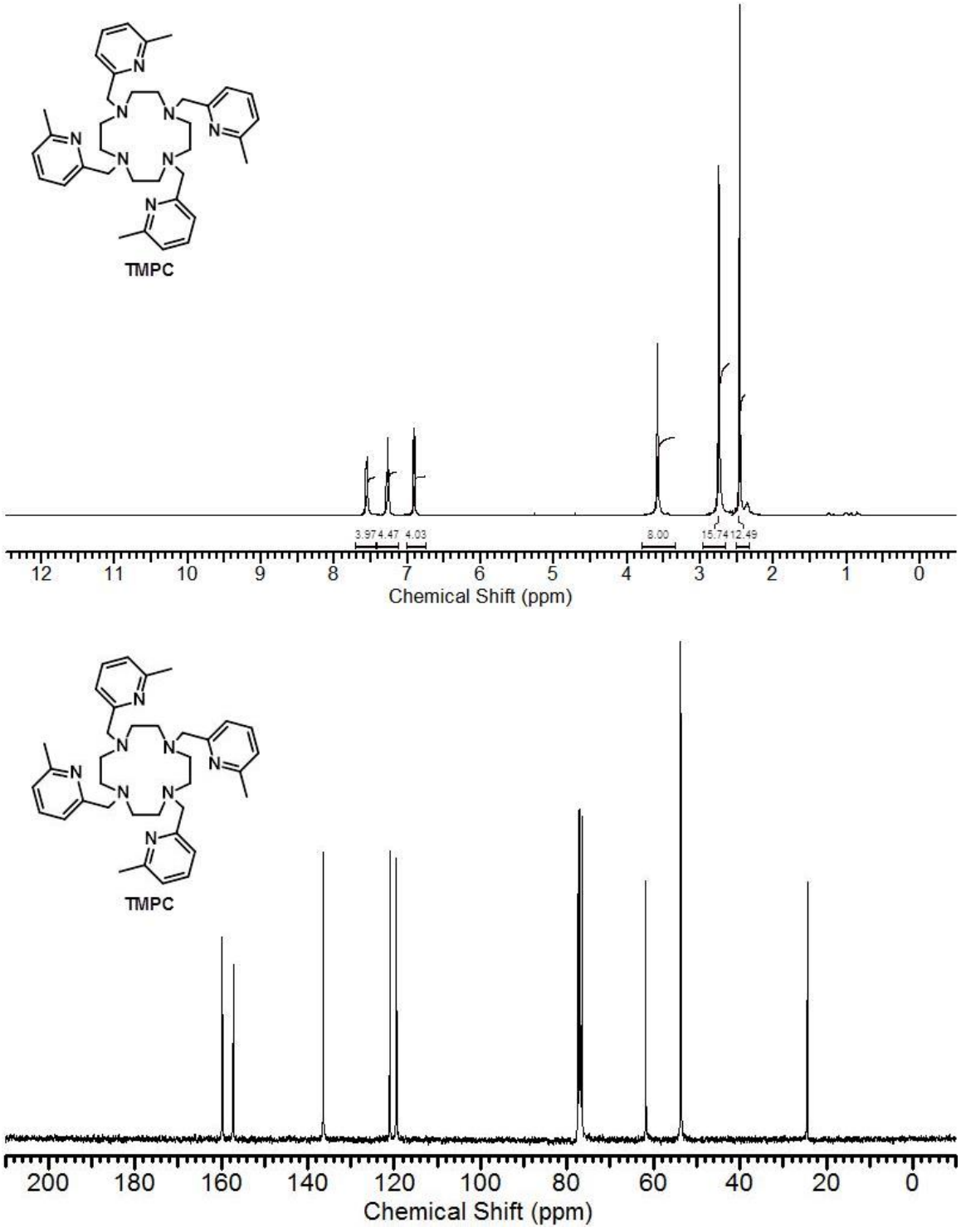


Figure S42. ^{1}H and ^{13}C NMR spectra of TMPC ligand in chloroform-*d*.

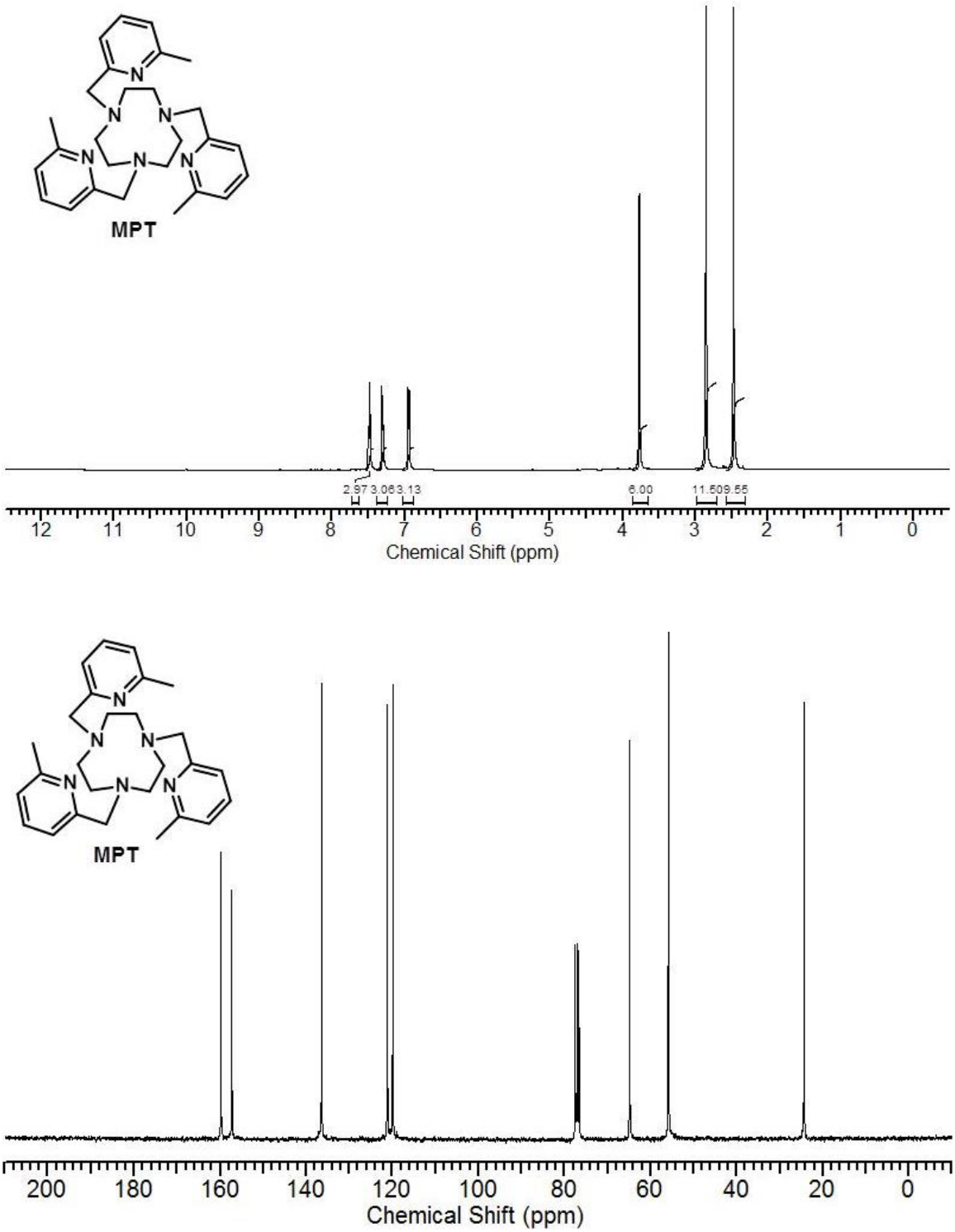


Figure S43. ^{1}H and ^{13}C NMR spectra of MPT ligand (free base) in chloroform-*d*.

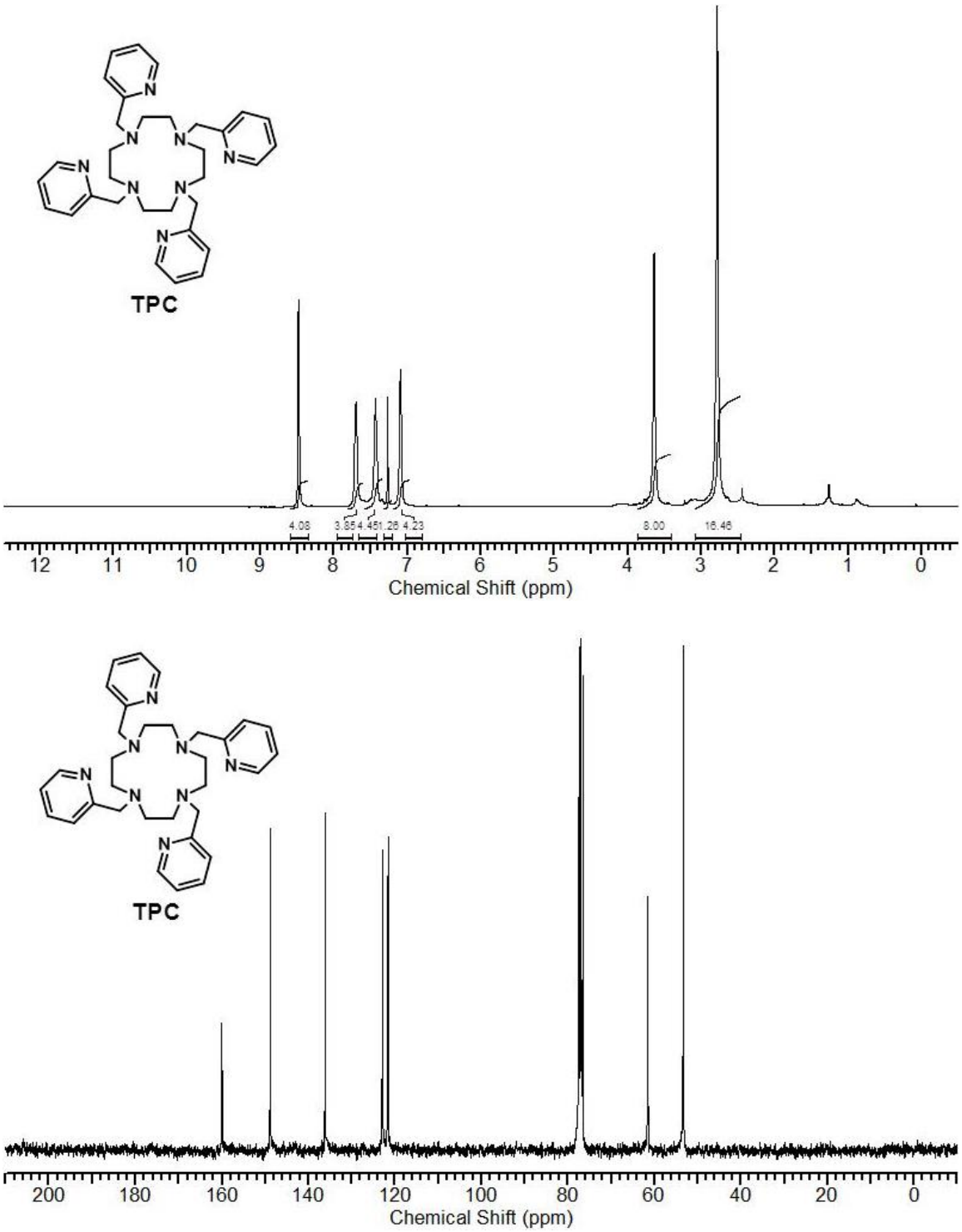


Figure S44. ^{1}H and ^{13}C NMR spectra of TPC ligand in chloroform-*d*.

Appendix 2. X-ray diffraction data

Fe(MPT)

Table S7. Crystal data and structure refinement for Fe(MPT).

Identification code	Fe(MPT)
Empirical formula	$C_{29.5}H_{36.5}F_{7.5}FeN_6Na_{0.5}O_{7.75}S_{2.5}$
Formula weight	889.14
Temperature/K	90
Crystal system	monoclinic
Space group	$P2_1$
a/Å	14.0975(17)
b/Å	13.7505(16)
c/Å	37.868(4)
α/°	90.00
β/°	96.079(4)
γ/°	90.00
Volume/Å^3	7299.3(15)
Z	8
ρ_{calc}g/cm^3	1.618
μ/mm^{-1}	0.657
F(000)	3652.0
Crystal size/mm^3	0.22 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.16 to 59.22
Index ranges	$-19 \leq h \leq 19$, $-19 \leq k \leq 19$, $-52 \leq l \leq 52$
Reflections collected	160296
Independent reflections	40994 [R_{int} = 0.0510, R_{sigma} = 0.0515]
Data/restraints/parameters	40994/1/1987
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0537, wR_2 = 0.1358
Final R indexes [all data]	R_1 = 0.0662, wR_2 = 0.1446
Largest diff. peak/hole / e Å^{-3}	1.57/-1.01
Flack parameter	0.449(8)

Table S8. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Fe(MPT). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
Fe1	2627.0(3)	4824.0(3)	2674.08(12)	13.80(9)
N1	1595(2)	5517(2)	3002.1(7)	17.9(6)
N2	1251(2)	4260(2)	2417.8(8)	18.2(6)
N3	2498.1(19)	6309(2)	2446.6(8)	16.7(5)
N4	3623.5(19)	4776(2)	2250.3(7)	14.6(5)
N5	3604(2)	5631(2)	3063.3(7)	17.3(5)
N6	3160(2)	3665(2)	3056.9(8)	19.1(6)
C1	772(2)	4861(3)	2980.9(9)	21.0(7)
C2	511(2)	4521(3)	2603.0(9)	18.6(6)
C3	-421(3)	4460(3)	2460.7(10)	23.9(7)
C4	-632(3)	4079(3)	2117.4(11)	28.1(8)
C5	110(3)	3752(3)	1941.7(10)	25.2(8)
C6	1052(3)	3849(3)	2095.8(9)	19.5(6)
C7	1853(3)	3493(3)	1900.1(10)	22.5(7)
C8	1295(3)	6508(3)	2865.9(9)	20.8(7)
C9	1521(2)	6641(3)	2483.9(10)	20.6(7)
C10	2648(2)	6186(3)	2068.9(8)	18.0(6)
C11	3501(2)	5559(2)	2030.8(9)	16.3(6)
C12	4099(2)	5768(3)	1776.1(9)	18.4(6)
C13	4880(3)	5166(3)	1744.6(9)	22.8(7)
C14	4996(2)	4360(3)	1963.3(9)	19.6(7)
C15	4361(2)	4168(2)	2205.8(9)	16.0(6)
C16	4447(3)	3254(3)	2425.3(9)	20.7(7)
C17	3225(3)	6977(3)	2634.6(10)	21.9(7)
C18	4007(2)	6421(3)	2858.9(9)	19.3(7)
C19	4348(2)	4936(3)	3197.3(9)	21.9(7)
C20	3936(3)	3958(3)	3271.9(9)	21.1(7)
C21	4408(3)	3374(3)	3531(1)	29.8(8)
C22	4078(3)	2433(4)	3573.0(12)	36.3(10)
C23	3295(3)	2123(3)	3354.0(12)	34.5(9)
C24	2839(3)	2741(3)	3101.2(10)	23.0(7)
C25	1988(3)	2399(3)	2861.3(11)	26.9(8)
C26	3080(3)	6028(3)	3353.3(9)	22.4(7)
C27	2100(2)	5558(3)	3366.3(9)	21.2(7)

Fe3	2717.3(3)	3899.9(3)	7731.67(12)	15.28(9)
N13	3543(2)	3348(2)	8216.5(8)	23.5(6)
N14	3061(2)	5250(2)	8086.4(8)	21.7(6)
N15	3027(2)	2375(2)	7576.6(8)	20.5(6)
N16	3743(2)	4032(2)	7310.3(7)	16.3(5)
N17	1632(2)	3041(2)	7989.3(8)	21.5(6)
N18	1339(2)	4389(2)	7445.9(8)	18.7(6)
C55	4281(3)	4085(3)	8316.9(10)	24.5(7)
C56	3850(3)	5081(3)	8309.7(10)	25.4(8)
C57	4294(3)	5797(4)	8525.6(12)	37(1)
C58	3910(4)	6717(4)	8514.9(15)	50.6(14)
C59	3079(4)	6899(3)	8293.0(13)	39.5(11)
C60	2668(3)	6158(3)	8081.9(10)	26.4(8)
C61	1785(3)	6360(3)	7845.1(12)	29.6(9)
C62	3981(3)	2390(3)	8165.3(10)	26.4(8)
C63	3985(3)	2161(3)	7773.9(10)	25.2(8)
C64	3069(3)	2409(3)	7189.2(9)	21.7(7)
C65	3685(2)	3246(2)	7094.8(9)	15.8(6)
C66	4174(3)	3175(3)	6796.9(9)	19.6(7)
C67	4772(3)	3916(3)	6721.9(9)	22.7(7)
C68	4858(2)	4717(3)	6946.9(9)	20.2(7)
C69	4331(2)	4764(3)	7235.9(9)	17.2(6)
C70	4400(3)	5643(3)	7471.4(10)	22.6(7)
C71	2304(3)	1663(3)	7669.4(11)	25.6(8)
C72	1400(3)	2191(3)	7746.7(11)	25.5(8)
C73	804(3)	3692(3)	7983.9(10)	26.1(8)
C74	585(3)	4148(3)	7622.3(10)	22.7(7)
C75	-356(3)	4320(3)	7487.7(11)	27.8(8)
C76	-547(3)	4766(3)	7161.2(12)	31.4(8)
C77	217(3)	5045(3)	6979.3(11)	28.2(8)
C78	1150(3)	4849(3)	7126.9(10)	21.9(7)
C79	1968(3)	5146(3)	6930.5(10)	24.6(7)
C80	1973(3)	2734(3)	8353.7(10)	27.3(8)
C81	2850(3)	3293(3)	8488.2(10)	27.8(8)
Fe2	2123.3(3)	2858.3(3)	136.61(12)	14.47(9)
N7	3441(2)	2423(2)	-103.9(8)	19.3(6)
N8	2619(2)	4270(2)	-69.8(7)	16.8(5)
N9	1517(2)	2311(2)	-387.3(8)	22.0(6)

N10	559(2)	3069(2)	159.5(8)	19.2(6)
N11	2170(2)	1258(2)	231.4(8)	20.9(6)
N12	2732(2)	2762(2)	697.6(7)	18.4(6)
C28	4058(3)	3298(3)	-60.2(10)	22.2(7)
C29	3495(3)	4184(3)	-184.8(9)	20.9(7)
C30	3866(3)	4876(3)	-396.5(11)	29.8(8)
C31	3334(4)	5690(3)	-490.3(13)	38.3(11)
C32	2464(3)	5803(3)	-367.6(11)	28.6(8)
C33	2117(3)	5086(2)	-153.1(9)	18.7(6)
C34	1181(3)	5234(3)	-3.6(10)	23.8(7)
C35	3209(3)	2161(3)	-487.5(10)	25.9(8)
C36	2242(3)	2518(3)	-636.9(9)	24.1(7)
C37	644(3)	2898(3)	-476.2(9)	25.2(7)
C38	67(3)	2963(3)	-164.5(10)	22.7(7)
C39	-914(3)	2995(3)	-220.2(11)	27.8(8)
C40	-1422(3)	3161(3)	67.8(13)	33.2(9)
C41	-935(3)	3290(3)	398.7(12)	29.1(8)
C42	66(3)	3228(3)	439.4(10)	22.3(7)
C43	596(3)	3373(3)	800.7(11)	31.6(9)
C44	1297(3)	1249(3)	-371.2(10)	28.3(8)
C45	1313(3)	885(3)	8.1(10)	26.0(8)
C46	2067(3)	1132(3)	611.4(10)	24.1(7)
C47	2667(3)	1848(3)	833.8(9)	21.3(7)
C48	3056(3)	1597(3)	1170.6(10)	28.7(8)
C49	3505(3)	2327(4)	1381.9(11)	36.3(10)
C50	3544(3)	3252(4)	1254.1(11)	37(1)
C51	3157(3)	3468(3)	906.9(9)	21.8(7)
C52	3212(3)	4475(3)	768.7(10)	27.7(8)
C53	3071(3)	821(3)	132.4(11)	26.3(8)
C54	3842(3)	1586(3)	107.0(11)	25.0(7)
Fe4	2344.3(4)	6141.2(3)	5056.14(12)	17.29(10)
N19	2379(2)	7747(2)	5103.9(7)	20.9(6)
N20	2804(2)	6349(2)	5629.1(7)	18.7(6)
N21	1885(2)	6590(2)	4497.1(8)	21.8(6)
N22	778(2)	5976(2)	5018.3(8)	19.4(6)
N23	3726(2)	6473(2)	4850.9(8)	22.0(6)
N24	2817(2)	4662(2)	4915.8(7)	19.3(6)
C82	2166(3)	7963(2)	5470.3(9)	21.3(7)

C83	2700(3)	7280(3)	5732.4(9)	20.7(7)
C84	2995(3)	7613(3)	6072.0(9)	23.3(7)
C85	3391(3)	6950(3)	6320.1(9)	26.5(8)
C86	3469(3)	5993(3)	6220.5(9)	25.2(8)
C87	3189(3)	5706(3)	5874.1(9)	19.4(6)
C88	3285(3)	4661(3)	5769.7(10)	23.2(7)
C89	1613(3)	8106(2)	4841.4(9)	24.9(8)
C90	1708(3)	7658(3)	4478.3(10)	28.5(8)
C91	1018(3)	6028(3)	4390.3(9)	26.6(8)
C92	365(3)	6013(2)	4678.5(9)	21.6(7)
C93	-608(3)	5981(3)	4591.4(10)	26.7(8)
C94	-1197(3)	5902(3)	4864.3(12)	34.8(9)
C95	-771(3)	5848(3)	5210.7(11)	26.7(8)
C96	211(3)	5882(2)	5281.0(9)	21.2(7)
C97	649(3)	5775(3)	5656.6(9)	23.0(7)
C98	2664(3)	6320(3)	4282.7(10)	27.7(8)
C99	3631(3)	6668(3)	4457.7(10)	27.8(8)
C100	4295(3)	5583(3)	4933.6(10)	25.2(7)
C101	3709(3)	4707(3)	4806.8(9)	21.6(7)
C102	4067(3)	3986(3)	4601.6(10)	27.1(8)
C103	3502(3)	3185(3)	4509.1(11)	30.9(9)
C104	2606(3)	3114(3)	4631.8(11)	27.8(8)
C105	2289(3)	3856(3)	4837.1(9)	19.9(6)
C106	1351(3)	3755(3)	4983.7(10)	22.1(7)
C107	4097(3)	7325(3)	5057.8(10)	26.6(8)
C108	3335(3)	8123(3)	5043(1)	27.7(8)
S1	6854.3(6)	4310.9(6)	7977.6(2)	21.28(17)
S2	6217.2(7)	3208.4(7)	9115.9(3)	25.06(18)
S3	8767.2(7)	1082.2(7)	8840.8(2)	26.87(19)
S4	10109.3(8)	4989.0(9)	8885.3(3)	33.8(2)
Na1	7954.5(10)	3606.5(10)	8680.9(4)	19.9(3)
F1	6578.2(19)	6075.7(19)	7723.6(9)	47.5(7)
F2	8049.2(18)	5716.2(19)	7861.4(8)	41.1(6)
F3	7307(2)	5111(2)	7391.1(7)	46.1(7)
F4	6281.5(19)	2540(2)	9765.2(7)	43.5(7)
F5	7107.9(17)	1708.0(18)	9425.0(7)	35.5(6)
F6	5571.3(19)	1591(2)	9366.8(10)	52.0(8)
F7	10532(2)	1611(3)	8780.9(7)	56.2(9)

F8	10281(2)	90(3)	8709.4(8)	52.8(8)
F9	9767(2)	1100(2)	8292.7(6)	43.1(7)
F10	9151(2)	6498(2)	8628.1(8)	48.4(7)
F11	9916(2)	5742(3)	8248.6(8)	57.0(9)
F12	10658(3)	6641(3)	8624.2(13)	79.5(13)
O1	7666(2)	3662(2)	7983.7(8)	26.8(6)
O2	5998.9(19)	3979(2)	7769.3(7)	25.4(5)
O3	6726(2)	4715(2)	8318.6(8)	31.9(6)
O4	7083(2)	3751(2)	9213.5(8)	35.2(7)
O5	6208(2)	2745(2)	8775.3(8)	32.0(6)
O6	5348(2)	3691(3)	9182.1(8)	41.1(8)
O7	8210(2)	308(3)	8671.3(7)	37.8(8)
O8	9052(2)	947(3)	9212.6(7)	36.5(7)
O9	8477(3)	2041(3)	8736.7(11)	54.8(10)
O10	11006(2)	4589(3)	8829.4(9)	45.6(9)
O11	10113(3)	5483(5)	9227.6(10)	79.0(17)
O12	9289(4)	4446(4)	8786.2(16)	89.8(19)
C109	7218(3)	5356(3)	7723.6(12)	29.9(8)
C110	6300(3)	2209(3)	9434.5(13)	32.0(9)
C111	9887(3)	982(4)	8643.4(10)	34.8(10)
C112	9942(4)	6037(4)	8590.6(13)	41.2(11)
S5	6936.1(6)	4460.4(6)	2957.3(2)	17.14(15)
S6	9579.7(7)	7381.5(7)	3527.5(2)	24.86(18)
S7	6375.8(6)	5778.1(6)	4032.0(2)	20.91(17)
S8	10036.0(7)	3509.7(7)	3926.7(3)	27.3(2)
Na2	8139(1)	5211.9(10)	3637.3(3)	19.6(3)
F13	7415.0(19)	3547(2)	2393.6(7)	37.1(6)
F14	6572.8(18)	2690.8(17)	2723.4(8)	38.7(6)
F15	8049.4(18)	2954.6(19)	2893.0(8)	38.0(6)
F16	9258(3)	9163(2)	3727.5(8)	57.7(9)
F17	8051(2)	8242(3)	3702.9(8)	54.5(9)
F18	9172(2)	8093(2)	4134.9(6)	39.7(6)
F19	7259.1(17)	7316.1(17)	4319.4(7)	33.2(5)
F20	5737.0(19)	7474.4(19)	4213.8(9)	44.8(7)
F21	6330(2)	6609(2)	4654.3(7)	43.0(7)
F22	9918.3(19)	2883(2)	3266.6(6)	37.6(6)
F23	9157.5(19)	2019(2)	3612.2(6)	37.1(6)
F24	10678(2)	1931(2)	3640.4(9)	51.9(8)

O13	7817.1(18)	5016.0(19)	2995.0(7)	22.9(5)
O14	6184.5(18)	4871(2)	2717.9(6)	22.0(5)
O15	6666(2)	4101(2)	3289.2(7)	27.6(6)
O16	9260(2)	7634(2)	3166.2(7)	28.2(6)
O17	10569(2)	7530(3)	3637.2(8)	46.1(9)
O18	9223(3)	6479(2)	3650.4(9)	44.9(9)
O19	6446(2)	6178(2)	3683.3(8)	32.3(6)
O20	7210(2)	5224(2)	4167.7(8)	31.4(6)
O21	5470(2)	5341(2)	4086.7(8)	31.3(6)
O22	10879(3)	4040(3)	3852.5(9)	45.2(9)
O23	10113(3)	3001(3)	4258.8(8)	43.0(8)
O24	9155(3)	4034(3)	3836.2(11)	50.7(9)
C113	7265(3)	3356(3)	2734.2(11)	27.1(8)
C114	8991(3)	8265(3)	3788.7(10)	31.5(9)
C115	6429(3)	6851(3)	4317.8(11)	26.4(8)
C116	9952(3)	2551(3)	3592.9(10)	26.7(8)
S9	6065.0(9)	4992.5(8)	5879.4(3)	37.9(2)
F25	7463(2)	6235(2)	5883.4(8)	43.8(6)
F26	7873(2)	4751(2)	5807.7(11)	60.0(9)
F27	7070(2)	5536(3)	5377.4(8)	55.1(8)
O25	6320(3)	4878(3)	6263.2(10)	51.0(9)
O26	5445(2)	5793(3)	5785.8(9)	40.1(7)
O27	5871(3)	4110(3)	5688.9(11)	50.7(10)
O31	7643(4)	3391(4)	6600.6(15)	79.5(16)
C117	7167(4)	5409(4)	5727.9(14)	41.1(11)
S10	7105.0(9)	4720(1)	1144.1(3)	43.1(3)
F28	5893(4)	4631(3)	564.4(11)	93.0(16)
F29	6400(3)	3266(3)	756.1(12)	83.1(13)
F30	5376(3)	3990(4)	1009.9(12)	87.2(14)
O28	7859(3)	4747(4)	919.8(15)	78.6(15)
O29	6696(4)	5669(3)	1193.8(13)	68.2(12)
O30	7134(5)	4140(3)	1450.3(12)	86.1(18)
C118	6235(4)	4092(4)	814(2)	67(2)

Table S9. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Fe(MPT). 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	15.5(2)	13.5(2)	12.50(19)	-0.53(16)	1.83(16)	-0.73(17)
N1	18.8(14)	20.2(14)	14.8(13)	-4.3(10)	2.3(10)	-0.8(11)
N2	17.3(13)	18.0(13)	19.3(13)	-1.6(11)	2.7(11)	-4.1(11)
N3	14.8(13)	14.5(13)	20.7(13)	-0.4(10)	1.7(10)	1.4(10)
N4	16.4(12)	13.7(12)	13.7(12)	-0.1(10)	0.8(9)	-0.5(10)
N5	17.7(13)	19.9(14)	14.2(12)	1.1(10)	0.9(10)	-1.7(11)
N6	19.2(14)	21.3(14)	17.5(13)	2.1(11)	5.6(11)	1.6(11)
C1	18.9(15)	28.5(18)	16.8(15)	-2.8(14)	7.1(12)	-4.0(14)
C2	19.8(16)	19.1(15)	17.6(15)	-2.0(12)	5.7(12)	-2.9(13)
C3	19.6(16)	24.1(17)	28.6(18)	-3.6(15)	5.8(14)	-3.4(14)
C4	20.1(17)	34(2)	28.9(19)	-3.8(16)	-1.4(14)	-6.5(15)
C5	25.6(18)	31(2)	18.7(16)	-3.4(14)	0.1(13)	-8.3(15)
C6	23.3(17)	17.6(15)	18.2(15)	-2.2(13)	4.8(12)	-4.5(13)
C7	24.4(17)	22.9(17)	20.6(16)	-8.0(14)	4.3(13)	-2.9(14)
C8	20.5(16)	18.7(16)	23.2(17)	-7.9(13)	2.4(13)	2.1(13)
C9	19.7(16)	16.8(15)	25.4(17)	0.7(13)	1.9(13)	4.1(13)
C10	20.3(15)	17.4(15)	16.0(14)	2.8(12)	0.9(12)	2.8(13)
C11	17.0(15)	16.3(15)	14.8(14)	-0.1(11)	-1.9(12)	-3.2(12)
C12	23.2(16)	17.4(15)	14.6(14)	0.4(12)	2.6(12)	-4.9(13)
C13	25.8(18)	27.0(18)	16.4(15)	-3.2(13)	5.3(13)	-8.7(14)
C14	20.9(16)	18.8(16)	19.4(15)	-6.1(13)	3.6(13)	-2.7(13)
C15	15.5(14)	15.8(14)	16.0(14)	-2.5(11)	-1.3(11)	-1.0(11)
C16	23.8(17)	17.6(15)	20.5(16)	-0.9(13)	1.2(13)	4.3(13)
C17	20.7(16)	17.5(16)	26.9(18)	-1.1(13)	0.0(13)	-3.7(13)
C18	18.3(16)	18.2(16)	20.9(16)	-2.4(12)	0.1(12)	-5.1(12)
C19	19.6(16)	28.2(18)	17.5(15)	1.1(14)	-0.5(12)	-2.5(14)
C20	20.0(16)	27.7(18)	16.3(15)	4.4(13)	5.2(12)	5.5(14)
C21	29(2)	40(2)	20.6(17)	9.0(16)	2.0(15)	3.9(17)
C22	37(2)	41(2)	31(2)	17.4(19)	1.1(17)	5.8(19)
C23	40(2)	28(2)	37(2)	15.2(17)	11.7(18)	3.8(18)
C24	27.0(18)	19.3(16)	24.2(17)	3.9(13)	9.9(14)	0.9(14)
C25	29.9(19)	18.7(17)	33(2)	4.1(15)	5.6(15)	-3.5(15)
C26	26.7(17)	23.3(17)	16.8(15)	-7.7(13)	0.5(13)	-1.8(14)
C27	20.3(16)	28.5(18)	14.9(15)	-5.2(13)	2.7(12)	-1.8(14)
Fe3	17.2(2)	13.0(2)	16.2(2)	-1.19(17)	4.43(17)	-0.01(17)

N13	29.0(16)	20.8(15)	20.3(14)	1.7(11)	0.7(12)	1.4(12)
N14	23.5(15)	20.8(14)	22.2(14)	-3.8(12)	9.6(12)	-3.7(12)
N15	25.4(15)	15.0(13)	22.2(14)	0.4(11)	7.6(12)	-3.1(11)
N16	14.5(12)	17.7(13)	16.7(12)	0.5(10)	2(1)	1.7(10)
N17	24.8(15)	19.0(14)	22.3(14)	3.5(11)	9.2(12)	-0.2(12)
N18	18.5(14)	15.7(13)	22.7(14)	0.5(11)	5.7(11)	-0.1(11)
C55	24.1(17)	27.0(19)	22.0(17)	-3.1(14)	0.9(14)	-4.7(14)
C56	33(2)	23.5(18)	20.8(17)	-3.5(14)	8.5(15)	-5.8(15)
C57	37(2)	40(2)	34(2)	-15.3(19)	-0.7(18)	-5.0(19)
C58	57(3)	37(3)	56(3)	-31(2)	-1(3)	-6(2)
C59	50(3)	24(2)	47(3)	-15.7(19)	14(2)	1.5(19)
C60	35(2)	18.5(16)	27.7(18)	-4.8(14)	13.5(15)	-4.1(15)
C61	35(2)	15.1(16)	41(2)	-1.7(15)	15.2(18)	3.8(15)
C62	33(2)	24.3(18)	21.8(17)	3.5(14)	1.2(15)	4.2(16)
C63	30.4(19)	22.4(18)	23.6(17)	3.6(14)	7.3(15)	7.5(15)
C64	25.9(18)	18.6(16)	21.8(16)	-1.9(13)	8.1(13)	-2.2(14)
C65	15.2(14)	14.4(14)	17.6(15)	1.5(11)	0.9(11)	2.3(12)
C66	22.7(17)	19.8(16)	16.2(15)	-0.4(12)	2.1(12)	4.3(13)
C67	21.2(16)	29.1(18)	18.5(15)	5.7(14)	6.0(13)	2.9(14)
C68	20.4(16)	22.3(16)	18.0(15)	6.8(13)	2.8(12)	-2.4(13)
C69	15.2(14)	15.9(14)	20.1(15)	4.3(12)	0.5(12)	3.7(12)
C70	24.2(17)	15.6(16)	27.9(18)	-2.5(13)	2.1(14)	-3.5(13)
C71	31(2)	17.6(16)	29.6(19)	1.5(14)	8.5(15)	-2.9(14)
C72	26.2(18)	17.8(17)	34(2)	-1.7(14)	9.1(15)	-5.2(14)
C73	26.4(18)	24.9(18)	28.4(19)	2.2(15)	9.9(15)	1.1(15)
C74	20.3(16)	16.3(16)	32.7(19)	-2.4(14)	9.0(14)	0.4(13)
C75	21.5(18)	23.0(18)	40(2)	-2.8(16)	7.9(16)	2.0(15)
C76	23.6(18)	30(2)	40(2)	2.9(18)	0.5(16)	7.4(16)
C77	24.4(18)	26.8(19)	33(2)	4.2(15)	0.2(15)	9.5(15)
C78	22.3(16)	14.6(15)	29.3(18)	0.4(14)	5.0(14)	1.8(13)
C79	24.1(18)	25.8(18)	24.5(17)	7.5(14)	5.2(14)	4.3(14)
C80	31(2)	29(2)	22.7(17)	5.5(15)	6.9(15)	-1.2(16)
C81	37(2)	28.8(19)	18.4(17)	4.1(14)	9.2(15)	0.0(16)
Fe2	17.3(2)	13.9(2)	12.2(2)	-0.87(16)	1.39(16)	-0.59(17)
N7	22.5(14)	14.6(13)	21.4(14)	-0.4(11)	6.0(11)	1.6(11)
N8	20.7(14)	13.6(12)	16.5(13)	-0.8(10)	4(1)	1.2(11)
N9	24.1(15)	25.6(15)	16.1(13)	-5.1(11)	1.0(11)	-3.7(12)
N10	18.6(14)	18.4(14)	20.3(14)	3.5(11)	0.1(11)	0.4(11)

N11	23.2(14)	16.9(14)	22.5(14)	-0.7(11)	1.2(11)	-0.7(11)
N12	20.3(14)	19.1(14)	15.4(13)	0.4(11)	1(1)	-2.4(11)
C28	20.3(16)	17.9(16)	29.0(18)	0.6(14)	6.2(14)	-1.1(13)
C29	23.0(17)	18.8(16)	21.4(16)	-1.7(13)	5.4(13)	-1.4(13)
C30	26.6(18)	23.7(18)	42(2)	3.1(17)	19.1(16)	-2.4(16)
C31	45(3)	22.0(19)	52(3)	13.0(19)	24(2)	3.0(18)
C32	39(2)	17.5(16)	31(2)	7.2(15)	10.5(17)	6.7(16)
C33	23.0(16)	16.5(15)	16.8(15)	-1.8(12)	3.0(12)	3.6(12)
C34	25.6(18)	19.4(16)	27.7(18)	2.6(14)	7.9(14)	6.4(14)
C35	37(2)	23.5(18)	18.9(16)	-4.3(13)	12.9(15)	3.5(15)
C36	30.1(19)	29.6(19)	13.1(15)	-3.3(13)	4.5(13)	-6.1(15)
C37	26.7(18)	30.6(19)	16.4(15)	0.3(14)	-6.5(13)	-1.2(16)
C38	21.2(17)	20.2(16)	26.4(17)	3.2(14)	0.9(13)	-0.5(14)
C39	21.6(18)	23.6(18)	37(2)	4.5(16)	-3.7(15)	-2.9(14)
C40	20.9(18)	23.2(19)	55(3)	9.7(18)	3.0(17)	-0.2(15)
C41	25.1(19)	21.7(18)	42(2)	4.1(16)	10.8(16)	0.5(15)
C42	22.4(17)	18.2(16)	27.4(18)	4.6(13)	7.4(14)	0.9(13)
C43	34(2)	38(2)	24.2(19)	-1.1(16)	8.4(16)	6.7(18)
C44	36(2)	22.9(18)	25.2(18)	-8.0(15)	-1.1(15)	-7.3(16)
C45	31.1(19)	17.8(16)	29.0(19)	-3.6(14)	2.8(15)	-10.7(14)
C46	29.1(18)	19.7(16)	24.1(17)	8.2(14)	5.6(14)	0.0(15)
C47	22.5(17)	22.3(17)	19.3(16)	5.5(13)	2.5(13)	1.9(13)
C48	31(2)	34(2)	21.2(18)	10.5(15)	0.4(15)	0.3(16)
C49	38(2)	53(3)	16.9(17)	7.8(18)	-3.0(16)	-2(2)
C50	44(3)	47(3)	18.4(18)	-1.3(17)	-5.1(17)	-4(2)
C51	24.0(17)	24.0(17)	16.5(15)	-3.2(13)	-1.3(13)	-2.3(14)
C52	35(2)	23.6(18)	23.8(18)	-7.9(14)	-0.7(15)	-3.7(16)
C53	28.8(19)	15.0(15)	36(2)	3.1(15)	10.8(16)	4.4(14)
C54	23.7(18)	21.5(17)	30.2(19)	0.6(14)	4.7(15)	4.9(14)
Fe4	25.3(2)	13.8(2)	12.4(2)	-0.85(17)	0.28(17)	-0.83(19)
N19	31.5(16)	16.0(13)	14.8(13)	-0.9(11)	0.3(11)	-2.1(12)
N20	22.5(14)	18.5(14)	14.8(13)	-0.5(10)	0.0(11)	-2.3(11)
N21	33.1(17)	17.3(14)	14.5(13)	-0.7(11)	0.1(12)	1.0(12)
N22	25.3(15)	13.5(13)	18.2(13)	-1.9(10)	-3.3(11)	-0.3(11)
N23	30.8(16)	18.1(14)	17.2(14)	-1.3(11)	2.7(12)	-4.2(12)
N24	24.4(15)	19.0(14)	14.2(12)	-0.3(10)	0.2(11)	-0.5(11)
C82	32.4(19)	13.9(15)	17.1(15)	-3.2(12)	0.7(13)	-1.0(14)
C83	27.3(18)	19.1(16)	16.0(15)	-3.4(12)	3.1(13)	-3.5(13)

C84	28.2(18)	22.4(17)	19.3(16)	-6.1(13)	2.0(14)	-1.2(14)
C85	30.2(19)	34(2)	14.2(15)	-4.6(14)	-1.2(14)	2.6(16)
C86	30.2(19)	31(2)	14.4(15)	-0.9(14)	0.0(13)	2.9(15)
C87	21.9(16)	17.3(15)	19.3(15)	0.8(12)	2.9(13)	1.6(13)
C88	31.9(19)	16.1(16)	21.5(16)	2.3(13)	2.3(14)	4.5(14)
C89	44(2)	10.8(15)	18.1(16)	0.5(12)	-3.4(15)	2.5(14)
C90	48(2)	19.6(18)	16.8(16)	1.1(13)	-2.0(16)	-0.7(16)
C91	36(2)	24.5(18)	17.7(16)	-1.0(14)	-3.3(14)	-2.3(16)
C92	32.7(19)	12.3(15)	18.3(15)	-2.1(12)	-4.5(13)	1.6(13)
C93	34(2)	23.8(18)	20.1(17)	-0.4(14)	-7.0(14)	2.5(15)
C94	30(2)	32(2)	40(2)	-0.5(18)	-7.3(18)	2.9(17)
C95	28.4(19)	20.5(17)	31.1(19)	1.3(14)	2.8(15)	4.0(14)
C96	31.8(19)	11.0(14)	19.9(16)	0.4(12)	-1.7(14)	1.2(13)
C97	27.8(18)	20.9(16)	20.2(16)	0.7(13)	2.0(14)	0.2(14)
C98	40(2)	27.1(19)	16.6(16)	-1.9(14)	4.4(15)	-4.3(16)
C99	37(2)	27.8(19)	19.7(17)	-2.1(14)	5.7(15)	-2.3(16)
C100	26.9(19)	23.0(18)	25.6(18)	-3.4(14)	2.8(14)	-3.4(15)
C101	25.2(17)	21.8(17)	18.1(15)	0.3(13)	3.3(13)	1.9(14)
C102	28.8(19)	27.7(19)	26.0(18)	-2.1(15)	9.1(15)	2.3(16)
C103	33(2)	26.9(19)	33(2)	-10.5(16)	7.0(17)	4.8(16)
C104	35(2)	17.8(17)	31(2)	-7.2(14)	2.9(16)	-2.3(15)
C105	24.9(17)	16.1(15)	18.7(15)	-1.3(13)	2.2(13)	0.6(13)
C106	24.8(17)	18.3(16)	23.2(17)	-1.7(13)	2.8(13)	-3.9(13)
C107	32(2)	23.3(18)	24.8(18)	-4.5(14)	5.8(15)	-7.9(15)
C108	40(2)	19.7(17)	23.6(18)	-3.5(14)	5.3(16)	-10.8(16)
S1	23.4(4)	16.5(4)	24.0(4)	-3.8(3)	2.7(3)	0.0(3)
S2	25.8(4)	22.1(4)	26.8(4)	-4.2(3)	0.2(3)	3.1(3)
S3	34.0(5)	27.9(5)	18.5(4)	2.8(3)	2.2(3)	-9.4(4)
S4	28.0(5)	46.0(6)	26.8(5)	13.0(4)	-0.2(4)	0.4(4)
Na1	26.5(7)	18.5(6)	15.1(6)	2.9(5)	4.4(5)	3.7(5)
F1	30.2(13)	21.3(12)	91(2)	13.5(14)	6.3(14)	6.8(10)
F2	25.1(12)	28.7(13)	69.0(19)	8.3(13)	2.7(12)	-3.9(10)
F3	45.9(16)	55.9(18)	37.9(15)	15.6(13)	11.1(12)	-2.1(14)
F4	33.0(14)	60.4(19)	38.5(14)	12.9(13)	10.3(11)	16.8(13)
F5	25.0(12)	27.7(12)	54.6(16)	7.8(11)	8.0(11)	8.3(10)
F6	25.3(13)	43.9(16)	85(2)	16.2(16)	-1.9(14)	-14.2(12)
F7	55.1(18)	85(2)	28.5(13)	-10.3(14)	5.4(12)	-50.3(18)
F8	46.5(17)	71(2)	43.0(16)	4.9(15)	13.6(13)	7.1(16)

F9	48.1(15)	66.0(19)	16.0(11)	1.5(12)	7.1(10)	-25.1(14)
F10	57.3(18)	44.3(16)	45.7(16)	-0.4(13)	15.7(14)	26.6(14)
F11	67(2)	74(2)	32.6(15)	11.0(15)	15.3(14)	24.2(18)
F12	62(2)	59(2)	115(3)	35(2)	-4(2)	-24.4(19)
O1	28.8(14)	20.1(13)	30.8(14)	-1.1(10)	-0.3(11)	5.2(11)
O2	21.9(12)	24.7(13)	29.1(13)	-4.1(11)	-0.3(10)	0.3(11)
O3	39.6(16)	28.6(15)	28.6(14)	-11.7(12)	8.5(12)	-6.1(13)
O4	42.9(17)	24.3(15)	36.7(16)	-3.0(12)	-4.2(13)	-10.0(13)
O5	34.6(15)	30.2(15)	30.3(14)	-8.8(12)	-1.4(12)	1.9(12)
O6	39.3(18)	50(2)	34.0(16)	1.9(14)	4.1(13)	24.5(15)
O7	42.4(18)	50.0(19)	19.6(13)	2.5(13)	-2.9(12)	-24.8(15)
O8	40.9(17)	52(2)	16.7(12)	-0.8(12)	2.1(11)	-20.0(15)
O9	77(3)	33.7(18)	57(2)	11.1(17)	21(2)	6.1(19)
O10	41.7(19)	53(2)	42.8(19)	0.7(16)	10.5(15)	18.9(16)
O11	68(3)	144(5)	25.1(18)	0(2)	3.7(17)	53(3)
O12	65(3)	72(3)	124(5)	40(3)	-29(3)	-30(3)
C109	24.3(19)	25.1(19)	41(2)	7.7(17)	5.6(16)	4.4(15)
C110	18.3(17)	31(2)	47(2)	6.6(18)	3.9(16)	0.0(15)
C111	40(2)	48(3)	17.1(17)	-6.5(17)	7.8(16)	-20(2)
C112	46(3)	32(2)	46(3)	2(2)	12(2)	9(2)
S5	19.1(4)	15.4(4)	17.1(4)	1.9(3)	2.5(3)	-0.2(3)
S6	31.3(5)	27.0(4)	16.6(4)	-0.7(3)	3.6(3)	8.8(4)
S7	23.0(4)	15.4(4)	23.9(4)	1.5(3)	0.5(3)	-0.3(3)
S8	31.6(5)	24.0(4)	26.7(5)	-9.1(4)	4.7(4)	-4.8(4)
Na2	24.2(7)	22.7(7)	12.9(6)	-5.3(5)	6.6(5)	-7.9(6)
F13	38.4(14)	41.9(15)	32.9(13)	-14.3(11)	12.9(11)	0.6(11)
F14	27.4(12)	19.6(11)	69.1(18)	-11.0(11)	5.7(12)	-6.4(9)
F15	27.2(12)	27.3(12)	57.2(17)	-7.5(12)	-5.8(11)	11.6(10)
F16	118(3)	21.9(13)	34.3(15)	-4.2(11)	11.0(16)	2.6(15)
F17	40.4(16)	86(2)	40.1(16)	6.0(15)	17.1(13)	25.9(16)
F18	61.9(18)	41.1(15)	18.0(11)	-2.7(10)	12.6(11)	7.7(13)
F19	26.6(12)	23.0(11)	50.5(15)	-3(1)	5.9(11)	-9.7(9)
F20	30.6(13)	22.2(12)	81(2)	-9.1(13)	2.8(13)	3.5(10)
F21	48.3(16)	49.3(16)	34.0(14)	-15.4(12)	16.0(12)	-20.0(13)
F22	45.3(15)	46.2(15)	22.5(11)	-3.7(11)	9.4(10)	-18.6(13)
F23	45.0(15)	39.0(14)	27.3(12)	-3.3(10)	4.2(10)	-20.7(12)
F24	46.6(17)	46.4(17)	60.5(19)	-19.4(15)	-5.5(14)	18.8(14)
O13	20.7(12)	20.2(12)	27.8(13)	-2.3(10)	2(1)	-2.4(10)

O14	21.0(12)	24.4(13)	20.6(12)	2(1)	1.6(9)	2.2(10)
O15	32.2(15)	28.5(14)	22.7(13)	9.1(11)	6.3(11)	2.9(11)
O16	31.5(15)	35.9(16)	17.1(12)	-0.3(11)	2.1(10)	6.8(12)
O17	31.2(16)	85(3)	22.0(14)	2.2(16)	2.5(12)	11.0(17)
O18	78(3)	24.0(15)	31.7(16)	0.5(13)	-0.3(16)	2.0(16)
O19	40.2(16)	28.8(14)	27.7(14)	7.5(12)	3.2(12)	0.6(13)
O20	29.8(15)	23.2(14)	38.7(16)	-0.2(12)	-7.8(12)	5.3(11)
O21	28.4(15)	26.5(14)	39.3(16)	-4.9(12)	5.0(12)	-10.0(12)
O22	55(2)	41.6(19)	39.1(18)	-5.7(15)	6.8(15)	-25.9(17)
O23	60(2)	46(2)	23.3(14)	-4.2(13)	5.0(14)	-20.4(17)
O24	51(2)	41(2)	61(2)	-6.3(17)	10.1(18)	11.8(17)
C113	22.2(18)	23.2(18)	36(2)	-4.8(15)	4.2(15)	-1.3(14)
C114	46(2)	30(2)	19.5(18)	3.3(15)	7.2(16)	5.7(18)
C115	24.7(18)	19.1(17)	36(2)	-0.8(15)	6.5(15)	-1.5(14)
C116	32(2)	22.6(18)	25.5(18)	-1.9(14)	4.1(15)	-2.0(15)
S9	43.2(6)	28.9(5)	43.0(6)	-6.8(5)	11.8(5)	-9.8(5)
F25	45.7(15)	29.3(13)	58.5(17)	-2.8(12)	15.4(13)	-9.3(12)
F26	47.7(17)	34.9(15)	104(3)	-4.8(17)	36.7(18)	2.6(14)
F27	56.4(19)	76(2)	35.8(15)	-8.1(15)	17.8(14)	-12.0(17)
O25	66(2)	41.7(19)	51(2)	-0.6(17)	32.9(18)	-5.8(18)
O26	45.7(19)	39.6(18)	35.3(17)	-11.3(14)	6.3(14)	-4.6(15)
O27	52(2)	36.5(19)	69(2)	-27.1(17)	29.9(18)	-19.2(16)
O31	66(3)	83(3)	93(4)	49(3)	24(3)	18(3)
C117	42(3)	36(2)	48(3)	2(2)	18(2)	-3(2)
S10	45.6(7)	44.0(7)	42.1(6)	-2.3(5)	16.5(5)	-3.0(5)
F28	122(4)	76(3)	71(3)	24(2)	-36(2)	-44(3)
F29	97(3)	73(3)	78(3)	-30(2)	9(2)	1(2)
F30	52(2)	115(4)	96(3)	3(3)	17(2)	-18(2)
O28	58(3)	80(3)	103(4)	-18(3)	31(3)	-22(3)
O29	100(4)	41(2)	67(3)	-1(2)	23(3)	3(2)
O30	149(5)	44(2)	58(3)	22(2)	-24(3)	-27(3)
C118	44(3)	34(3)	115(5)	49(3)	-29(3)	-21(2)

Table S10. Bond Lengths for Fe(MPT).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	N1	2.225(3)	Fe4	N20	2.216(3)
Fe1	N2	2.215(3)	Fe4	N21	2.234(3)
Fe1	N3	2.216(3)	Fe4	N22	2.209(3)
Fe1	N4	2.243(3)	Fe4	N23	2.220(3)
Fe1	N5	2.207(3)	Fe4	N24	2.222(3)
Fe1	N6	2.230(3)	N19	C82	1.480(4)
N1	C1	1.465(4)	N19	C89	1.472(5)
N1	C8	1.502(5)	N19	C108	1.484(5)
N1	C27	1.484(4)	N20	C83	1.351(5)
N2	C2	1.366(4)	N20	C87	1.353(4)
N2	C6	1.347(4)	N21	C90	1.490(5)
N3	C9	1.473(4)	N21	C91	1.467(5)
N3	C10	1.477(4)	N21	C98	1.480(5)
N3	C17	1.499(4)	N22	C92	1.356(4)
N4	C11	1.361(4)	N22	C96	1.347(5)
N4	C15	1.358(4)	N23	C99	1.505(5)
N5	C18	1.482(4)	N23	C100	1.478(5)
N5	C19	1.470(5)	N23	C107	1.475(5)
N5	C26	1.490(4)	N24	C101	1.367(5)
N6	C20	1.353(5)	N24	C105	1.350(5)
N6	C24	1.366(5)	C82	C83	1.508(5)
C1	C2	1.513(5)	C83	C84	1.387(5)
C2	C3	1.369(5)	C84	C85	1.383(5)
C3	C4	1.404(5)	C85	C86	1.378(6)
C4	C5	1.374(6)	C86	C87	1.386(5)
C5	C6	1.398(5)	C87	C88	1.500(5)
C6	C7	1.498(5)	C89	C90	1.526(5)
C8	C9	1.524(5)	C91	C92	1.500(5)
C10	C11	1.499(5)	C92	C93	1.377(5)
C11	C12	1.377(5)	C93	C94	1.397(6)
C12	C13	1.392(5)	C94	C95	1.386(6)
C13	C14	1.383(5)	C95	C96	1.383(5)
C14	C15	1.375(5)	C96	C97	1.497(5)
C15	C16	1.504(5)	C98	C99	1.528(6)
C17	C18	1.525(5)	C100	C101	1.510(5)
C19	C20	1.504(5)	C101	C102	1.387(5)

C20	C21	1.383(5)	C102	C103	1.383(6)
C21	C22	1.389(6)	C103	C104	1.395(6)
C22	C23	1.376(7)	C104	C105	1.385(5)
C23	C24	1.386(5)	C105	C106	1.495(5)
C24	C25	1.502(6)	C107	C108	1.533(6)
C26	C27	1.531(5)	S1	Na1	3.0922(17)
Fe3	N13	2.202(3)	S1	O1	1.449(3)
Fe3	N14	2.313(3)	S1	O2	1.443(3)
Fe3	N15	2.234(3)	S1	O3	1.435(3)
Fe3	N16	2.271(3)	S1	C109	1.833(4)
Fe3	N17	2.237(3)	S2	Na1	3.1410(17)
Fe3	N18	2.226(3)	S2	O4	1.445(3)
N13	C55	1.472(5)	S2	O5	1.437(3)
N13	C62	1.476(5)	S2	O6	1.439(3)
N13	C81	1.494(5)	S2	C110	1.824(4)
N14	C56	1.345(5)	S3	O7	1.434(3)
N14	C60	1.364(5)	S3	O8	1.435(3)
N15	C63	1.501(5)	S3	O9	1.424(4)
N15	C64	1.475(4)	S3	C111	1.822(5)
N15	C71	1.481(5)	S4	O10	1.415(3)
N16	C65	1.352(4)	S4	O11	1.463(4)
N16	C69	1.353(4)	S4	O12	1.394(5)
N17	C72	1.500(5)	S4	C112	1.822(5)
N17	C73	1.470(5)	Na1	O1	2.629(3)
N17	C80	1.474(5)	Na1	O3	2.589(4)
N18	C74	1.355(4)	Na1	O4	2.478(4)
N18	C78	1.365(5)	Na1	O5	2.789(3)
C55	C56	1.497(6)	Na1	O9	2.278(4)
C56	C57	1.385(6)	Na1	O12	2.207(5)
C57	C58	1.375(7)	F1	C109	1.338(5)
C58	C59	1.390(8)	F2	C109	1.327(5)
C59	C60	1.384(6)	F3	C109	1.323(5)
C60	C61	1.482(6)	F4	C110	1.335(5)
C62	C63	1.516(5)	F5	C110	1.335(5)
C64	C65	1.507(5)	F6	C110	1.337(5)
C65	C66	1.386(5)	F7	C111	1.323(5)
C66	C67	1.371(5)	F8	C111	1.358(6)
C67	C68	1.389(5)	F9	C111	1.331(4)

C68	C69	1.388(5)	F10	C112	1.304(5)
C69	C70	1.499(5)	F11	C112	1.354(6)
C71	C72	1.522(5)	F12	C112	1.303(6)
C73	C74	1.508(5)	S5	Na2	3.1063(16)
C74	C75	1.389(5)	S5	O13	1.452(3)
C75	C76	1.381(6)	S5	O14	1.435(3)
C76	C77	1.393(6)	S5	O15	1.438(3)
C77	C78	1.399(5)	S5	C113	1.821(4)
C78	C79	1.493(5)	S6	O16	1.437(3)
C80	C81	1.499(6)	S6	O17	1.427(4)
Fe2	N7	2.235(3)	S6	O18	1.435(4)
Fe2	N8	2.232(3)	S6	C114	1.821(4)
Fe2	N9	2.208(3)	S7	Na2	3.1315(17)
Fe2	N10	2.235(3)	S7	O19	1.443(3)
Fe2	N11	2.229(3)	S7	O20	1.448(3)
Fe2	N12	2.209(3)	S7	O21	1.446(3)
N7	C28	1.483(5)	S7	C115	1.827(4)
N7	C35	1.498(5)	S8	O22	1.447(3)
N7	C54	1.480(5)	S8	O23	1.433(3)
N8	C29	1.358(4)	S8	O24	1.445(4)
N8	C33	1.347(4)	S8	C116	1.822(4)
N9	C36	1.491(5)	Na2	O13	2.441(3)
N9	C37	1.479(5)	Na2	O15	2.793(3)
N9	C44	1.495(5)	Na2	O18	2.315(4)
N10	C38	1.352(5)	Na2	O19	2.753(3)
N10	C42	1.345(5)	Na2	O20	2.512(3)
N11	C45	1.490(5)	Na2	O24	2.239(4)
N11	C46	1.471(5)	F13	C113	1.355(5)
N11	C53	1.489(5)	F14	C113	1.335(4)
N12	C47	1.366(5)	F15	C113	1.322(5)
N12	C51	1.352(4)	F16	C114	1.318(5)
C28	C29	1.503(5)	F17	C114	1.331(6)
C29	C30	1.382(5)	F18	C114	1.330(5)
C30	C31	1.374(6)	F19	C115	1.333(4)
C31	C32	1.365(6)	F20	C115	1.327(5)
C32	C33	1.398(5)	F21	C115	1.338(5)
C33	C34	1.503(5)	F22	C116	1.314(5)
C35	C36	1.502(6)	F23	C116	1.345(5)

C37	C38	1.506(5)	F24	C116	1.329(5)
C38	C39	1.377(5)	S9	O25	1.468(4)
C39	C40	1.385(6)	S9	O26	1.427(4)
C40	C41	1.375(6)	S9	O27	1.424(3)
C41	C42	1.406(5)	S9	C117	1.805(5)
C42	C43	1.501(6)	F25	C117	1.326(6)
C44	C45	1.519(5)	F26	C117	1.356(6)
C46	C47	1.497(5)	F27	C117	1.331(6)
C47	C48	1.378(5)	S10	O28	1.429(5)
C48	C49	1.393(6)	S10	O29	1.446(5)
C49	C50	1.364(7)	S10	O30	1.404(4)
C50	C51	1.401(5)	S10	C118	1.868(6)
C51	C52	1.485(5)	F28	C118	1.256(6)
C53	C54	1.524(5)	F29	C118	1.185(7)
Fe4	N19	2.216(3)	F30	C118	1.493(8)

Table S11. Bond Angles for Fe(MPT).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Fe1	N4	155.28(11)	C90	N21	Fe4	110.3(2)
N1	Fe1	N6	97.95(11)	C91	N21	Fe4	105.4(2)
N2	Fe1	N1	78.48(11)	C91	N21	C90	112.1(3)
N2	Fe1	N3	96.91(11)	C91	N21	C98	111.2(3)
N2	Fe1	N4	105.18(10)	C98	N21	Fe4	107.1(2)
N2	Fe1	N6	104.72(11)	C98	N21	C90	110.5(3)
N3	Fe1	N1	77.94(11)	C92	N22	Fe4	112.5(2)
N3	Fe1	N4	77.35(10)	C96	N22	Fe4	129.0(2)
N3	Fe1	N6	156.77(11)	C96	N22	C92	118.4(3)
N5	Fe1	N1	79.08(11)	C99	N23	Fe4	113.2(2)
N5	Fe1	N2	157.54(11)	C100	N23	Fe4	103.4(2)
N5	Fe1	N3	79.39(11)	C100	N23	C99	110.3(3)
N5	Fe1	N4	95.68(10)	C107	N23	Fe4	104.6(2)
N5	Fe1	N6	77.39(11)	C107	N23	C99	111.9(3)
N6	Fe1	N4	104.50(10)	C107	N23	C100	113.1(3)
C1	N1	Fe1	105.4(2)	C101	N24	Fe4	109.8(2)
C1	N1	C8	110.4(3)	C105	N24	Fe4	129.2(2)
C1	N1	C27	111.9(3)	C105	N24	C101	118.3(3)
C8	N1	Fe1	111.9(2)	N19	C82	C83	110.8(3)
C27	N1	Fe1	104.9(2)	N20	C83	C82	117.4(3)
C27	N1	C8	112.0(3)	N20	C83	C84	123.4(3)
C2	N2	Fe1	111.4(2)	C84	C83	C82	119.0(3)
C6	N2	Fe1	129.3(2)	C85	C84	C83	118.2(3)
C6	N2	C2	118.5(3)	C86	C85	C84	118.8(3)
C9	N3	Fe1	106.7(2)	C85	C86	C87	120.5(3)
C9	N3	C10	111.1(3)	N20	C87	C86	121.1(3)
C9	N3	C17	111.3(3)	N20	C87	C88	119.1(3)
C10	N3	Fe1	104.9(2)	C86	C87	C88	119.8(3)
C10	N3	C17	111.7(3)	N19	C89	C90	110.2(3)
C17	N3	Fe1	110.9(2)	N21	C90	C89	112.7(3)
C11	N4	Fe1	111.4(2)	N21	C91	C92	111.3(3)
C15	N4	Fe1	130.7(2)	N22	C92	C91	117.1(3)
C15	N4	C11	117.4(3)	N22	C92	C93	122.9(3)
C18	N5	Fe1	105.5(2)	C93	C92	C91	119.9(3)
C18	N5	C26	111.4(3)	C92	C93	C94	118.7(3)
C19	N5	Fe1	106.0(2)	C95	C94	C93	118.2(4)

C19	N5	C18	110.9(3)	C96	C95	C94	120.4(4)
C19	N5	C26	112.0(3)	N22	C96	C95	121.4(3)
C26	N5	Fe1	110.7(2)	N22	C96	C97	119.6(3)
C20	N6	Fe1	112.0(2)	C95	C96	C97	118.9(3)
C20	N6	C24	117.4(3)	N21	C98	C99	111.3(3)
C24	N6	Fe1	130.6(3)	N23	C99	C98	110.8(3)
N1	C1	C2	110.7(3)	N23	C100	C101	109.1(3)
N2	C2	C1	116.4(3)	N24	C101	C100	115.5(3)
N2	C2	C3	122.4(3)	N24	C101	C102	122.6(3)
C3	C2	C1	121.2(3)	C102	C101	C100	121.9(3)
C2	C3	C4	119.2(3)	C103	C102	C101	118.5(4)
C5	C4	C3	118.2(3)	C102	C103	C104	119.3(4)
C4	C5	C6	120.3(3)	C105	C104	C103	119.5(4)
N2	C6	C5	121.0(3)	N24	C105	C104	121.7(3)
N2	C6	C7	119.3(3)	N24	C105	C106	118.9(3)
C5	C6	C7	119.7(3)	C104	C105	C106	119.4(3)
N1	C8	C9	110.9(3)	N23	C107	C108	110.0(3)
N3	C9	C8	110.2(3)	N19	C108	C107	112.9(3)
N3	C10	C11	110.9(3)	O1	S1	Na1	58.01(12)
N4	C11	C10	116.6(3)	O1	S1	C109	103.13(18)
N4	C11	C12	123.0(3)	O2	S1	Na1	133.27(13)
C12	C11	C10	120.3(3)	O2	S1	O1	115.25(17)
C11	C12	C13	119.0(3)	O2	S1	C109	103.02(18)
C14	C13	C12	118.0(3)	O3	S1	Na1	56.34(14)
C15	C14	C13	120.6(3)	O3	S1	O1	113.50(18)
N4	C15	C14	121.7(3)	O3	S1	O2	115.87(17)
N4	C15	C16	117.6(3)	O3	S1	C109	103.7(2)
C14	C15	C16	120.6(3)	C109	S1	Na1	123.71(15)
N3	C17	C18	112.0(3)	O4	S2	Na1	50.19(14)
N5	C18	C17	111.3(3)	O4	S2	C110	103.13(19)
N5	C19	C20	111.7(3)	O5	S2	Na1	62.62(13)
N6	C20	C19	117.2(3)	O5	S2	O4	112.69(19)
N6	C20	C21	123.5(4)	O5	S2	O6	115.71(19)
C21	C20	C19	119.1(3)	O5	S2	C110	104.7(2)
C20	C21	C22	118.7(4)	O6	S2	Na1	137.47(16)
C23	C22	C21	118.5(4)	O6	S2	O4	115.4(2)
C22	C23	C24	120.7(4)	O6	S2	C110	103.2(2)
N6	C24	C23	121.3(4)	C110	S2	Na1	118.66(14)

N6	C24	C25	118.1(3)	O7	S3	O8	115.21(18)
C23	C24	C25	120.6(4)	O7	S3	C111	102.6(2)
N5	C26	C27	112.9(3)	O8	S3	C111	103.2(2)
N1	C27	C26	109.4(3)	O9	S3	O7	115.8(2)
N13	Fe3	N14	74.48(12)	O9	S3	O8	115.7(2)
N13	Fe3	N15	78.17(12)	O9	S3	C111	101.1(2)
N13	Fe3	N16	107.08(11)	O10	S4	O11	113.2(2)
N13	Fe3	N17	77.30(12)	O10	S4	C112	106.0(2)
N13	Fe3	N18	150.08(12)	O11	S4	C112	99.4(3)
N15	Fe3	N14	150.67(12)	O12	S4	O10	118.7(3)
N15	Fe3	N16	74.56(11)	O12	S4	O11	114.3(4)
N15	Fe3	N17	77.32(11)	O12	S4	C112	102.0(3)
N16	Fe3	N14	103.53(11)	S1	Na1	S2	99.12(5)
N17	Fe3	N14	106.36(11)	O1	Na1	S1	27.87(6)
N17	Fe3	N16	149.81(11)	O1	Na1	S2	119.03(8)
N18	Fe3	N14	99.10(11)	O1	Na1	O5	95.52(10)
N18	Fe3	N15	109.94(11)	O3	Na1	S1	27.47(6)
N18	Fe3	N16	102.84(10)	O3	Na1	S2	82.26(8)
N18	Fe3	N17	76.66(11)	O3	Na1	O1	55.05(9)
C55	N13	Fe3	106.0(2)	O3	Na1	O5	76.56(10)
C55	N13	C62	110.7(3)	O4	Na1	S1	115.41(9)
C55	N13	C81	110.7(3)	O4	Na1	S2	26.61(7)
C62	N13	Fe3	112.9(2)	O4	Na1	O1	141.03(11)
C62	N13	C81	111.0(3)	O4	Na1	O3	91.28(11)
C81	N13	Fe3	105.4(2)	O4	Na1	O5	53.80(9)
C56	N14	Fe3	109.6(2)	O5	Na1	S1	82.78(7)
C56	N14	C60	118.3(3)	O5	Na1	S2	27.23(6)
C60	N14	Fe3	131.8(3)	O9	Na1	S1	120.25(12)
C63	N15	Fe3	104.1(2)	O9	Na1	S2	92.81(11)
C64	N15	Fe3	105.1(2)	O9	Na1	O1	97.74(13)
C64	N15	C63	111.9(3)	O9	Na1	O3	142.86(15)
C64	N15	C71	111.0(3)	O9	Na1	O4	100.59(13)
C71	N15	Fe3	113.5(2)	O9	Na1	O5	82.41(13)
C71	N15	C63	110.9(3)	O12	Na1	S1	109.38(14)
C65	N16	Fe3	111.0(2)	O12	Na1	S2	133.89(19)
C65	N16	C69	117.9(3)	O12	Na1	O1	101.80(18)
C69	N16	Fe3	131.0(2)	O12	Na1	O3	107.29(16)
C72	N17	Fe3	105.0(2)	O12	Na1	O4	107.3(2)

C73	N17	Fe3	104.6(2)	O12	Na1	O5	161.1(2)
C73	N17	C72	110.2(3)	O12	Na1	O9	102.5(2)
C73	N17	C80	111.5(3)	S1	O1	Na1	94.12(14)
C80	N17	Fe3	112.9(2)	S1	O3	Na1	96.19(16)
C80	N17	C72	112.2(3)	S2	O4	Na1	103.20(16)
C74	N18	Fe3	112.1(2)	S2	O5	Na1	90.14(14)
C74	N18	C78	117.4(3)	S3	O9	Na1	169.0(3)
C78	N18	Fe3	130.4(2)	S4	O12	Na1	174.6(5)
N13	C55	C56	110.5(3)	F1	C109	S1	110.7(3)
N14	C56	C55	118.5(3)	F2	C109	S1	111.7(3)
N14	C56	C57	122.7(4)	F2	C109	F1	107.0(3)
C57	C56	C55	118.9(4)	F3	C109	S1	111.0(3)
C58	C57	C56	119.0(4)	F3	C109	F1	108.7(4)
C57	C58	C59	119.1(4)	F3	C109	F2	107.5(3)
C60	C59	C58	119.4(4)	F4	C110	S2	110.9(3)
N14	C60	C59	121.5(4)	F4	C110	F5	107.6(3)
N14	C60	C61	119.6(3)	F4	C110	F6	107.8(4)
C59	C60	C61	119.0(4)	F5	C110	S2	111.4(3)
N13	C62	C63	111.1(3)	F5	C110	F6	107.9(4)
N15	C63	C62	110.5(3)	F6	C110	S2	111.0(3)
N15	C64	C65	110.2(3)	F7	C111	S3	112.3(3)
N16	C65	C64	117.8(3)	F7	C111	F8	105.5(4)
N16	C65	C66	123.0(3)	F7	C111	F9	108.8(3)
C66	C65	C64	119.2(3)	F8	C111	S3	110.4(3)
C67	C66	C65	119.1(3)	F9	C111	S3	112.1(3)
C66	C67	C68	118.5(3)	F9	C111	F8	107.5(4)
C69	C68	C67	120.1(3)	F10	C112	S4	112.0(3)
N16	C69	C68	121.3(3)	F10	C112	F11	108.2(4)
N16	C69	C70	118.6(3)	F11	C112	S4	109.8(3)
C68	C69	C70	120.1(3)	F12	C112	S4	113.3(4)
N15	C71	C72	110.0(3)	F12	C112	F10	110.0(4)
N17	C72	C71	110.9(3)	F12	C112	F11	103.1(4)
N17	C73	C74	110.6(3)	O13	S5	Na2	50.01(11)
N18	C74	C73	117.0(3)	O13	S5	C113	103.13(17)
N18	C74	C75	123.0(4)	O14	S5	Na2	133.99(12)
C75	C74	C73	120.0(3)	O14	S5	O13	114.95(16)
C76	C75	C74	119.5(4)	O14	S5	O15	116.18(16)
C75	C76	C77	118.5(4)	O14	S5	C113	104.01(18)

C76	C77	C78	119.5(4)	O15	S5	Na2	64.00(12)
N18	C78	C77	122.0(3)	O15	S5	O13	113.40(17)
N18	C78	C79	118.6(3)	O15	S5	C113	102.88(18)
C77	C78	C79	119.4(3)	C113	S5	Na2	121.23(14)
N17	C80	C81	110.3(3)	O16	S6	C114	103.92(18)
N13	C81	C80	111.6(3)	O17	S6	O16	116.17(19)
N7	Fe2	N10	156.42(11)	O17	S6	O18	113.3(2)
N8	Fe2	N7	77.62(11)	O17	S6	C114	103.5(2)
N8	Fe2	N10	104.32(11)	O18	S6	O16	115.6(2)
N9	Fe2	N7	78.59(11)	O18	S6	C114	101.8(2)
N9	Fe2	N8	95.01(11)	O19	S7	Na2	61.52(13)
N9	Fe2	N10	77.83(11)	O19	S7	O20	113.14(19)
N9	Fe2	N11	79.07(12)	O19	S7	O21	115.89(19)
N9	Fe2	N12	156.60(12)	O19	S7	C115	103.42(19)
N11	Fe2	N7	77.88(11)	O20	S7	Na2	51.92(13)
N11	Fe2	N8	155.47(11)	O20	S7	C115	103.49(18)
N11	Fe2	N10	97.71(11)	O21	S7	Na2	136.27(13)
N12	Fe2	N7	96.95(11)	O21	S7	O20	115.24(19)
N12	Fe2	N8	106.55(11)	O21	S7	C115	103.44(18)
N12	Fe2	N10	104.76(11)	C115	S7	Na2	119.92(13)
N12	Fe2	N11	77.54(11)	O22	S8	C116	102.96(19)
C28	N7	Fe2	103.9(2)	O23	S8	O22	115.4(2)
C28	N7	C35	111.6(3)	O23	S8	O24	115.8(2)
C35	N7	Fe2	110.7(2)	O23	S8	C116	104.39(19)
C54	N7	Fe2	106.0(2)	O24	S8	O22	113.9(2)
C54	N7	C28	112.6(3)	O24	S8	C116	101.9(2)
C54	N7	C35	111.6(3)	S5	Na2	S7	95.00(5)
C29	N8	Fe2	111.5(2)	O13	Na2	S5	27.11(6)
C33	N8	Fe2	129.1(2)	O13	Na2	S7	115.45(8)
C33	N8	C29	118.1(3)	O13	Na2	O15	54.48(8)
C36	N9	Fe2	106.1(2)	O13	Na2	O19	92.60(10)
C36	N9	C44	111.8(3)	O13	Na2	O20	137.71(11)
C37	N9	Fe2	104.6(2)	O15	Na2	S5	27.57(6)
C37	N9	C36	111.2(3)	O15	Na2	S7	76.89(7)
C37	N9	C44	111.8(3)	O18	Na2	S5	124.71(10)
C44	N9	Fe2	111.0(2)	O18	Na2	S7	110.98(11)
C38	N10	Fe2	111.3(2)	O18	Na2	O13	99.04(11)
C42	N10	Fe2	130.2(2)	O18	Na2	O15	151.37(11)

C42	N10	C38	118.4(3)	O18	Na2	O19	102.12(12)
C45	N11	Fe2	103.9(2)	O18	Na2	O20	112.13(12)
C46	N11	Fe2	105.6(2)	O19	Na2	S5	79.17(7)
C46	N11	C45	110.9(3)	O19	Na2	S7	27.44(6)
C46	N11	C53	111.9(3)	O19	Na2	O15	71.80(9)
C53	N11	Fe2	111.7(2)	O20	Na2	S5	112.33(8)
C53	N11	C45	112.3(3)	O20	Na2	S7	26.99(7)
C47	N12	Fe2	112.6(2)	O20	Na2	O15	87.51(10)
C51	N12	Fe2	128.5(2)	O20	Na2	O19	54.33(9)
C51	N12	C47	118.9(3)	O24	Na2	S5	108.18(11)
N7	C28	C29	109.8(3)	O24	Na2	S7	122.08(12)
N8	C29	C28	116.0(3)	O24	Na2	O13	107.47(13)
N8	C29	C30	122.7(3)	O24	Na2	O15	100.40(13)
C30	C29	C28	121.4(3)	O24	Na2	O18	98.05(15)
C31	C30	C29	118.7(4)	O24	Na2	O19	148.84(13)
C32	C31	C30	119.4(4)	O24	Na2	O20	96.04(13)
C31	C32	C33	120.0(4)	S5	O13	Na2	102.88(14)
N8	C33	C32	121.1(3)	S5	O15	Na2	88.43(14)
N8	C33	C34	119.0(3)	S6	O18	Na2	153.8(2)
C32	C33	C34	119.9(3)	S7	O19	Na2	91.05(14)
N7	C35	C36	112.5(3)	S7	O20	Na2	101.09(16)
N9	C36	C35	110.8(3)	S8	O24	Na2	160.7(3)
N9	C37	C38	111.1(3)	F13	C113	S5	110.7(3)
N10	C38	C37	116.8(3)	F14	C113	S5	111.4(3)
N10	C38	C39	123.1(4)	F14	C113	F13	106.9(3)
C39	C38	C37	119.9(3)	F15	C113	S5	112.3(3)
C38	C39	C40	118.6(4)	F15	C113	F13	107.9(3)
C41	C40	C39	119.3(4)	F15	C113	F14	107.5(3)
C40	C41	C42	119.4(4)	F16	C114	S6	112.0(3)
N10	C42	C41	121.3(4)	F16	C114	F17	105.9(4)
N10	C42	C43	119.5(3)	F16	C114	F18	108.2(4)
C41	C42	C43	119.2(3)	F17	C114	S6	110.5(3)
N9	C44	C45	112.2(3)	F18	C114	S6	111.4(3)
N11	C45	C44	110.7(3)	F18	C114	F17	108.6(3)
N11	C46	C47	111.4(3)	F19	C115	S7	111.8(3)
N12	C47	C46	116.6(3)	F19	C115	F21	107.1(3)
N12	C47	C48	123.0(4)	F20	C115	S7	111.3(3)
C48	C47	C46	120.2(3)	F20	C115	F19	108.0(3)

C47	C48	C49	117.6(4)	F20	C115	F21	107.2(3)
C50	C49	C48	120.1(4)	F21	C115	S7	111.2(3)
C49	C50	C51	120.3(4)	F22	C116	S8	113.2(3)
N12	C51	C50	120.1(4)	F22	C116	F23	107.0(3)
N12	C51	C52	120.0(3)	F22	C116	F24	107.5(3)
C50	C51	C52	119.9(4)	F23	C116	S8	110.4(3)
N11	C53	C54	111.8(3)	F24	C116	S8	112.2(3)
N7	C54	C53	109.7(3)	F24	C116	F23	106.1(3)
N19	Fe4	N20	77.88(11)	O25	S9	C117	102.7(2)
N19	Fe4	N21	78.68(11)	O26	S9	O25	114.1(2)
N19	Fe4	N23	79.14(12)	O26	S9	C117	101.6(2)
N19	Fe4	N24	158.01(12)	O27	S9	O25	115.1(2)
N20	Fe4	N21	156.56(11)	O27	S9	O26	116.9(2)
N20	Fe4	N23	98.05(11)	O27	S9	C117	103.6(2)
N20	Fe4	N24	106.77(11)	F25	C117	S9	111.8(3)
N22	Fe4	N19	96.95(11)	F25	C117	F26	106.4(4)
N22	Fe4	N20	105.26(11)	F25	C117	F27	109.0(4)
N22	Fe4	N21	77.27(11)	F26	C117	S9	110.7(3)
N22	Fe4	N23	155.04(11)	F27	C117	S9	111.0(4)
N22	Fe4	N24	102.29(11)	F27	C117	F26	107.7(4)
N23	Fe4	N21	77.79(12)	O28	S10	O29	112.7(3)
N23	Fe4	N24	78.93(11)	O28	S10	C118	95.2(3)
N24	Fe4	N21	95.17(11)	O29	S10	C118	105.1(3)
C82	N19	Fe4	105.7(2)	O30	S10	O28	123.1(4)
C82	N19	C108	110.7(3)	O30	S10	O29	112.5(3)
C89	N19	Fe4	105.7(2)	O30	S10	C118	104.5(3)
C89	N19	C82	111.0(3)	F28	C118	S10	113.8(4)
C89	N19	C108	113.0(3)	F28	C118	F30	99.4(5)
C108	N19	Fe4	110.3(2)	F29	C118	S10	116.1(4)
C83	N20	Fe4	112.1(2)	F29	C118	F28	119.6(8)
C83	N20	C87	117.9(3)	F29	C118	F30	100.7(5)
C87	N20	Fe4	129.9(2)	F30	C118	S10	102.8(5)

Table S12. Torsion Angles for Fe(MPT).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Fe1	N1	C1	C2	-44.2(3)	Fe4	N20	C87	C88	-4.7(5)
Fe1	N1	C8	C9	17.8(3)	Fe4	N21	C90	C89	-15.9(4)
Fe1	N1	C27	C26	51.4(3)	Fe4	N21	C91	C92	43.5(3)
Fe1	N2	C2	C1	-16.9(4)	Fe4	N21	C98	C99	-48.8(3)
Fe1	N2	C2	C3	164.6(3)	Fe4	N22	C92	C91	7.6(4)
Fe1	N2	C6	C5	-164.1(3)	Fe4	N22	C92	C93	-176.3(3)
Fe1	N2	C6	C7	15.7(5)	Fe4	N22	C96	C95	175.7(3)
Fe1	N3	C9	C8	51.3(3)	Fe4	N22	C96	C97	-6.5(5)
Fe1	N3	C10	C11	-46.8(3)	Fe4	N23	C99	C98	-15.6(4)
Fe1	N3	C17	C18	14.9(3)	Fe4	N23	C100	C101	49.3(3)
Fe1	N4	C11	C10	-10.3(3)	Fe4	N23	C107	C108	-51.6(3)
Fe1	N4	C11	C12	171.8(3)	Fe4	N24	C101	C100	22.4(4)
Fe1	N4	C15	C14	-168.2(2)	Fe4	N24	C101	C102	-159.2(3)
Fe1	N4	C15	C16	13.4(4)	Fe4	N24	C105	C104	155.3(3)
Fe1	N5	C18	C17	49.7(3)	Fe4	N24	C105	C106	-26.3(5)
Fe1	N5	C19	C20	-43.0(3)	N19	Fe4	N20	C83	11.7(2)
Fe1	N5	C26	C27	15.7(4)	N19	Fe4	N20	C87	-165.5(3)
Fe1	N6	C20	C19	-5.5(4)	N19	Fe4	N21	C90	-9.0(3)
Fe1	N6	C20	C21	-179.5(3)	N19	Fe4	N21	C91	-130.2(2)
Fe1	N6	C24	C23	178.5(3)	N19	Fe4	N21	C98	111.3(2)
Fe1	N6	C24	C25	0.0(5)	N19	Fe4	N22	C92	89.8(2)
N1	Fe1	N2	C2	-6.3(2)	N19	Fe4	N22	C96	-87.7(3)
N1	Fe1	N2	C6	163.0(3)	N19	Fe4	N23	C99	-88.5(3)
N1	Fe1	N3	C9	-31.3(2)	N19	Fe4	N23	C100	152.2(2)
N1	Fe1	N3	C10	-149.2(2)	N19	Fe4	N23	C107	33.6(2)
N1	Fe1	N3	C17	90.1(2)	N19	Fe4	N24	C101	8.7(4)
N1	Fe1	N4	C11	-14.0(4)	N19	Fe4	N24	C105	-152.2(3)
N1	Fe1	N4	C15	158.3(3)	N19	C82	C83	N20	-36.9(4)
N1	Fe1	N5	C18	-110.9(2)	N19	C82	C83	C84	147.9(3)
N1	Fe1	N5	C19	131.3(2)	N19	C89	C90	N21	46.0(5)
N1	Fe1	N5	C26	9.6(2)	N20	Fe4	N19	C82	-29.5(2)
N1	Fe1	N6	C20	-91.2(2)	N20	Fe4	N19	C89	-147.3(2)
N1	Fe1	N6	C24	89.6(3)	N20	Fe4	N19	C108	90.2(2)
N1	C1	C2	N2	43.2(4)	N20	Fe4	N21	C90	-8.1(5)
N1	C1	C2	C3	-138.3(3)	N20	Fe4	N21	C91	-129.3(3)
N1	C8	C9	N3	-46.6(4)	N20	Fe4	N21	C98	112.2(3)

N2	Fe1	N1	C1	27.5(2)	N20	Fe4	N22	C92	169.1(2)
N2	Fe1	N1	C8	-92.6(2)	N20	Fe4	N22	C96	-8.4(3)
N2	Fe1	N1	C27	145.8(2)	N20	Fe4	N23	C99	-164.4(2)
N2	Fe1	N3	C9	45.3(2)	N20	Fe4	N23	C100	76.3(2)
N2	Fe1	N3	C10	-72.6(2)	N20	Fe4	N23	C107	-42.3(2)
N2	Fe1	N3	C17	166.7(2)	N20	Fe4	N24	C101	-90.6(2)
N2	Fe1	N4	C11	81.4(2)	N20	Fe4	N24	C105	108.6(3)
N2	Fe1	N4	C15	-106.3(3)	N20	C83	C84	C85	-1.8(6)
N2	Fe1	N5	C18	-113.7(3)	N21	Fe4	N19	C82	150.2(2)
N2	Fe1	N5	C19	128.6(3)	N21	Fe4	N19	C89	32.4(2)
N2	Fe1	N5	C26	6.9(4)	N21	Fe4	N19	C108	-90.1(2)
N2	Fe1	N6	C20	-171.3(2)	N21	Fe4	N20	C83	10.9(5)
N2	Fe1	N6	C24	9.5(3)	N21	Fe4	N20	C87	-166.4(3)
N2	C2	C3	C4	2.7(6)	N21	Fe4	N22	C92	13.1(2)
N3	Fe1	N1	C1	127.2(2)	N21	Fe4	N22	C96	-164.4(3)
N3	Fe1	N1	C8	7.2(2)	N21	Fe4	N23	C99	-7.8(2)
N3	Fe1	N1	C27	-114.4(2)	N21	Fe4	N23	C100	-127.2(2)
N3	Fe1	N2	C2	-82.4(2)	N21	Fe4	N23	C107	114.2(2)
N3	Fe1	N2	C6	86.9(3)	N21	Fe4	N24	C101	81.1(2)
N3	Fe1	N4	C11	-12.4(2)	N21	Fe4	N24	C105	-79.8(3)
N3	Fe1	N4	C15	159.9(3)	N21	C91	C92	N22	-36.1(4)
N3	Fe1	N5	C18	-31.3(2)	N21	C91	C92	C93	147.6(3)
N3	Fe1	N5	C19	-149.1(2)	N21	C98	C99	N23	43.4(4)
N3	Fe1	N5	C26	89.2(2)	N22	Fe4	N19	C82	74.7(2)
N3	Fe1	N6	C20	-13.3(4)	N22	Fe4	N19	C89	-43.1(2)
N3	Fe1	N6	C24	167.5(3)	N22	Fe4	N19	C108	-165.6(2)
N3	C10	C11	N4	40.1(4)	N22	Fe4	N20	C83	-82.3(3)
N3	C10	C11	C12	-142.0(3)	N22	Fe4	N20	C87	100.5(3)
N3	C17	C18	N5	-44.3(4)	N22	Fe4	N21	C90	90.9(3)
N4	Fe1	N1	C1	128.8(3)	N22	Fe4	N21	C91	-30.3(2)
N4	Fe1	N1	C8	8.8(4)	N22	Fe4	N21	C98	-148.8(2)
N4	Fe1	N1	C27	-112.8(3)	N22	Fe4	N23	C99	-5.4(4)
N4	Fe1	N2	C2	-161.1(2)	N22	Fe4	N23	C100	-124.7(3)
N4	Fe1	N2	C6	8.2(3)	N22	Fe4	N23	C107	116.7(3)
N4	Fe1	N3	C9	149.4(2)	N22	Fe4	N24	C101	159.1(2)
N4	Fe1	N3	C10	31.46(19)	N22	Fe4	N24	C105	-1.7(3)
N4	Fe1	N3	C17	-89.2(2)	N22	C92	C93	C94	-0.3(6)
N4	Fe1	N5	C18	44.6(2)	N23	Fe4	N19	C82	-130.2(2)

N4	Fe1	N5	C19	-73.1(2)	N23	Fe4	N19	C89	111.9(2)
N4	Fe1	N5	C26	165.2(2)	N23	Fe4	N19	C108	-10.5(2)
N4	Fe1	N6	C20	78.3(2)	N23	Fe4	N20	C83	88.7(3)
N4	Fe1	N6	C24	-100.9(3)	N23	Fe4	N20	C87	-88.6(3)
N4	C11	C12	C13	-1.5(5)	N23	Fe4	N21	C90	-90.2(3)
N5	Fe1	N1	C1	-151.4(2)	N23	Fe4	N21	C91	148.6(2)
N5	Fe1	N1	C8	88.5(2)	N23	Fe4	N21	C98	30.2(2)
N5	Fe1	N1	C27	-33.1(2)	N23	Fe4	N22	C92	10.6(4)
N5	Fe1	N2	C2	-3.5(4)	N23	Fe4	N22	C96	-166.8(3)
N5	Fe1	N2	C6	165.8(3)	N23	Fe4	N24	C101	4.6(2)
N5	Fe1	N3	C9	-112.3(2)	N23	Fe4	N24	C105	-156.2(3)
N5	Fe1	N3	C10	129.8(2)	N23	C100	C101	N24	-51.1(4)
N5	Fe1	N3	C17	9.1(2)	N23	C100	C101	C102	130.5(4)
N5	Fe1	N4	C11	-90.2(2)	N23	C107	C108	N19	45.7(4)
N5	Fe1	N4	C15	82.1(3)	N24	Fe4	N19	C82	-134.3(3)
N5	Fe1	N6	C20	-14.4(2)	N24	Fe4	N19	C89	107.9(3)
N5	Fe1	N6	C24	166.5(3)	N24	Fe4	N19	C108	-14.6(4)
N5	C19	C20	N6	34.0(4)	N24	Fe4	N20	C83	169.5(2)
N5	C19	C20	C21	-151.8(3)	N24	Fe4	N20	C87	-7.8(3)
N5	C26	C27	N1	-46.2(4)	N24	Fe4	N21	C90	-167.6(3)
N6	Fe1	N1	C1	-76.0(2)	N24	Fe4	N21	C91	71.2(2)
N6	Fe1	N1	C8	164.0(2)	N24	Fe4	N21	C98	-47.3(2)
N6	Fe1	N1	C27	42.3(2)	N24	Fe4	N22	C92	-79.5(2)
N6	Fe1	N2	C2	89.0(2)	N24	Fe4	N22	C96	103.0(3)
N6	Fe1	N2	C6	-101.7(3)	N24	Fe4	N23	C99	90.0(2)
N6	Fe1	N3	C9	-113.3(3)	N24	Fe4	N23	C100	-29.4(2)
N6	Fe1	N3	C10	128.8(3)	N24	Fe4	N23	C107	-148.0(2)
N6	Fe1	N3	C17	8.1(4)	N24	C101	C102	C103	-1.1(6)
N6	Fe1	N4	C11	-168.6(2)	C82	N19	C89	C90	-165.4(3)
N6	Fe1	N4	C15	3.7(3)	C82	N19	C108	C107	102.2(3)
N6	Fe1	N5	C18	148.2(2)	C82	C83	C84	C85	173.1(3)
N6	Fe1	N5	C19	30.5(2)	C83	N20	C87	C86	0.0(5)
N6	Fe1	N5	C26	-91.2(2)	C83	N20	C87	C88	178.2(3)
N6	C20	C21	C22	0.5(6)	C83	C84	C85	C86	-0.5(6)
C1	N1	C8	C9	-99.3(3)	C84	C85	C86	C87	2.5(6)
C1	N1	C27	C26	165.3(3)	C85	C86	C87	N20	-2.3(6)
C1	C2	C3	C4	-175.7(4)	C85	C86	C87	C88	179.6(4)
C2	N2	C6	C5	4.6(5)	C87	N20	C83	C82	-173.0(3)

C2	N2	C6	C7	-175.6(3)	C87	N20	C83	C84	2.1(5)
C2	C3	C4	C5	2.1(6)	C89	N19	C82	C83	157.2(3)
C3	C4	C5	C6	-3.4(6)	C89	N19	C108	C107	-132.5(3)
C4	C5	C6	N2	0.1(6)	C90	N21	C91	C92	-76.5(4)
C4	C5	C6	C7	-179.7(4)	C90	N21	C98	C99	71.4(4)
C6	N2	C2	C1	172.5(3)	C91	N21	C90	C89	101.2(4)
C6	N2	C2	C3	-6.0(5)	C91	N21	C98	C99	-163.4(3)
C8	N1	C1	C2	76.8(4)	C91	C92	C93	C94	175.8(4)
C8	N1	C27	C26	-70.2(4)	C92	N22	C96	C95	-1.6(5)
C9	N3	C10	C11	-161.8(3)	C92	N22	C96	C97	176.1(3)
C9	N3	C17	C18	133.6(3)	C92	C93	C94	C95	-0.8(6)
C10	N3	C9	C8	165.1(3)	C93	C94	C95	C96	0.6(6)
C10	N3	C17	C18	-101.7(3)	C94	C95	C96	N22	0.6(6)
C10	C11	C12	C13	-179.3(3)	C94	C95	C96	C97	-177.2(4)
C11	N4	C15	C14	3.7(5)	C96	N22	C92	C91	-174.7(3)
C11	N4	C15	C16	-174.7(3)	C96	N22	C92	C93	1.5(5)
C11	C12	C13	C14	2.5(5)	C98	N21	C90	C89	-134.1(4)
C12	C13	C14	C15	-0.5(5)	C98	N21	C91	C92	159.2(3)
C13	C14	C15	N4	-2.7(5)	C99	N23	C100	C101	-72.0(4)
C13	C14	C15	C16	175.6(3)	C99	N23	C107	C108	71.2(4)
C15	N4	C11	C10	176.3(3)	C100	N23	C99	C98	99.7(4)
C15	N4	C11	C12	-1.6(5)	C100	N23	C107	C108	-163.5(3)
C17	N3	C9	C8	-69.8(4)	C100	C101	C102	C103	177.2(4)
C17	N3	C10	C11	73.3(3)	C101	N24	C105	C104	-4.2(5)
C18	N5	C19	C20	-157.0(3)	C101	N24	C105	C106	174.3(3)
C18	N5	C26	C27	132.7(3)	C101	C102	C103	C104	-1.7(6)
C19	N5	C18	C17	164.1(3)	C102	C103	C104	C105	1.5(6)
C19	N5	C26	C27	-102.4(3)	C103	C104	C105	N24	1.5(6)
C19	C20	C21	C22	-173.4(4)	C103	C104	C105	C106	-176.9(4)
C20	N6	C24	C23	-0.7(5)	C105	N24	C101	C100	-174.4(3)
C20	N6	C24	C25	-179.1(3)	C105	N24	C101	C102	4.0(5)
C20	C21	C22	C23	0.1(6)	C107	N23	C99	C98	-133.5(3)
C21	C22	C23	C24	-1.0(7)	C107	N23	C100	C101	161.9(3)
C22	C23	C24	N6	1.3(6)	C108	N19	C82	C83	-76.4(4)
C22	C23	C24	C25	179.7(4)	C108	N19	C89	C90	69.5(4)
C24	N6	C20	C19	173.8(3)	S1	Na1	O4	S2	56.18(18)
C24	N6	C20	C21	-0.2(5)	S1	Na1	O5	S2	-126.52(14)
C26	N5	C18	C17	-70.4(4)	S1	Na1	O9	S3	-146.3(15)

C26	N5	C19	C20	77.8(4)	S1	Na1	O12	S4	132(4)
C27	N1	C1	C2	-157.7(3)	S2	Na1	O1	S1	48.55(15)
C27	N1	C8	C9	135.3(3)	S2	Na1	O3	S1	-127.44(14)
Fe3	N13	C55	C56	47.8(3)	S2	Na1	O9	S3	-44.0(16)
Fe3	N13	C62	C63	15.8(4)	S2	Na1	O12	S4	8(4)
Fe3	N13	C81	C80	52.3(3)	Na1	S1	C109	F1	-113.6(3)
Fe3	N14	C56	C55	-5.9(4)	Na1	S1	C109	F2	5.5(4)
Fe3	N14	C56	C57	172.3(3)	Na1	S1	C109	F3	125.5(3)
Fe3	N14	C60	C59	-171.1(3)	Na1	S2	C110	F4	115.6(2)
Fe3	N14	C60	C61	8.7(5)	Na1	S2	C110	F5	-4.2(4)
Fe3	N15	C63	C62	52.0(3)	Na1	S2	C110	F6	-124.5(3)
Fe3	N15	C64	C65	47.6(3)	O1	S1	Na1	S2	-138.42(14)
Fe3	N15	C71	C72	16.6(4)	O1	S1	Na1	O3	168.8(2)
Fe3	N16	C65	C64	-6.5(4)	O1	S1	Na1	O4	-160.56(17)
Fe3	N16	C65	C66	174.4(3)	O1	S1	Na1	O5	-116.55(15)
Fe3	N16	C69	C68	-175.6(2)	O1	S1	Na1	O9	-39.74(19)
Fe3	N16	C69	C70	3.9(5)	O1	S1	Na1	O12	78.4(2)
Fe3	N17	C72	C71	52.5(3)	O1	S1	O3	Na1	-10.39(19)
Fe3	N17	C73	C74	46.8(3)	O1	S1	C109	F1	-173.7(3)
Fe3	N17	C80	C81	14.8(4)	O1	S1	C109	F2	-54.6(3)
Fe3	N18	C74	C73	5.4(4)	O1	S1	C109	F3	65.4(3)
Fe3	N18	C74	C75	-175.9(3)	O1	Na1	O3	S1	6.39(12)
Fe3	N18	C78	C77	175.8(3)	O1	Na1	O4	S2	41.9(3)
Fe3	N18	C78	C79	-3.9(5)	O1	Na1	O5	S2	-151.37(14)
N13	Fe3	N14	C56	24.9(2)	O1	Na1	O9	S3	-163.8(15)
N13	Fe3	N14	C60	-161.8(3)	O1	Na1	O12	S4	160(4)
N13	Fe3	N15	C63	-32.5(2)	O2	S1	Na1	S2	-42.51(17)
N13	Fe3	N15	C64	-150.2(2)	O2	S1	Na1	O1	95.9(2)
N13	Fe3	N15	C71	88.3(3)	O2	S1	Na1	O3	-95.3(2)
N13	Fe3	N16	C65	97.4(2)	O2	S1	Na1	O4	-64.66(19)
N13	Fe3	N16	C69	-86.5(3)	O2	S1	Na1	O5	-20.65(18)
N13	Fe3	N17	C72	-112.5(2)	O2	S1	Na1	O9	56.2(2)
N13	Fe3	N17	C73	131.5(2)	O2	S1	Na1	O12	174.3(2)
N13	Fe3	N17	C80	10.1(2)	O2	S1	O1	Na1	-126.79(15)
N13	Fe3	N18	C74	-13.9(4)	O2	S1	O3	Na1	126.32(15)
N13	Fe3	N18	C78	168.3(3)	O2	S1	C109	F1	66.0(3)
N13	C55	C56	N14	-28.2(5)	O2	S1	C109	F2	-174.8(3)
N13	C55	C56	C57	153.5(4)	O2	S1	C109	F3	-54.8(3)

N13	C62	C63	N15	-46.5(4)	O3	S1	Na1	S2	52.83(15)
N14	Fe3	N13	C55	-38.2(2)	O3	S1	Na1	O1	-168.8(2)
N14	Fe3	N13	C62	-159.6(3)	O3	S1	Na1	O4	30.69(17)
N14	Fe3	N13	C81	79.1(2)	O3	S1	Na1	O5	74.69(16)
N14	Fe3	N15	C63	-11.0(3)	O3	S1	Na1	O9	151.5(2)
N14	Fe3	N15	C64	-128.8(2)	O3	S1	Na1	O12	-90.4(2)
N14	Fe3	N15	C71	109.7(3)	O3	S1	O1	Na1	10.19(19)
N14	Fe3	N16	C65	175.1(2)	O3	S1	C109	F1	-55.1(4)
N14	Fe3	N16	C69	-8.8(3)	O3	S1	C109	F2	64.0(3)
N14	Fe3	N17	C72	178.1(2)	O3	S1	C109	F3	-176.0(3)
N14	Fe3	N17	C73	62.1(2)	O3	Na1	O1	S1	-6.30(12)
N14	Fe3	N17	C80	-59.3(3)	O3	Na1	O4	S2	69.80(17)
N14	Fe3	N18	C74	-88.6(2)	O3	Na1	O5	S2	-99.30(15)
N14	Fe3	N18	C78	93.7(3)	O3	Na1	O9	S3	-124.9(15)
N14	C56	C57	C58	0.6(7)	O3	Na1	O12	S4	104(4)
N15	Fe3	N13	C55	131.0(2)	O4	S2	Na1	S1	-130.53(17)
N15	Fe3	N13	C62	9.7(2)	O4	S2	Na1	O1	-151.31(19)
N15	Fe3	N13	C81	-111.6(2)	O4	S2	Na1	O3	-108.75(18)
N15	Fe3	N14	C56	3.1(4)	O4	S2	Na1	O5	175.6(2)
N15	Fe3	N14	C60	176.4(3)	O4	S2	Na1	O9	108.2(2)
N15	Fe3	N16	C65	25.3(2)	O4	S2	Na1	O12	-2.2(3)
N15	Fe3	N16	C69	-158.6(3)	O4	S2	O5	Na1	-3.64(19)
N15	Fe3	N17	C72	-32.0(2)	O4	S2	C110	F4	64.1(3)
N15	Fe3	N17	C73	-148.0(2)	O4	S2	C110	F5	-55.8(4)
N15	Fe3	N17	C80	90.6(3)	O4	S2	C110	F6	-176.1(3)
N15	Fe3	N18	C74	87.2(3)	O4	Na1	O1	S1	28.6(2)
N15	Fe3	N18	C78	-90.6(3)	O4	Na1	O3	S1	-152.54(15)
N15	C64	C65	N16	-28.5(4)	O4	Na1	O5	S2	2.43(13)
N15	C64	C65	C66	150.7(3)	O4	Na1	O9	S3	-18.4(16)
N15	C71	C72	N17	-46.8(4)	O4	Na1	O12	S4	7(4)
N16	Fe3	N13	C55	61.5(2)	O5	S2	Na1	S1	53.84(14)
N16	Fe3	N13	C62	-59.9(3)	O5	S2	Na1	O1	33.06(16)
N16	Fe3	N13	C81	178.8(2)	O5	S2	Na1	O3	75.62(16)
N16	Fe3	N14	C56	-79.4(2)	O5	S2	Na1	O4	-175.6(2)
N16	Fe3	N14	C60	93.9(3)	O5	S2	Na1	O9	-67.40(18)
N16	Fe3	N15	C63	79.2(2)	O5	S2	Na1	O12	-177.8(2)
N16	Fe3	N15	C64	-38.6(2)	O5	S2	O4	Na1	4.2(2)
N16	Fe3	N15	C71	-160.1(3)	O5	S2	C110	F4	-177.9(3)

N16	Fe3	N17	C72	-10.3(4)	O5	S2	C110	F5	62.3(3)
N16	Fe3	N17	C73	-126.3(3)	O5	S2	C110	F6	-58.0(4)
N16	Fe3	N17	C80	112.3(3)	O5	Na1	O1	S1	63.07(14)
N16	Fe3	N18	C74	165.2(2)	O5	Na1	O3	S1	-100.33(15)
N16	Fe3	N18	C78	-12.5(3)	O5	Na1	O4	S2	-2.48(13)
N16	C65	C66	C67	2.4(5)	O5	Na1	O9	S3	-69.3(16)
N17	Fe3	N13	C55	-149.5(2)	O5	Na1	O12	S4	4(4)
N17	Fe3	N13	C62	89.1(3)	O6	S2	Na1	S1	-45.3(2)
N17	Fe3	N13	C81	-32.1(2)	O6	S2	Na1	O1	-66.0(2)
N17	Fe3	N14	C56	96.3(2)	O6	S2	Na1	O3	-23.5(2)
N17	Fe3	N14	C60	-90.4(3)	O6	S2	Na1	O4	85.3(3)
N17	Fe3	N15	C63	-111.9(2)	O6	S2	Na1	O5	-99.1(3)
N17	Fe3	N15	C64	130.3(2)	O6	S2	Na1	O9	-166.5(2)
N17	Fe3	N15	C71	8.8(2)	O6	S2	Na1	O12	83.1(3)
N17	Fe3	N16	C65	3.4(4)	O6	S2	O4	Na1	-131.77(18)
N17	Fe3	N16	C69	179.5(3)	O6	S2	O5	Na1	132.20(19)
N17	Fe3	N18	C74	16.2(2)	O6	S2	C110	F4	-56.4(3)
N17	Fe3	N18	C78	-161.5(3)	O6	S2	C110	F5	-176.3(3)
N17	C73	C74	N18	-36.9(5)	O6	S2	C110	F6	63.5(4)
N17	C73	C74	C75	144.3(4)	O7	S3	O9	Na1	116.2(15)
N17	C80	C81	N13	-45.2(4)	O7	S3	C111	F7	-176.5(3)
N18	Fe3	N13	C55	-119.4(3)	O7	S3	C111	F8	-59.1(3)
N18	Fe3	N13	C62	119.2(3)	O7	S3	C111	F9	60.7(4)
N18	Fe3	N13	C81	-2.1(4)	O8	S3	O9	Na1	-23.1(16)
N18	Fe3	N14	C56	174.9(2)	O8	S3	C111	F7	-56.5(4)
N18	Fe3	N14	C60	-11.7(3)	O8	S3	C111	F8	60.9(3)
N18	Fe3	N15	C63	177.5(2)	O8	S3	C111	F9	-179.3(3)
N18	Fe3	N15	C64	59.8(2)	O9	S3	C111	F7	63.5(4)
N18	Fe3	N15	C71	-61.7(3)	O9	S3	C111	F8	-179.1(3)
N18	Fe3	N16	C65	-82.1(2)	O9	S3	C111	F9	-59.3(4)
N18	Fe3	N16	C69	94.0(3)	O9	Na1	O1	S1	146.13(16)
N18	Fe3	N17	C72	82.4(2)	O9	Na1	O3	S1	-43.0(3)
N18	Fe3	N17	C73	-33.6(2)	O9	Na1	O4	S2	-74.8(2)
N18	Fe3	N17	C80	-155.0(3)	O9	Na1	O5	S2	111.53(17)
N18	C74	C75	C76	-0.8(6)	O9	Na1	O12	S4	-99(4)
C55	N13	C62	C63	-102.8(4)	O10	S4	O12	Na1	126(4)
C55	N13	C81	C80	166.4(3)	O10	S4	C112	F10	-177.3(4)
C55	C56	C57	C58	178.8(4)	O10	S4	C112	F11	62.5(4)

C56	N14	C60	C59	1.8(6)	O10	S4	C112	F12	-52.2(4)
C56	N14	C60	C61	-178.5(3)	O11	S4	O12	Na1	-12(4)
C56	C57	C58	C59	1.2(8)	O11	S4	C112	F10	-59.8(4)
C57	C58	C59	C60	-1.5(8)	O11	S4	C112	F11	-179.9(4)
C58	C59	C60	N14	0.0(7)	O11	S4	C112	F12	65.4(4)
C58	C59	C60	C61	-179.7(5)	O12	S4	C112	F10	57.8(5)
C60	N14	C56	C55	179.7(3)	O12	S4	C112	F11	-62.4(5)
C60	N14	C56	C57	-2.1(6)	O12	S4	C112	F12	-177.1(5)
C62	N13	C55	C56	170.6(3)	O12	Na1	O1	S1	-109.3(2)
C62	N13	C81	C80	-70.3(4)	O12	Na1	O3	S1	98.9(2)
C63	N15	C64	C65	-64.7(4)	O12	Na1	O4	S2	178.37(19)
C63	N15	C71	C72	133.4(3)	O12	Na1	O5	S2	4.9(6)
C64	N15	C63	C62	165.0(3)	O12	Na1	O9	S3	92.2(16)
C64	N15	C71	C72	-101.6(4)	C109	S1	Na1	S2	137.02(17)
C64	C65	C66	C67	-176.7(3)	C109	S1	Na1	O1	-84.6(2)
C65	N16	C69	C68	0.3(5)	C109	S1	Na1	O3	84.2(2)
C65	N16	C69	C70	179.7(3)	C109	S1	Na1	O4	114.88(19)
C65	C66	C67	C68	-0.6(5)	C109	S1	Na1	O5	158.89(17)
C66	C67	C68	C69	-1.3(5)	C109	S1	Na1	O9	-124.3(2)
C67	C68	C69	N16	1.5(5)	C109	S1	Na1	O12	-6.2(3)
C67	C68	C69	C70	-178.0(3)	C109	S1	O1	Na1	121.75(17)
C69	N16	C65	C64	176.9(3)	C109	S1	O3	Na1	-121.57(16)
C69	N16	C65	C66	-2.3(5)	C110	S2	Na1	S1	146.27(17)
C71	N15	C63	C62	-70.4(4)	C110	S2	Na1	O1	125.49(19)
C71	N15	C64	C65	170.7(3)	C110	S2	Na1	O3	168.05(18)
C72	N17	C73	C74	-65.5(4)	C110	S2	Na1	O4	-83.2(2)
C72	N17	C80	C81	133.2(3)	C110	S2	Na1	O5	92.4(2)
C73	N17	C72	C71	164.6(3)	C110	S2	Na1	O9	25.0(2)
C73	N17	C80	C81	-102.6(4)	C110	S2	Na1	O12	-85.4(3)
C73	C74	C75	C76	177.9(4)	C110	S2	O4	Na1	116.53(18)
C74	N18	C78	C77	-1.8(5)	C110	S2	O5	Na1	-115.00(15)
C74	N18	C78	C79	178.5(3)	C111	S3	O9	Na1	-133.8(15)
C74	C75	C76	C77	-1.0(6)	C112	S4	O12	Na1	-118(4)
C75	C76	C77	C78	1.3(6)	S5	Na2	O18	S6	30.4(6)
C76	C77	C78	N18	0.1(6)	S5	Na2	O19	S7	124.11(14)
C76	C77	C78	C79	179.8(4)	S5	Na2	O20	S7	-53.20(16)
C78	N18	C74	C73	-176.6(3)	S5	Na2	O24	S8	111.6(8)
C78	N18	C74	C75	2.2(5)	S7	Na2	O13	S5	-44.13(16)

C80	N17	C72	C71	-70.5(4)	S7	Na2	O15	S5	129.71(13)
C80	N17	C73	C74	169.1(3)	S7	Na2	O18	S6	-81.9(5)
C81	N13	C55	C56	-65.9(4)	S7	Na2	O24	S8	-140.1(7)
C81	N13	C62	C63	133.9(3)	Na2	S5	C113	F13	-121.3(2)
Fe2	N7	C28	C29	-48.6(3)	Na2	S5	C113	F14	120.0(3)
Fe2	N7	C35	C36	16.2(4)	Na2	S5	C113	F15	-0.7(4)
Fe2	N7	C54	C53	51.5(3)	Na2	S7	C115	F19	1.6(3)
Fe2	N8	C29	C28	-16.8(4)	Na2	S7	C115	F20	122.5(2)
Fe2	N8	C29	C30	164.7(3)	Na2	S7	C115	F21	-118.1(2)
Fe2	N8	C33	C32	-162.2(3)	O13	S5	Na2	S7	140.87(15)
Fe2	N8	C33	C34	19.5(5)	O13	S5	Na2	O15	-170.4(2)
Fe2	N9	C36	C35	50.1(3)	O13	S5	Na2	O18	21.02(19)
Fe2	N9	C37	C38	-46.2(3)	O13	S5	Na2	O19	118.35(16)
Fe2	N9	C44	C45	14.0(4)	O13	S5	Na2	O20	162.27(17)
Fe2	N10	C38	C37	-9.8(4)	O13	S5	Na2	O24	-92.98(18)
Fe2	N10	C38	C39	175.8(3)	O13	S5	O15	Na2	8.04(16)
Fe2	N10	C42	C41	-176.5(3)	O13	S5	C113	F13	-70.3(3)
Fe2	N10	C42	C43	5.5(5)	O13	S5	C113	F14	170.9(3)
Fe2	N11	C45	C44	51.9(3)	O13	S5	C113	F15	50.2(3)
Fe2	N11	C46	C47	-43.5(3)	O13	Na2	O15	S5	-5.38(11)
Fe2	N11	C53	C54	18.2(4)	O13	Na2	O18	S6	39.9(5)
Fe2	N12	C47	C46	-10.1(4)	O13	Na2	O19	S7	147.78(15)
Fe2	N12	C47	C48	175.5(3)	O13	Na2	O20	S7	-41.3(2)
Fe2	N12	C51	C50	-176.8(3)	O13	Na2	O24	S8	83.1(8)
Fe2	N12	C51	C52	3.3(5)	O14	S5	Na2	S7	53.43(16)
N7	Fe2	N8	C29	-8.5(2)	O14	S5	Na2	O13	-87.4(2)
N7	Fe2	N8	C33	157.8(3)	O14	S5	Na2	O15	102.2(2)
N7	Fe2	N9	C36	-31.0(2)	O14	S5	Na2	O18	-66.4(2)
N7	Fe2	N9	C37	-148.6(2)	O14	S5	Na2	O19	30.91(17)
N7	Fe2	N9	C44	90.7(3)	O14	S5	Na2	O20	74.82(18)
N7	Fe2	N10	C38	-12.3(4)	O14	S5	Na2	O24	179.58(19)
N7	Fe2	N10	C42	163.9(3)	O14	S5	O13	Na2	127.56(15)
N7	Fe2	N11	C45	-113.9(2)	O14	S5	O15	Na2	-128.41(14)
N7	Fe2	N11	C46	129.2(2)	O14	S5	C113	F13	50.0(3)
N7	Fe2	N11	C53	7.3(2)	O14	S5	C113	F14	-68.8(3)
N7	Fe2	N12	C47	-87.0(2)	O14	S5	C113	F15	170.5(3)
N7	Fe2	N12	C51	91.5(3)	O15	S5	Na2	S7	-48.77(13)
N7	C28	C29	N8	46.2(4)	O15	S5	Na2	O13	170.4(2)

N7	C28	C29	C30	-135.3(4)	O15	S5	Na2	O18	-168.62(19)
N7	C35	C36	N9	-45.0(4)	O15	S5	Na2	O19	-71.29(15)
N8	Fe2	N7	C28	30.6(2)	O15	S5	Na2	O20	-27.38(15)
N8	Fe2	N7	C35	-89.4(2)	O15	S5	Na2	O24	77.38(18)
N8	Fe2	N7	C54	149.5(2)	O15	S5	O13	Na2	-9.44(19)
N8	Fe2	N9	C36	45.3(2)	O15	S5	C113	F13	171.5(3)
N8	Fe2	N9	C37	-72.3(2)	O15	S5	C113	F14	52.7(3)
N8	Fe2	N9	C44	167.0(2)	O15	S5	C113	F15	-67.9(3)
N8	Fe2	N10	C38	79.5(2)	O15	Na2	O13	S5	5.47(11)
N8	Fe2	N10	C42	-104.3(3)	O15	Na2	O18	S6	19.4(7)
N8	Fe2	N11	C45	-111.4(3)	O15	Na2	O19	S7	96.62(15)
N8	Fe2	N11	C46	131.8(3)	O15	Na2	O20	S7	-65.50(15)
N8	Fe2	N11	C53	9.9(4)	O15	Na2	O24	S8	139.0(8)
N8	Fe2	N12	C47	-166.1(2)	O16	S6	O18	Na2	-22.9(6)
N8	Fe2	N12	C51	12.4(3)	O16	S6	C114	F16	-62.4(4)
N8	C29	C30	C31	1.0(6)	O16	S6	C114	F17	55.5(3)
N9	Fe2	N7	C28	128.4(2)	O16	S6	C114	F18	176.3(3)
N9	Fe2	N7	C35	8.4(2)	O17	S6	O18	Na2	-160.5(5)
N9	Fe2	N7	C54	-112.7(2)	O17	S6	C114	F16	59.4(4)
N9	Fe2	N8	C29	-85.6(2)	O17	S6	C114	F17	177.3(3)
N9	Fe2	N8	C33	80.7(3)	O17	S6	C114	F18	-61.9(4)
N9	Fe2	N10	C38	-12.6(2)	O18	S6	C114	F16	177.2(3)
N9	Fe2	N10	C42	163.6(3)	O18	S6	C114	F17	-65.0(3)
N9	Fe2	N11	C45	-33.4(2)	O18	S6	C114	F18	55.8(4)
N9	Fe2	N11	C46	-150.3(2)	O18	Na2	O13	S5	-162.63(15)
N9	Fe2	N11	C53	87.9(3)	O18	Na2	O15	S5	19.8(3)
N9	Fe2	N12	C47	-9.8(4)	O18	Na2	O19	S7	-112.40(16)
N9	Fe2	N12	C51	168.8(3)	O18	Na2	O20	S7	93.05(17)
N9	C37	C38	N10	39.5(5)	O18	Na2	O24	S8	-19.0(8)
N9	C37	C38	C39	-146.0(4)	O19	S7	Na2	S5	-54.72(15)
N9	C44	C45	N11	-45.6(4)	O19	S7	Na2	O13	-36.15(17)
N10	Fe2	N7	C28	128.1(3)	O19	S7	Na2	O15	-75.67(16)
N10	Fe2	N7	C35	8.1(4)	O19	S7	Na2	O18	75.49(18)
N10	Fe2	N7	C54	-113.0(3)	O19	S7	Na2	O20	173.3(2)
N10	Fe2	N8	C29	-164.3(2)	O19	S7	Na2	O24	-169.8(2)
N10	Fe2	N8	C33	2.0(3)	O19	S7	O20	Na2	-6.4(2)
N10	Fe2	N9	C36	148.9(3)	O19	S7	C115	F19	-63.0(3)
N10	Fe2	N9	C37	31.3(2)	O19	S7	C115	F20	57.9(3)

N10	Fe2	N9	C44	-89.4(3)	O19	S7	C115	F21	177.3(3)
N10	Fe2	N11	C45	42.5(2)	O19	Na2	O13	S5	-59.91(14)
N10	Fe2	N11	C46	-74.3(2)	O19	Na2	O15	S5	101.68(14)
N10	Fe2	N11	C53	163.8(2)	O19	Na2	O18	S6	-54.7(5)
N10	Fe2	N12	C47	83.7(3)	O19	Na2	O20	S7	3.79(12)
N10	Fe2	N12	C51	-97.8(3)	O19	Na2	O24	S8	-149.1(6)
N10	C38	C39	C40	1.1(6)	O20	S7	Na2	S5	131.97(16)
N11	Fe2	N7	C28	-150.5(2)	O20	S7	Na2	O13	150.54(18)
N11	Fe2	N7	C35	89.5(2)	O20	S7	Na2	O15	111.02(17)
N11	Fe2	N7	C54	-31.6(2)	O20	S7	Na2	O18	-97.82(18)
N11	Fe2	N8	C29	-11.1(4)	O20	S7	Na2	O19	-173.3(2)
N11	Fe2	N8	C33	155.2(3)	O20	S7	Na2	O24	16.8(2)
N11	Fe2	N9	C36	-110.7(2)	O20	S7	O19	Na2	5.72(19)
N11	Fe2	N9	C37	131.7(2)	O20	S7	C115	F19	55.2(3)
N11	Fe2	N9	C44	11.0(2)	O20	S7	C115	F20	176.1(3)
N11	Fe2	N10	C38	-89.6(2)	O20	S7	C115	F21	-64.5(3)
N11	Fe2	N10	C42	86.6(3)	O20	Na2	O13	S5	-24.8(2)
N11	Fe2	N12	C47	-11.1(2)	O20	Na2	O15	S5	154.80(14)
N11	Fe2	N12	C51	167.4(3)	O20	Na2	O18	S6	-110.9(5)
N11	C46	C47	N12	37.7(4)	O20	Na2	O19	S7	-3.73(12)
N11	C46	C47	C48	-147.7(4)	O20	Na2	O24	S8	-132.5(8)
N11	C53	C54	N7	-47.5(4)	O21	S7	Na2	S5	44.0(2)
N12	Fe2	N7	C28	-74.9(2)	O21	S7	Na2	O13	62.6(2)
N12	Fe2	N7	C35	165.2(2)	O21	S7	Na2	O15	23.1(2)
N12	Fe2	N7	C54	44.0(2)	O21	S7	Na2	O18	174.2(2)
N12	Fe2	N8	C29	85.2(2)	O21	S7	Na2	O19	98.7(2)
N12	Fe2	N8	C33	-108.5(3)	O21	S7	Na2	O20	-88.0(2)
N12	Fe2	N9	C36	-112.0(3)	O21	S7	Na2	O24	-71.1(2)
N12	Fe2	N9	C37	130.3(3)	O21	S7	O19	Na2	-130.58(16)
N12	Fe2	N9	C44	9.6(4)	O21	S7	O20	Na2	130.21(16)
N12	Fe2	N10	C38	-168.7(2)	O21	S7	C115	F19	175.8(3)
N12	Fe2	N10	C42	7.5(3)	O21	S7	C115	F20	-63.4(3)
N12	Fe2	N11	C45	146.0(2)	O21	S7	C115	F21	56.1(3)
N12	Fe2	N11	C46	29.2(2)	O22	S8	O24	Na2	1.4(9)
N12	Fe2	N11	C53	-92.7(3)	O22	S8	C116	F22	-56.2(3)
N12	C47	C48	C49	2.2(6)	O22	S8	C116	F23	-176.2(3)
C28	N7	C35	C36	-99.0(4)	O22	S8	C116	F24	65.6(3)
C28	N7	C54	C53	164.5(3)	O23	S8	O24	Na2	138.8(7)

C28	C29	C30	C31	-177.4(4)	O23	S8	C116	F22	-177.1(3)
C29	N8	C33	C32	3.4(5)	O23	S8	C116	F23	62.9(3)
C29	N8	C33	C34	-175.0(3)	O23	S8	C116	F24	-55.2(4)
C29	C30	C31	C32	1.1(7)	O24	S8	C116	F22	62.0(3)
C30	C31	C32	C33	-1.0(7)	O24	S8	C116	F23	-57.9(3)
C31	C32	C33	N8	-1.3(6)	O24	S8	C116	F24	-176.1(3)
C31	C32	C33	C34	177.0(4)	O24	Na2	O13	S5	95.91(17)
C33	N8	C29	C28	175.2(3)	O24	Na2	O15	S5	-109.51(16)
C33	N8	C29	C30	-3.3(5)	O24	Na2	O18	S6	149.2(5)
C35	N7	C28	C29	70.8(4)	O24	Na2	O19	S7	16.8(3)
C35	N7	C54	C53	-69.1(4)	O24	Na2	O20	S7	-165.70(17)
C36	N9	C37	C38	-160.3(3)	C113	S5	Na2	S7	-138.44(16)
C36	N9	C44	C45	132.3(3)	C113	S5	Na2	O13	80.7(2)
C37	N9	C36	C35	163.3(3)	C113	S5	Na2	O15	-89.7(2)
C37	N9	C44	C45	-102.3(4)	C113	S5	Na2	O18	101.7(2)
C37	C38	C39	C40	-173.1(4)	C113	S5	Na2	O19	-160.96(17)
C38	N10	C42	C41	-0.5(5)	C113	S5	Na2	O20	-117.04(18)
C38	N10	C42	C43	-178.5(3)	C113	S5	Na2	O24	-12.3(2)
C38	C39	C40	C41	0.2(6)	C113	S5	O13	Na2	-119.94(17)
C39	C40	C41	C42	-1.5(6)	C113	S5	O15	Na2	118.70(14)
C40	C41	C42	N10	1.7(6)	C114	S6	O18	Na2	89.0(5)
C40	C41	C42	C43	179.7(4)	C115	S7	Na2	S5	-144.28(16)
C42	N10	C38	C37	173.4(3)	C115	S7	Na2	O13	-125.71(17)
C42	N10	C38	C39	-1.0(5)	C115	S7	Na2	O15	-165.23(16)
C44	N9	C36	C35	-71.0(4)	C115	S7	Na2	O18	-14.07(19)
C44	N9	C37	C38	74.0(4)	C115	S7	Na2	O19	-89.6(2)
C45	N11	C46	C47	-155.4(3)	C115	S7	Na2	O20	83.8(2)
C45	N11	C53	C54	134.5(3)	C115	S7	Na2	O24	100.6(2)
C46	N11	C45	C44	165.0(3)	C115	S7	O19	Na2	117.00(15)
C46	N11	C53	C54	-100.0(4)	C115	S7	O20	Na2	-117.62(16)
C46	C47	C48	C49	-172.0(4)	C116	S8	O24	Na2	-108.7(8)
C47	N12	C51	C50	1.7(5)	O25	S9	C117	F25	-59.3(4)
C47	N12	C51	C52	-178.3(3)	O25	S9	C117	F26	59.2(4)
C47	C48	C49	C50	0.3(7)	O25	S9	C117	F27	178.8(3)
C48	C49	C50	C51	-1.8(7)	O26	S9	C117	F25	59.0(4)
C49	C50	C51	N12	0.8(7)	O26	S9	C117	F26	177.5(3)
C49	C50	C51	C52	-179.3(4)	O26	S9	C117	F27	-62.9(4)
C51	N12	C47	C46	171.2(3)	O27	S9	C117	F25	-179.4(4)

C51	N12	C47	C48	-3.2(5)	O27	S9	C117	F26	-60.9(4)
C53	N11	C45	C44	-68.9(4)	O27	S9	C117	F27	58.7(4)
C53	N11	C46	C47	78.3(4)	O28	S10	C118	F28	-74.1(7)
C54	N7	C28	C29	-162.8(3)	O28	S10	C118	F29	70.6(6)
C54	N7	C35	C36	134.0(3)	O28	S10	C118	F30	179.5(4)
Fe4	N19	C82	C83	43.0(3)	O29	S10	C118	F28	41.0(7)
Fe4	N19	C89	C90	-51.2(3)	O29	S10	C118	F29	-174.2(6)
Fe4	N19	C108	C107	-14.4(4)	O29	S10	C118	F30	-65.3(4)
Fe4	N20	C83	C82	9.4(4)	O30	S10	C118	F28	159.6(6)
Fe4	N20	C83	C84	-175.6(3)	O30	S10	C118	F29	-55.6(7)
Fe4	N20	C87	C86	177.2(3)	O30	S10	C118	F30	53.3(4)

Table S13. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Fe(MPT).

Atom	*x*	*y*	*z*	U(eq)
H1A	222	5202	3066	25
H1B	925	4291	3136	25
H3	-919	4673	2593	29
H4	-1271	4049	2010	34
H5	-17	3459	1714	30
H7A	2076	4023	1757	34
H7B	1629	2952	1744	34
H7C	2379	3270	2071	34
H8A	1633	7011	3018	25
H8B	602	6591	2877	25
H9A	1061	6264	2322	25
H9B	1457	7336	2417	25
H10A	2741	6831	1962	22
H10B	2075	5884	1940	22
H12	3981	6314	1624	22
H13	5320	5305	1578	27
H14	5520	3935	1946	24
H16A	4778	3400	2660	31
H16B	4810	2767	2307	31
H16C	3809	3000	2452	31
H17A	2904	7423	2789	26
H17B	3516	7376	2457	26
H18A	4455	6140	2702	23
H18B	4370	6876	3025	23
H19A	4697	5195	3418	26
H19B	4810	4861	3020	26
H21	4947	3611	3677	36
H22	4385	2014	3749	44
H23	3066	1479	3376	41
H25A	1447	2833	2885	40
H25B	1821	1737	2928	40
H25C	2139	2403	2615	40
H26A	2997	6738	3319	27
H26B	3467	5923	3584	27
H27A	2177	4893	3465	25

H27B	1721	5943	3522	25
H55A	4775	4058	8150	29
H55B	4591	3944	8558	29
H57	4854	5654	8679	44
H58	4208	7222	8657	61
H59	2795	7526	8286	47
H61A	1911	6282	7597	44
H61B	1575	7028	7884	44
H61C	1284	5905	7898	44
H62A	3620	1881	8279	32
H62B	4644	2388	8281	32
H63A	4479	2556	7674	30
H63B	4143	1466	7745	30
H64A	2418	2488	7067	26
H64B	3335	1791	7108	26
H66	4096	2621	6647	24
H67	5120	3883	6521	27
H68	5278	5232	6903	24
H70A	3758	5854	7514	34
H70B	4720	6169	7356	34
H70C	4766	5482	7698	34
H71A	2561	1285	7881	31
H71B	2155	1203	7470	31
H72A	1055	2423	7521	31
H72B	978	1735	7858	31
H73A	938	4209	8164	31
H73B	243	3319	8045	31
H75	-863	4132	7619	33
H76	-1186	4881	7063	38
H77	106	5366	6757	34
H79A	2438	5500	7091	37
H79B	1736	5568	6731	37
H79C	2266	4566	6840	37
H80A	2119	2029	8356	33
H80B	1467	2847	8511	33
H81A	2666	3959	8553	33
H81B	3159	2974	8705	33
H28A	4609	3220	-200	27

H28B	4306	3375	193	27
H30	4478	4789	-476	36
H31	3569	6171	-639	46
H32	2095	6369	-428	34
H34A	667	4939	-163	36
H34B	1059	5932	19	36
H34C	1206	4928	231	36
H35A	3233	1445	-513	31
H35B	3698	2444	-626	31
H36A	2269	3227	-680	29
H36B	2053	2194	-867	29
H37A	252	2598	-680	30
H37B	824	3560	-547	30
H39	-1236	2906	-451	33
H40	-2099	3185	37	40
H41	-1272	3419	598	35
H43A	932	2773	877	47
H43B	143	3540	970	47
H43C	1058	3902	791	47
H44A	1770	880	-493	34
H44B	659	1126	-499	34
H45A	729	1103	109	31
H45B	1321	165	9	31
H46A	2259	464	685	29
H46B	1390	1220	651	29
H48	3020	950	1256	34
H49	3785	2181	1615	44
H50	3835	3752	1401	44
H52A	3666	4496	590	42
H52B	3426	4916	964	42
H52C	2581	4678	660	42
H53A	2943	486	-99	32
H53B	3302	329	312	32
H54A	4091	1806	348	30
H54B	4378	1301	-7	30
H82A	1472	7896	5485	26
H82B	2349	8642	5531	26
H84	2927	8278	6133	28

H85	3606	7152	6555	32
H86	3716	5525	6391	30
H88A	2721	4465	5612	35
H88B	3342	4253	5983	35
H88C	3856	4583	5645	35
H89A	1651	8823	4825	30
H89B	985	7934	4918	30
H90A	1116	7783	4320	34
H90B	2241	7977	4373	34
H91A	1195	5353	4334	32
H91B	679	6317	4173	32
H93	-873	6012	4350	32
H94	-1872	5886	4814	42
H95	-1155	5787	5401	32
H97A	1159	5288	5667	35
H97B	161	5567	5806	35
H97C	915	6401	5742	35
H98A	2540	6613	4043	33
H98B	2677	5605	4254	33
H99A	4147	6328	4349	33
H99B	3697	7374	4416	33
H10C	4476	5538	5193	30
H10D	4886	5607	4814	30
H102	4687	4042	4526	32
H103	3722	2689	4364	37
H104	2216	2561	4575	33
H10E	1357	4139	5202	33
H10F	1239	3069	5037	33
H10G	840	3990	4809	33
H10H	4673	7576	4960	32
H10I	4279	7133	5308	32
H10J	3532	8621	5225	33
H10K	3293	8443	4808	33
H31A	8236	3488	6592	119
H31B	7329	3650	6421	119

Co(MPT)

Table S14. Crystal data and structure refinement for Co(MPT).

Identification code	Co(MPT)
Empirical formula	$C_{27}H_{36}CoN_8O_6$
Formula weight	627.57
Temperature/K	90
Crystal system	orthorhombic
Space group	Pbca
a/Å	18.3433(7)
b/Å	18.0221(7)
c/Å	18.9080(7)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	6250.7(4)
Z	8
ρ_{calc}g/cm^3	1.334
μ/mm^{-1}	0.601
F(000)	2632.0
Crystal size/mm^3	0.2 × 0.2 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.84 to 60.1
Index ranges	$-25 \leq h \leq 25$, $-25 \leq k \leq 25$, $-26 \leq l \leq 26$
Reflections collected	141678
Independent reflections	9149 [R_{int} = 0.0680, R_{sigma} = 0.0298]
Data/restraints/parameters	9149/0/382
Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ (I)]	R_1 = 0.0463, wR_2 = 0.1178
Final R indexes [all data]	R_1 = 0.0642, wR_2 = 0.1251
Largest diff. peak/hole / e Å^{-3}	0.99/-0.58

Table S15. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Co(MPT). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Co1	8145.10(13)	7078.64(13)	1983.89(13)	18.36(7)
N1	7401.3(8)	6978.8(8)	1099.7(8)	19.9(3)
N2	7393.7(9)	6225.8(10)	2381.8(9)	27.2(3)
N3	7430.8(9)	8007.1(9)	2198.5(9)	24.9(3)
N4	8640.3(8)	7536.8(9)	2965.3(8)	22.7(3)
N5	8629.6(9)	7879.8(9)	1282.5(9)	23.6(3)
N6	9038.7(9)	6422.8(9)	1519.9(9)	24.5(3)
C1	7134.9(10)	6211.2(10)	1117.6(10)	23.3(4)
C2	6936.7(10)	5991.2(10)	1861.9(10)	23.3(4)
C3	6341(1)	5541.1(11)	1989.7(11)	26.9(4)
C4	6206.5(11)	5302.0(12)	2671.0(12)	31.8(4)
C5	6683.0(13)	5507.7(13)	3197.4(13)	37.1(5)
C6	7274.0(12)	5969.0(14)	3044.0(12)	35.6(5)
C7	7795.7(17)	6176(2)	3619.7(14)	62.9(9)
C8	6784.1(10)	7512.8(10)	1166.4(10)	23.0(4)
C9	6702.8(11)	7794.7(12)	1923.3(11)	27.3(4)
C10	7427.8(11)	8091.4(14)	2974.0(11)	33.5(5)
C11	8198(1)	8063.0(11)	3252.1(10)	25.2(4)
C12	8409.4(11)	8530.6(11)	3791.5(10)	25.7(4)
C13	9103.9(11)	8454.6(11)	4069.6(10)	26.7(4)
C14	9547.6(11)	7902.3(12)	3807.5(11)	29.3(4)
C15	9309.5(10)	7449.4(11)	3256.7(11)	25.1(4)
C16	9794.0(12)	6845.0(13)	2982.6(12)	35.2(5)
C17	7715.3(12)	8685.6(11)	1842.2(12)	30.7(4)
C18	8509.0(12)	8610.7(11)	1621.5(11)	28.4(4)
C19	9410.7(11)	7687.2(12)	1253.4(11)	29.7(4)
C20	9506(1)	6868.0(12)	1159.2(10)	27.7(4)
C21	10069.4(12)	6595.6(16)	748.6(11)	39.0(6)
C22	10169.4(14)	5837.3(17)	702.5(12)	47.9(7)
C23	9708.7(14)	5382.5(15)	1074.1(13)	44.2(6)
C24	9148.1(12)	5679.2(12)	1486.7(12)	32.5(5)
C25	8667.1(13)	5180.3(12)	1905.6(16)	44.1(6)
C26	8281.0(11)	7841.3(11)	566.7(11)	27.3(4)
C27	7846.2(11)	7126.8(10)	464.1(10)	24.3(4)

O1	8313.2(9)	5185.8(8)	-79.5(8)	35.6(4)
O2	8386.6(15)	4066.1(10)	300.5(13)	71.9(7)
O3	7362.8(12)	4639.5(10)	366.8(13)	65.8(7)
N7	8022.9(13)	4631.3(10)	197.8(10)	38.3(5)
O4	10093.8(11)	8917.1(11)	2545.5(12)	55.3(5)
O5	10170.2(14)	9703.3(18)	1675.1(15)	97.5(11)
O6	10906.9(16)	8790(2)	1758.3(17)	124.5(14)
N8	10401.3(12)	9135.1(17)	1987.9(14)	59.9(7)

Table S16. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Co(MPT). 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}
Co1	17.18(12)	18.75(12)	19.14(12)	-0.07(9)	0.83(9)	3.02(9)
N1	22.5(7)	17.6(7)	19.6(7)	-1.4(5)	0.4(6)	2.9(6)
N2	24.1(8)	30.6(8)	27.0(8)	7.1(7)	-1.2(6)	-2.5(7)
N3	21.3(7)	29.1(8)	24.2(8)	-8.5(6)	-3.9(6)	8.1(6)
N4	19.9(7)	26.3(8)	22.0(7)	-1.3(6)	-1.1(6)	2.0(6)
N5	23.3(7)	23.1(8)	24.3(8)	0.9(6)	-0.4(6)	-0.5(6)
N6	22.1(7)	25.1(8)	26.3(8)	-6.2(6)	-1.6(6)	7.0(6)
C1	24.0(9)	17.7(8)	28.3(9)	-2.4(7)	-1.0(7)	0.1(7)
C2	22.3(9)	18.8(8)	28.6(9)	1.3(7)	1.3(7)	3.7(7)
C3	20.8(8)	20.9(9)	39.0(11)	1.2(8)	2.3(8)	2.1(7)
C4	25.2(10)	29(1)	41.2(12)	4.8(9)	6.3(8)	-1.7(8)
C5	36.2(11)	40.0(12)	35.2(11)	12.7(9)	4.6(9)	-6.2(10)
C6	32.4(11)	43.7(13)	30.8(11)	12.6(9)	-3.1(9)	-6.6(9)
C7	60.9(18)	92(2)	35.6(14)	30.5(15)	-16.1(13)	-37.1(17)
C8	22.9(9)	21.3(8)	24.8(9)	-3.4(7)	-3.7(7)	5.6(7)
C9	20.8(8)	31.4(10)	29.7(10)	-9.0(8)	-5.2(7)	8.9(7)
C10	23.8(9)	50.4(13)	26.4(10)	-15.6(9)	-2.9(8)	11.8(9)
C11	22.4(9)	32.7(10)	20.6(8)	-4.4(7)	-0.8(7)	4.7(7)
C12	27.5(9)	28.1(9)	21.6(9)	-2.2(7)	-0.2(7)	2.7(8)
C13	30.2(10)	27.2(9)	22.6(9)	-1.7(7)	-3.2(8)	-3.6(8)
C14	24.1(9)	34(1)	29.8(10)	-0.8(8)	-7.5(8)	0.3(8)
C15	20.2(8)	28.2(9)	27.0(9)	-1.9(7)	-3.5(7)	1.5(7)
C16	27.1(10)	39.9(11)	38.4(12)	-10.2(9)	-11.0(9)	10.7(9)
C17	34.6(11)	18.2(8)	39.5(11)	-7.6(8)	-13.9(9)	8.7(8)
C18	34.4(11)	17.7(8)	33.2(10)	0.3(7)	-5.7(8)	-2.0(7)
C19	23.2(9)	35.4(10)	30.5(10)	2.5(8)	4.1(8)	-4.7(8)
C20	20.5(9)	40.1(11)	22.5(9)	-3.5(8)	-0.6(7)	4.4(8)
C21	25(1)	69.8(17)	22.1(10)	-3.7(10)	-0.1(8)	15.2(10)
C22	37.7(12)	80.7(19)	25.4(11)	-15.5(12)	-5.2(9)	35.4(13)
C23	45.3(13)	45.9(14)	41.3(13)	-21.3(11)	-17.8(11)	29.0(11)
C24	29.6(10)	28.4(10)	39.6(11)	-9.9(9)	-13.6(9)	11.3(8)
C25	37.6(12)	19.6(10)	75.1(18)	3.2(10)	-12.1(12)	6.2(9)
C26	31.8(10)	27.3(10)	22.8(9)	4.0(7)	0.3(8)	-4.0(8)
C27	29.1(9)	24.5(9)	19.2(8)	0.7(7)	1.7(7)	1.2(7)
O1	50.2(9)	23.2(7)	33.3(8)	5.8(6)	10.7(7)	-4.4(6)

O2	105.1(18)	31.6(10)	79.1(16)	24.6(10)	40.6(14)	15.6(11)
O3	70.9(14)	37.6(10)	89.0(16)	-19.8(10)	48.2(12)	-21.7(9)
N7	66.6(14)	21.5(8)	26.7(9)	-4.7(7)	17.8(9)	-4.7(8)
O4	48.1(11)	61.3(12)	56.4(12)	3.8(10)	-6.1(9)	-9.6(9)
O5	60.9(14)	136(3)	95(2)	68.0(19)	27.0(14)	49.0(16)
O6	73.6(19)	214(4)	86(2)	-13(2)	3.1(16)	79(2)
N8	30.6(11)	91(2)	57.9(15)	-12.8(14)	-11.4(11)	13.8(12)

Table S17. Bond Lengths for Co(MPT).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	N1	2.1654(15)	C4	C5	1.376(3)
Co1	N2	2.1973(16)	C5	C6	1.396(3)
Co1	N3	2.1636(15)	C6	C7	1.497(3)
Co1	N4	2.2249(16)	C8	C9	1.526(3)
Co1	N5	2.1525(16)	C10	C11	1.508(3)
Co1	N6	2.2031(15)	C11	C12	1.379(3)
N1	C1	1.468(2)	C12	C13	1.385(3)
N1	C8	1.491(2)	C13	C14	1.378(3)
N1	C27	1.477(2)	C14	C15	1.393(3)
N2	C2	1.359(3)	C15	C16	1.498(3)
N2	C6	1.353(3)	C17	C18	1.521(3)
N3	C9	1.483(2)	C19	C20	1.497(3)
N3	C10	1.474(3)	C20	C21	1.383(3)
N3	C17	1.490(3)	C21	C22	1.382(4)
N4	C11	1.361(2)	C22	C23	1.371(4)
N4	C15	1.355(2)	C23	C24	1.397(3)
N5	C18	1.482(2)	C24	C25	1.488(4)
N5	C19	1.475(3)	C26	C27	1.527(3)
N5	C26	1.498(3)	O1	N7	1.248(2)
N6	C20	1.358(3)	O2	N7	1.233(3)
N6	C24	1.356(3)	O3	N7	1.252(3)
C1	C2	1.507(3)	O4	N8	1.259(3)
C2	C3	1.382(3)	O5	N8	1.256(4)
C3	C4	1.380(3)	O6	N8	1.198(3)

Table S18. Bond Angles for Co(MPT).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Co1	N2	79.11(6)	N1	C1	C2	110.49(15)
N1	Co1	N4	158.75(6)	N2	C2	C1	116.42(16)
N1	Co1	N6	96.71(6)	N2	C2	C3	122.93(18)
N2	Co1	N4	103.30(6)	C3	C2	C1	120.56(18)
N2	Co1	N6	103.16(6)	C4	C3	C2	119.2(2)
N3	Co1	N1	80.07(6)	C5	C4	C3	118.52(19)
N3	Co1	N2	95.56(7)	C4	C5	C6	120.2(2)
N3	Co1	N4	78.68(6)	N2	C6	C5	121.5(2)
N3	Co1	N6	160.08(7)	N2	C6	C7	119.0(2)
N5	Co1	N1	80.80(6)	C5	C6	C7	119.6(2)
N5	Co1	N2	159.91(6)	N1	C8	C9	111.62(15)
N5	Co1	N3	81.19(6)	N3	C9	C8	109.08(16)
N5	Co1	N4	95.53(6)	N3	C10	C11	109.86(16)
N5	Co1	N6	78.89(6)	N4	C11	C10	116.31(17)
N6	Co1	N4	103.15(6)	N4	C11	C12	123.58(18)
C1	N1	Co1	105.68(11)	C12	C11	C10	120.04(17)
C1	N1	C8	110.70(14)	C11	C12	C13	118.63(18)
C1	N1	C27	111.90(14)	C14	C13	C12	118.57(18)
C8	N1	Co1	111.07(11)	C13	C14	C15	120.45(18)
C27	N1	Co1	105.37(11)	N4	C15	C14	121.33(18)
C27	N1	C8	111.83(14)	N4	C15	C16	118.77(17)
C2	N2	Co1	110.90(12)	C14	C15	C16	119.90(17)
C6	N2	Co1	131.15(15)	N3	C17	C18	112.74(15)
C6	N2	C2	117.56(17)	N5	C18	C17	109.91(16)
C9	N3	Co1	106.25(11)	N5	C19	C20	110.48(16)
C9	N3	C17	111.61(16)	N6	C20	C19	116.69(17)
C10	N3	Co1	105.58(12)	N6	C20	C21	123.0(2)
C10	N3	C9	111.85(16)	C21	C20	C19	120.3(2)
C10	N3	C17	111.49(17)	C22	C21	C20	119.1(2)
C17	N3	Co1	109.73(12)	C23	C22	C21	118.5(2)
C11	N4	Co1	110.34(12)	C22	C23	C24	120.7(2)
C15	N4	Co1	131.76(13)	N6	C24	C23	120.8(2)
C15	N4	C11	117.34(16)	N6	C24	C25	118.99(19)
C18	N5	Co1	105.56(12)	C23	C24	C25	120.2(2)
C18	N5	C26	111.60(15)	N5	C26	C27	112.12(15)
C19	N5	Co1	105.43(12)	N1	C27	C26	109.72(15)

C19	N5	C18	111.73(16)	O1	N7	O3	120.7(2)
C19	N5	C26	111.72(16)	O2	N7	O1	119.8(2)
C26	N5	Co1	110.44(11)	O2	N7	O3	119.5(2)
C20	N6	Co1	110.65(12)	O5	N8	O4	119.8(2)
C24	N6	Co1	131.18(15)	O6	N8	O4	119.3(3)
C24	N6	C20	117.85(18)	O6	N8	O5	120.9(3)

Table S19. Torsion Angles for Co(MPT).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Co1	N1	C1	C2	44.62(16)	N4	Co1	N6	C24	105.44(18)
Co1	N1	C8	C9	-18.52(19)	N4	C11	C12	C13	-1.4(3)
Co1	N1	C27	C26	-49.74(16)	N5	Co1	N1	C1	150.50(12)
Co1	N2	C2	C1	13.4(2)	N5	Co1	N1	C8	-89.39(12)
Co1	N2	C2	C3	-170.07(15)	N5	Co1	N1	C27	31.88(11)
Co1	N2	C6	C5	169.22(18)	N5	Co1	N2	C2	8.5(3)
Co1	N2	C6	C7	-11.8(4)	N5	Co1	N2	C6	-164.08(19)
Co1	N3	C9	C8	-49.93(18)	N5	Co1	N3	C9	113.05(13)
Co1	N3	C10	C11	46.9(2)	N5	Co1	N3	C10	-128.02(14)
Co1	N3	C17	C18	-16.94(19)	N5	Co1	N3	C17	-7.76(12)
Co1	N4	C11	C10	14.3(2)	N5	Co1	N4	C11	89.43(14)
Co1	N4	C11	C12	-168.85(16)	N5	Co1	N4	C15	-81.50(18)
Co1	N4	C15	C14	167.65(15)	N5	Co1	N6	C20	11.88(13)
Co1	N4	C15	C16	-13.2(3)	N5	Co1	N6	C24	-161.40(19)
Co1	N5	C18	C17	-48.83(18)	N5	C19	C20	N6	-39.1(2)
Co1	N5	C19	C20	45.50(18)	N5	C19	C20	C21	143.93(19)
Co1	N5	C26	C27	-15.97(19)	N5	C26	C27	N1	44.9(2)
Co1	N6	C20	C19	10.6(2)	N6	Co1	N1	C1	72.95(12)
Co1	N6	C20	C21	-172.44(16)	N6	Co1	N1	C8	-166.94(12)
Co1	N6	C24	C23	170.71(15)	N6	Co1	N1	C27	-45.66(11)
Co1	N6	C24	C25	-10.1(3)	N6	Co1	N2	C2	-85.13(13)
N1	Co1	N2	C2	9.29(13)	N6	Co1	N2	C6	102.3(2)
N1	Co1	N2	C6	-163.3(2)	N6	Co1	N3	C9	113.16(19)
N1	Co1	N3	C9	30.93(13)	N6	Co1	N3	C10	-127.92(19)
N1	Co1	N3	C10	149.85(14)	N6	Co1	N3	C17	-7.6(2)
N1	Co1	N3	C17	-89.88(12)	N6	Co1	N4	C11	169.28(13)
N1	Co1	N4	C11	10.6(2)	N6	Co1	N4	C15	-1.65(19)
N1	Co1	N4	C15	-160.31(17)	N6	Co1	N5	C18	-149.21(13)
N1	Co1	N5	C18	112.03(12)	N6	Co1	N5	C19	-30.81(12)
N1	Co1	N5	C19	-129.58(13)	N6	Co1	N5	C26	90.03(13)
N1	Co1	N5	C26	-8.74(12)	N6	C20	C21	C22	-0.4(3)
N1	Co1	N6	C20	91.10(13)	C1	N1	C8	C9	98.56(18)
N1	Co1	N6	C24	-82.19(18)	C1	N1	C27	C26	-164.10(15)
N1	C1	C2	N2	-40.5(2)	C1	C2	C3	C4	174.99(18)
N1	C1	C2	C3	142.81(17)	C2	N2	C6	C5	-3.0(3)
N1	C8	C9	N3	46.2(2)	C2	N2	C6	C7	176.0(2)

N2	Co1	N1	C1	-29.22(11)	C2	C3	C4	C5	-1.5(3)
N2	Co1	N1	C8	90.88(12)	C3	C4	C5	C6	2.1(3)
N2	Co1	N1	C27	-147.84(12)	C4	C5	C6	N2	0.1(4)
N2	Co1	N3	C9	-46.96(13)	C4	C5	C6	C7	-178.8(3)
N2	Co1	N3	C10	71.96(14)	C6	N2	C2	C1	-172.92(19)
N2	Co1	N3	C17	-167.77(12)	C6	N2	C2	C3	3.6(3)
N2	Co1	N4	C11	-83.53(14)	C8	N1	C1	C2	-75.72(18)
N2	Co1	N4	C15	105.54(18)	C8	N1	C27	C26	71.04(19)
N2	Co1	N5	C18	112.8(2)	C9	N3	C10	C11	162.01(17)
N2	Co1	N5	C19	-128.79(19)	C9	N3	C17	C18	-134.45(17)
N2	Co1	N5	C26	-8.0(3)	C10	N3	C9	C8	-164.65(17)
N2	Co1	N6	C20	171.43(13)	C10	N3	C17	C18	99.67(19)
N2	Co1	N6	C24	-1.85(19)	C10	C11	C12	C13	175.4(2)
N2	C2	C3	C4	-1.4(3)	C11	N4	C15	C14	-2.8(3)
N3	Co1	N1	C1	-126.91(12)	C11	N4	C15	C16	176.41(19)
N3	Co1	N1	C8	-6.81(12)	C11	C12	C13	C14	-1.6(3)
N3	Co1	N1	C27	114.47(11)	C12	C13	C14	C15	2.3(3)
N3	Co1	N2	C2	88.03(13)	C13	C14	C15	N4	-0.1(3)
N3	Co1	N2	C6	-84.5(2)	C13	C14	C15	C16	-179.3(2)
N3	Co1	N4	C11	9.58(13)	C15	N4	C11	C10	-173.33(19)
N3	Co1	N4	C15	-161.35(19)	C15	N4	C11	C12	3.5(3)
N3	Co1	N5	C18	30.76(12)	C17	N3	C9	C8	69.7(2)
N3	Co1	N5	C19	149.15(13)	C17	N3	C10	C11	-72.2(2)
N3	Co1	N5	C26	-90.01(13)	C18	N5	C19	C20	159.68(16)
N3	Co1	N6	C20	11.8(3)	C18	N5	C26	C27	-133.06(18)
N3	Co1	N6	C24	-161.51(18)	C19	N5	C18	C17	-162.93(16)
N3	C10	C11	N4	-42.6(3)	C19	N5	C26	C27	101.04(19)
N3	C10	C11	C12	140.4(2)	C19	C20	C21	C22	176.4(2)
N3	C17	C18	N5	45.0(2)	C20	N6	C24	C23	-2.2(3)
N4	Co1	N1	C1	-127.95(16)	C20	N6	C24	C25	176.97(19)
N4	Co1	N1	C8	-7.8(2)	C20	C21	C22	C23	-0.7(3)
N4	Co1	N1	C27	113.43(17)	C21	C22	C23	C24	0.4(3)
N4	Co1	N2	C2	167.69(13)	C22	C23	C24	N6	1.1(3)
N4	Co1	N2	C6	-4.9(2)	C22	C23	C24	C25	-178.0(2)
N4	Co1	N3	C9	-149.45(14)	C24	N6	C20	C19	-175.08(18)
N4	Co1	N3	C10	-30.53(13)	C24	N6	C20	C21	1.8(3)
N4	Co1	N3	C17	89.74(12)	C26	N5	C18	C17	71.2(2)
N4	Co1	N5	C18	-46.86(12)	C26	N5	C19	C20	-74.5(2)

N4	Co1	N5	C19	71.54(12)	C27	N1	C1	C2	158.80(15)
N4	Co1	N5	C26	-167.63(12)	C27	N1	C8	C9	-135.93(17)
N4	Co1	N6	C20	-81.27(13)					

Table S20. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Co(MPT).

Atom	*x*	*y*	*z*	U(eq)
H1A	7517	5874	935	28
H1B	6702	6164	809	28
H3	6028	5398	1613	32
H4	5794	5002	2774	38
H5	6610	5335	3667	45
H7A	8295	6156	3438	94
H7B	7745	5827	4015	94
H7C	7689	6680	3784	94
H8A	6326	7266	1019	28
H8B	6868	7939	846	28
H9A	6373	8229	1933	33
H9B	6489	7402	2224	33
H10A	7136	7688	3190	40
H10B	7201	8571	3103	40
H12	8085	8897	3969	31
H13	9271	8776	4433	32
H14	10019	7830	4004	35
H16A	9496	6419	2842	53
H16B	10135	6694	3354	53
H16C	10067	7027	2573	53
H17A	7666	9113	2167	37
H17B	7416	8789	1418	37
H18A	8636	9012	1286	34
H18B	8827	8659	2042	34
H19A	9652	7847	1696	36
H19B	9644	7952	855	36
H21	10383	6925	502	47
H22	10549	5636	420	58
H23	9771	4860	1051	53
H25A	8648	5353	2397	66
H25B	8861	4674	1892	66
H25C	8175	5185	1704	66
H26A	8664	7872	199	33
H26B	7952	8272	506	33
H27A	7525	7175	46	29
H27B	8184	6707	381	29

Table S21. Solvent masks information for Co(MPT).

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	0.000	0.000	223.8	64.2	?
2	0.000	0.500	0.500	223.8	64.2	?
3	0.500	0.000	0.500	223.8	64.2	?
4	0.500	0.500	0.000	223.8	64.2	?

Fe(TMPC)

Table S22. Crystal data and structure refinement for Fe(TMPC).

Identification code	Fe(TMPC)
Empirical formula	$C_{19}H_{24}F_3Fe_{0.5}N_4O_3S$
Formula weight	706.39
Temperature/K	90.0
Crystal system	triclinic
Space group	P-1
a/Å	9.439(2)
b/Å	14.994(3)
c/Å	16.128(3)
α/°	106.106(6)
β/°	102.699(6)
γ/°	91.165(6)
Volume/Å^3	2131.4(8)
Z	4
ρ_{calc}g/cm^3	2.201
μ/mm^{-1}	1.029
F(000)	1432.0
Crystal size/mm^3	0.4 × 0.04 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.3 to 52.86
Index ranges	-11 ≤ h ≤ 11, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	29477
Independent reflections	8571 [R_{int} = 0.1168, R_{sigma} = 0.1513]
Data/restraints/parameters	8571/0/554
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.1116, wR_2 = 0.2740
Final R indexes [all data]	R_1 = 0.1775, wR_2 = 0.3013
Largest diff. peak/hole / e Å^{-3}	1.30/-1.01

Table S23. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Fe(TMPC). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	2392.7(13)	2611.2(9)	2596.3(9)	14.5(3)
S2	2287(2)	4933.9(16)	6827.9(16)	19.3(5)
S3	4569(3)	861.8(17)	8646.8(17)	21.6(5)
F4	2319(7)	3598(4)	7574(4)	38.6(16)
F5	2736(7)	3168(4)	6280(4)	33.6(14)
F6	4403(6)	3982(4)	7393(5)	39.4(16)
O7	5681(7)	620(5)	8160(5)	25.7(16)
O8	3144(7)	5138(5)	6256(5)	26.2(16)
F9	4445(8)	2383(4)	8151(5)	44.0(17)
O10	5103(7)	1422(5)	9554(5)	30.3(17)
F11	2889(8)	1260(5)	7284(4)	49.9(19)
O12	2548(8)	5598(5)	7699(5)	33.6(18)
F13	2545(7)	2021(5)	8544(5)	42.0(17)
O14	770(7)	4656(5)	6396(5)	29.8(17)
N15	2781(7)	3754(5)	3849(5)	15.2(16)
N16	935(8)	2160(5)	3370(5)	16.2(16)
N17	4359(8)	2068(5)	3451(5)	17.1(16)
O18	3455(7)	117(5)	8497(5)	33.9(18)
N19	946(8)	1870(5)	1311(5)	17.5(17)
N20	2270(9)	5061(6)	695(6)	25.1(19)
N21	2364(8)	3944(5)	2099(5)	17.8(17)
N22	3876(8)	2239(5)	1703(5)	16.5(16)
C23	2963(10)	3869(7)	7042(7)	23(2)
C24	5285(9)	1095(7)	4513(6)	20(2)
C25	4025(10)	1364(7)	3927(6)	19(2)
C26	-592(10)	1154(7)	3780(7)	25(2)
C27	936(10)	983(6)	-173(6)	21(2)
C28	1385(9)	3819(7)	4132(6)	19(2)
C29	1634(9)	1404(6)	715(6)	15.4(19)
C30	5933(10)	305(7)	4214(7)	21(2)
C31	2402(10)	4783(6)	2877(6)	19(2)
C32	7485(11)	615(7)	5655(7)	27(2)
C33	6807(11)	1434(7)	5919(7)	26(2)
C34	5388(9)	2131(7)	2176(7)	23(2)

C35	-811(10)	1878(7)	4467(6)	22(2)
C36	704(9)	2884(6)	4045(6)	16.6(19)
N37	5705(8)	1667(6)	5354(5)	22.8(18)
C38	3246(10)	4650(6)	3728(6)	19(2)
C39	490(10)	526(7)	2470(6)	22(2)
C40	281(9)	1297(7)	3239(6)	22(2)
C41	3807(10)	3914(7)	1865(6)	20(2)
C42	3940(10)	2981(6)	1256(6)	20(2)
C43	-518(9)	1913(6)	1060(6)	19(2)
C44	1183(10)	4006(7)	1334(7)	23(2)
C45	7048(10)	38(7)	4796(7)	27(2)
C46	5356(10)	1658(7)	2883(6)	21(2)
C47	-549(11)	1033(7)	-417(6)	24(2)
C48	2384(12)	5899(7)	525(7)	30(2)
C49	-149(10)	2763(7)	4604(7)	21(2)
C50	1219(10)	4936(7)	1113(6)	21(2)
C51	-1273(10)	2457(7)	1738(7)	25(2)
C52	5041(9)	2953(6)	4096(6)	16.5(19)
C53	7236(13)	2049(9)	6849(7)	38(3)
C54	-1287(10)	1477(6)	192(6)	20(2)
C55	3574(12)	1675(8)	8139(8)	35(3)
C56	1455(13)	6582(7)	761(7)	35(3)
C57	3913(10)	3492(7)	4521(6)	20(2)
C58	386(12)	6423(8)	1168(7)	35(3)
C59	3544(13)	6015(8)	55(8)	41(3)
C60	245(11)	5570(7)	1336(7)	26(2)
C61	3242(9)	1342(6)	1053(6)	16.7(19)

Table S24. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Fe(TMPC). 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	11.2(6)	15.2(7)	19.4(7)	6.1(5)	7.0(5)	2.6(5)
S2	18.8(11)	17.6(12)	24.0(13)	6.3(10)	9.7(10)	5.1(9)
S3	19.3(12)	22.4(13)	28.1(14)	11.0(11)	10.6(10)	7(1)
F4	47(4)	42(4)	44(4)	26(3)	28(3)	17(3)
F5	39(4)	23(3)	39(4)	5(3)	13(3)	7(3)
F6	22(3)	38(4)	56(4)	20(3)	-5(3)	4(3)
O7	26(4)	23(4)	36(4)	15(3)	15(3)	10(3)
O8	22(3)	29(4)	29(4)	7(3)	10(3)	4(3)
F9	56(4)	24(3)	66(5)	25(3)	25(4)	18(3)
O10	26(4)	36(4)	32(4)	11(3)	12(3)	10(3)
F11	53(4)	55(5)	37(4)	12(4)	0(3)	26(4)
O12	45(5)	34(4)	26(4)	8(3)	16(4)	9(4)
F13	43(4)	40(4)	56(4)	21(3)	27(3)	29(3)
O14	17(3)	29(4)	47(5)	18(4)	5(3)	6(3)
N15	11(4)	19(4)	19(4)	11(3)	4(3)	5(3)
N16	12(4)	19(4)	17(4)	5(3)	3(3)	4(3)
N17	14(4)	15(4)	27(4)	12(3)	8(3)	3(3)
O18	19(4)	24(4)	54(5)	4(4)	7(3)	-1(3)
N19	13(4)	16(4)	30(5)	14(3)	9(3)	2(3)
N20	24(4)	22(4)	31(5)	11(4)	6(4)	1(3)
N21	11(4)	19(4)	26(4)	7(3)	10(3)	1(3)
N22	14(4)	19(4)	18(4)	5(3)	6(3)	7(3)
C23	20(5)	20(5)	32(6)	8(4)	8(4)	8(4)
C24	14(4)	27(5)	25(5)	11(4)	9(4)	-4(4)
C25	16(4)	24(5)	18(5)	9(4)	2(4)	-2(4)
C26	17(5)	32(6)	30(6)	14(5)	5(4)	-1(4)
C27	25(5)	11(5)	25(5)	3(4)	2(4)	-1(4)
C28	14(4)	23(5)	21(5)	6(4)	7(4)	6(4)
C29	19(4)	9(4)	27(5)	13(4)	13(4)	3(4)
C30	18(5)	21(5)	28(5)	13(4)	8(4)	4(4)
C31	13(4)	16(5)	29(5)	7(4)	3(4)	2(4)
C32	22(5)	23(5)	39(6)	18(5)	2(5)	-3(4)
C33	28(5)	27(6)	29(6)	17(5)	11(5)	-2(4)
C34	8(4)	32(6)	27(5)	8(5)	0(4)	1(4)
C35	19(5)	26(5)	25(5)	10(4)	12(4)	-1(4)

C36	14(4)	18(5)	21(5)	8(4)	7(4)	5(4)
N37	20(4)	31(5)	24(4)	15(4)	9(4)	2(4)
C38	19(5)	16(5)	27(5)	12(4)	10(4)	1(4)
C39	21(5)	19(5)	23(5)	-1(4)	6(4)	2(4)
C40	9(4)	30(6)	27(5)	12(4)	2(4)	6(4)
C41	18(5)	23(5)	23(5)	13(4)	5(4)	1(4)
C42	18(5)	23(5)	26(5)	14(4)	9(4)	-2(4)
C43	13(4)	14(5)	30(5)	10(4)	3(4)	-2(4)
C44	12(4)	25(5)	30(6)	5(4)	8(4)	4(4)
C45	18(5)	28(6)	42(6)	20(5)	11(5)	9(4)
C46	14(4)	26(5)	25(5)	11(4)	8(4)	2(4)
C47	27(5)	24(5)	18(5)	2(4)	4(4)	2(4)
C48	34(6)	28(6)	22(5)	2(5)	-1(5)	-2(5)
C49	19(5)	19(5)	29(5)	6(4)	13(4)	8(4)
C50	20(5)	19(5)	23(5)	5(4)	6(4)	2(4)
C51	8(4)	36(6)	30(6)	7(5)	5(4)	6(4)
C52	10(4)	22(5)	22(5)	12(4)	4(4)	3(4)
C53	39(7)	49(7)	24(6)	12(5)	1(5)	0(6)
C54	15(5)	21(5)	30(6)	14(4)	6(4)	7(4)
C55	26(6)	39(7)	48(7)	18(6)	18(5)	16(5)
C56	48(7)	20(6)	32(6)	15(5)	-8(5)	-3(5)
C57	18(5)	19(5)	20(5)	3(4)	1(4)	5(4)
C58	36(6)	34(6)	33(6)	10(5)	2(5)	9(5)
C59	46(7)	33(7)	44(7)	16(6)	6(6)	-8(5)
C60	30(5)	25(5)	31(6)	14(5)	15(5)	4(4)
C61	16(4)	20(5)	19(5)	9(4)	10(4)	8(4)

Table S25. Bond Lengths for Fe(TMPC).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	N15	2.210(8)	N21	C44	1.497(12)
Fe1	N16	2.256(7)	N22	C34	1.498(11)
Fe1	N17	2.360(7)	N22	C42	1.491(11)
Fe1	N19	2.193(8)	N22	C61	1.475(12)
Fe1	N21	2.348(8)	C24	C25	1.486(13)
Fe1	N22	2.195(7)	C24	C30	1.360(13)
S2	O8	1.440(7)	C24	N37	1.355(12)
S2	O12	1.444(7)	C26	C35	1.376(14)
S2	O14	1.444(7)	C26	C40	1.378(13)
S2	C23	1.824(10)	C27	C29	1.397(13)
S3	O7	1.438(7)	C27	C47	1.380(13)
S3	O10	1.442(8)	C28	C36	1.488(13)
S3	O18	1.449(7)	C29	C61	1.509(12)
S3	C55	1.817(11)	C30	C45	1.393(13)
F4	C23	1.298(11)	C31	C38	1.495(13)
F5	C23	1.349(11)	C32	C33	1.401(15)
F6	C23	1.340(11)	C32	C45	1.380(15)
F9	C55	1.322(13)	C33	N37	1.345(13)
F11	C55	1.350(14)	C33	C53	1.489(15)
F13	C55	1.323(12)	C34	C46	1.506(13)
N15	C28	1.484(11)	C35	C49	1.395(13)
N15	C38	1.482(11)	C36	C49	1.377(12)
N15	C57	1.487(11)	C39	C40	1.494(13)
N16	C36	1.367(11)	C41	C42	1.496(13)
N16	C40	1.363(12)	C43	C51	1.497(13)
N17	C25	1.532(11)	C43	C54	1.393(13)
N17	C46	1.481(11)	C44	C50	1.532(13)
N17	C52	1.471(11)	C47	C54	1.360(13)
N19	C29	1.325(11)	C48	C56	1.388(16)
N19	C43	1.360(11)	C48	C59	1.495(15)
N20	C48	1.366(13)	C50	C60	1.368(13)
N20	C50	1.353(12)	C52	C57	1.518(12)
N21	C31	1.504(12)	C56	C58	1.369(16)
N21	C41	1.490(11)	C58	C60	1.388(15)

Table S26. Bond Angles for Fe(TMPC).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N15	Fe1	N16	76.0(3)	F4	C23	F6	108.5(8)
N15	Fe1	N17	80.3(3)	F5	C23	S2	110.7(7)
N15	Fe1	N21	77.6(3)	F6	C23	S2	111.3(7)
N16	Fe1	N17	88.2(3)	F6	C23	F5	106.7(8)
N16	Fe1	N21	129.0(3)	C30	C24	C25	121.0(9)
N19	Fe1	N15	149.0(3)	N37	C24	C25	115.9(8)
N19	Fe1	N16	93.0(3)	N37	C24	C30	123.1(9)
N19	Fe1	N17	128.9(3)	C24	C25	N17	116.8(7)
N19	Fe1	N21	88.0(3)	C35	C26	C40	120.6(9)
N19	Fe1	N22	76.2(3)	C47	C27	C29	117.3(9)
N21	Fe1	N17	128.7(3)	N15	C28	C36	111.6(7)
N22	Fe1	N15	126.8(3)	N19	C29	C27	123.0(8)
N22	Fe1	N16	148.8(3)	N19	C29	C61	115.9(8)
N22	Fe1	N17	77.0(3)	C27	C29	C61	121.1(8)
N22	Fe1	N21	80.4(3)	C24	C30	C45	119.6(10)
O8	S2	O12	114.8(4)	C38	C31	N21	111.9(7)
O8	S2	O14	113.9(4)	C45	C32	C33	120.2(9)
O8	S2	C23	104.0(4)	C32	C33	C53	120.8(10)
O12	S2	C23	104.1(5)	N37	C33	C32	121.1(10)
O14	S2	O12	115.0(4)	N37	C33	C53	117.9(9)
O14	S2	C23	103.0(4)	N22	C34	C46	111.0(7)
O7	S3	O10	114.5(4)	C26	C35	C49	119.0(8)
O7	S3	O18	115.1(4)	N16	C36	C28	116.7(8)
O7	S3	C55	103.4(4)	N16	C36	C49	122.0(8)
O10	S3	O18	116.1(5)	C49	C36	C28	121.3(8)
O10	S3	C55	102.3(5)	C33	N37	C24	118.1(9)
O18	S3	C55	102.8(5)	N15	C38	C31	111.9(7)
C28	N15	Fe1	106.5(5)	N16	C40	C26	120.7(9)
C28	N15	C57	109.6(7)	N16	C40	C39	118.0(8)
C38	N15	Fe1	111.5(5)	C26	C40	C39	121.3(9)
C38	N15	C28	110.4(7)	N21	C41	C42	110.7(7)
C38	N15	C57	110.7(7)	N22	C42	C41	110.7(7)
C57	N15	Fe1	108.0(5)	N19	C43	C51	118.1(8)
C36	N16	Fe1	112.3(6)	N19	C43	C54	120.9(9)
C40	N16	Fe1	128.8(6)	C54	C43	C51	121.0(8)
C40	N16	C36	118.8(8)	N21	C44	C50	115.1(8)

C25	N17	Fe1	118.5(5)	C32	C45	C30	117.7(9)
C46	N17	Fe1	109.0(5)	N17	C46	C34	112.4(8)
C46	N17	C25	107.9(7)	C54	C47	C27	120.6(9)
C52	N17	Fe1	100.2(5)	N20	C48	C56	121.5(10)
C52	N17	C25	110.7(7)	N20	C48	C59	115.4(10)
C52	N17	C46	110.2(7)	C56	C48	C59	123.1(10)
C29	N19	Fe1	114.1(6)	C36	C49	C35	118.8(9)
C29	N19	C43	118.8(8)	N20	C50	C44	114.8(8)
C43	N19	Fe1	126.8(6)	N20	C50	C60	124.4(9)
C50	N20	C48	116.6(9)	C60	C50	C44	120.8(8)
C31	N21	Fe1	108.3(5)	N17	C52	C57	110.4(7)
C41	N21	Fe1	99.2(5)	C47	C54	C43	119.2(9)
C41	N21	C31	109.3(7)	F9	C55	S3	111.8(7)
C41	N21	C44	110.7(7)	F9	C55	F11	107.4(9)
C44	N21	Fe1	119.9(5)	F9	C55	F13	107.7(9)
C44	N21	C31	108.8(7)	F11	C55	S3	111.7(8)
C34	N22	Fe1	112.9(5)	F13	C55	S3	112.0(8)
C42	N22	Fe1	108.6(5)	F13	C55	F11	106.0(9)
C42	N22	C34	109.0(7)	C58	C56	C48	120.3(10)
C61	N22	Fe1	105.9(5)	N15	C57	C52	111.1(7)
C61	N22	C34	109.4(7)	C56	C58	C60	119.0(10)
C61	N22	C42	111.0(7)	C50	C60	C58	118.2(9)
F4	C23	S2	112.0(7)	N22	C61	C29	108.8(7)
F4	C23	F5	107.5(8)				

Table S27. Torsion Angles for Fe(TMPC).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Fe1	N15	C28	C36	44.7(8)	N19	C43	C54	C47	-2.5(13)
Fe1	N15	C38	C31	41.2(8)	N20	C48	C56	C58	-0.6(16)
Fe1	N15	C57	C52	35.4(8)	N20	C50	C60	C58	-3.7(16)
Fe1	N16	C36	C28	2.1(9)	N21	Fe1	N15	C28	103.4(6)
Fe1	N16	C36	C49	-179.7(7)	N21	Fe1	N15	C38	-17.1(5)
Fe1	N16	C40	C26	-179.5(6)	N21	Fe1	N15	C57	-139.0(6)
Fe1	N16	C40	C39	-2.0(12)	N21	Fe1	N16	C36	-43.2(7)
Fe1	N17	C25	C24	-175.5(6)	N21	Fe1	N16	C40	135.9(7)
Fe1	N17	C46	C34	31.9(9)	N21	Fe1	N17	C25	161.6(6)
Fe1	N17	C52	C57	51.2(7)	N21	Fe1	N17	C46	-74.5(6)
Fe1	N19	C29	C27	-171.8(6)	N21	Fe1	N17	C52	41.1(6)
Fe1	N19	C29	C61	8.6(9)	N21	Fe1	N19	C29	94.7(6)
Fe1	N19	C43	C51	-5.2(11)	N21	Fe1	N19	C43	-79.4(7)
Fe1	N19	C43	C54	173.7(6)	N21	Fe1	N22	C34	117.2(6)
Fe1	N21	C31	C38	32.2(8)	N21	Fe1	N22	C42	-3.8(5)
Fe1	N21	C41	C42	52.6(8)	N21	Fe1	N22	C61	-123.1(5)
Fe1	N21	C44	C50	175.9(6)	N21	C31	C38	N15	-49.7(10)
Fe1	N22	C34	C46	39.4(9)	N21	C41	C42	N22	-63.0(10)
Fe1	N22	C42	C41	34.0(8)	N21	C44	C50	N20	75.2(10)
Fe1	N22	C61	C29	46.8(7)	N21	C44	C50	C60	-104.7(10)
O7	S3	C55	F9	-55.2(9)	N22	Fe1	N15	C28	171.2(5)
O7	S3	C55	F11	65.2(8)	N22	Fe1	N15	C38	50.7(6)
O7	S3	C55	F13	-176.1(8)	N22	Fe1	N15	C57	-71.2(6)
O8	S2	C23	F4	178.4(7)	N22	Fe1	N16	C36	158.9(6)
O8	S2	C23	F5	-61.8(7)	N22	Fe1	N16	C40	-21.9(10)
O8	S2	C23	F6	56.7(8)	N22	Fe1	N17	C25	-132.2(6)
O10	S3	C55	F9	64.0(9)	N22	Fe1	N17	C46	-8.3(5)
O10	S3	C55	F11	-175.6(7)	N22	Fe1	N17	C52	107.3(5)
O10	S3	C55	F13	-57.0(9)	N22	Fe1	N19	C29	14.0(6)
O12	S2	C23	F4	57.7(8)	N22	Fe1	N19	C43	-160.0(7)
O12	S2	C23	F5	177.6(6)	N22	Fe1	N21	C31	-139.3(5)
O12	S2	C23	F6	-63.9(8)	N22	Fe1	N21	C41	-25.3(5)
O14	S2	C23	F4	-62.6(8)	N22	Fe1	N21	C44	95.1(6)
O14	S2	C23	F5	57.3(7)	N22	C34	C46	N17	-47.8(11)
O14	S2	C23	F6	175.8(7)	C24	C30	C45	C32	-2.2(13)
N15	Fe1	N16	C36	17.6(6)	C25	N17	C46	C34	161.9(7)

N15	Fe1	N16	C40	-163.3(8)	C25	N17	C52	C57	-74.8(9)
N15	Fe1	N17	C25	96.2(6)	C25	C24	C30	C45	-175.7(8)
N15	Fe1	N17	C46	-139.9(6)	C25	C24	N37	C33	177.5(8)
N15	Fe1	N17	C52	-24.2(5)	C26	C35	C49	C36	0.0(14)
N15	Fe1	N19	C29	156.2(6)	C27	C29	C61	N22	142.1(8)
N15	Fe1	N19	C43	-17.9(10)	C27	C47	C54	C43	2.5(14)
N15	Fe1	N21	C31	-8.1(5)	C28	N15	C38	C31	-77.0(9)
N15	Fe1	N21	C41	105.9(5)	C28	N15	C57	C52	151.0(7)
N15	Fe1	N21	C44	-133.7(6)	C28	C36	C49	C35	177.2(9)
N15	Fe1	N22	C34	50.7(7)	C29	N19	C43	C51	-179.0(8)
N15	Fe1	N22	C42	-70.3(6)	C29	N19	C43	C54	-0.1(12)
N15	Fe1	N22	C61	170.4(5)	C29	C27	C47	C54	-0.1(14)
N15	C28	C36	N16	-32.2(11)	C30	C24	C25	N17	-96.6(10)
N15	C28	C36	C49	149.7(8)	C30	C24	N37	C33	-0.7(13)
N16	Fe1	N15	C28	-32.6(5)	C31	N21	C41	C42	165.8(7)
N16	Fe1	N15	C38	-153.1(6)	C31	N21	C44	C50	50.5(10)
N16	Fe1	N15	C57	85.0(6)	C32	C33	N37	C24	-1.2(13)
N16	Fe1	N17	C25	20.2(6)	C33	C32	C45	C30	0.4(14)
N16	Fe1	N17	C46	144.0(6)	C34	N22	C42	C41	-89.4(9)
N16	Fe1	N17	C52	-100.3(5)	C34	N22	C61	C29	168.8(7)
N16	Fe1	N19	C29	-136.4(6)	C35	C26	C40	N16	-0.5(14)
N16	Fe1	N19	C43	49.6(7)	C35	C26	C40	C39	-177.9(9)
N16	Fe1	N21	C31	52.1(6)	C36	N16	C40	C26	-0.4(13)
N16	Fe1	N21	C41	166.1(5)	C36	N16	C40	C39	177.1(8)
N16	Fe1	N21	C44	-73.5(7)	N37	C24	C25	N17	85.1(10)
N16	Fe1	N22	C34	-80.1(8)	N37	C24	C30	C45	2.5(14)
N16	Fe1	N22	C42	158.9(5)	C38	N15	C28	C36	165.9(7)
N16	Fe1	N22	C61	39.6(8)	C38	N15	C57	C52	-87.0(9)
N16	C36	C49	C35	-0.8(14)	C40	N16	C36	C28	-177.1(8)
N17	Fe1	N15	C28	-123.2(6)	C40	N16	C36	C49	1.0(13)
N17	Fe1	N15	C38	116.3(6)	C40	C26	C35	C49	0.7(14)
N17	Fe1	N15	C57	-5.6(5)	C41	N21	C31	C38	-74.9(9)
N17	Fe1	N16	C36	98.0(6)	C41	N21	C44	C50	-69.6(10)
N17	Fe1	N16	C40	-82.8(7)	C42	N22	C34	C46	160.1(8)
N17	Fe1	N19	C29	-46.2(7)	C42	N22	C61	C29	-70.9(8)
N17	Fe1	N19	C43	139.7(7)	C43	N19	C29	C27	2.7(12)
N17	Fe1	N21	C31	-74.6(6)	C43	N19	C29	C61	-176.8(7)
N17	Fe1	N21	C41	39.4(6)	C44	N21	C31	C38	164.1(7)

N17	Fe1	N21	C44	159.8(6)	C44	N21	C41	C42	-74.4(9)
N17	Fe1	N22	C34	-16.5(6)	C44	C50	C60	C58	176.2(9)
N17	Fe1	N22	C42	-137.4(6)	C45	C32	C33	N37	1.3(14)
N17	Fe1	N22	C61	103.3(5)	C45	C32	C33	C53	178.3(9)
N17	C52	C57	N15	-63.2(9)	C46	N17	C25	C24	60.1(10)
O18	S3	C55	F9	-175.3(8)	C46	N17	C52	C57	166.0(7)
O18	S3	C55	F11	-54.9(8)	C47	C27	C29	N19	-2.6(13)
O18	S3	C55	F13	63.7(9)	C47	C27	C29	C61	176.9(8)
N19	Fe1	N15	C28	39.3(8)	C48	N20	C50	C44	-177.0(8)
N19	Fe1	N15	C38	-81.2(7)	C48	N20	C50	C60	2.9(15)
N19	Fe1	N15	C57	156.9(6)	C48	C56	C58	C60	-0.2(16)
N19	Fe1	N16	C36	-133.1(6)	C50	N20	C48	C56	-0.7(14)
N19	Fe1	N16	C40	46.0(8)	C50	N20	C48	C59	-179.5(9)
N19	Fe1	N17	C25	-72.3(7)	C51	C43	C54	C47	176.4(9)
N19	Fe1	N17	C46	51.6(6)	C52	N17	C25	C24	-60.6(10)
N19	Fe1	N17	C52	167.2(5)	C52	N17	C46	C34	-77.1(9)
N19	Fe1	N21	C31	144.3(5)	C53	C33	N37	C24	-178.2(8)
N19	Fe1	N21	C41	-101.7(5)	C56	C58	C60	C50	2.2(16)
N19	Fe1	N21	C44	18.8(6)	C57	N15	C28	C36	-71.9(9)
N19	Fe1	N22	C34	-152.6(6)	C57	N15	C38	C31	161.5(7)
N19	Fe1	N22	C42	86.4(6)	C59	C48	C56	C58	178.1(10)
N19	Fe1	N22	C61	-32.9(5)	C61	N22	C34	C46	-78.4(9)
N19	C29	C61	N22	-38.3(10)	C61	N22	C42	C41	150.1(7)

Table S28. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Fe(TMPC).

Atom	*x*	*y*	*z*	U(eq)
H25A	3342	1620	4283	23
H25B	3537	803	3481	23
H26	-1036	562	3679	30
H27	1451	680	-584	25
H28A	718	4124	3772	23
H28B	1560	4198	4746	23
H30	5633	-54	3625	25
H31A	2841	5323	2777	23
H31B	1412	4903	2925	23
H32	8231	459	6059	32
H34A	5920	2740	2446	28
H34B	5892	1767	1751	28
H35	-1393	1778	4836	26
H38A	4275	4668	3732	22
H38B	3112	5159	4221	22
H39A	-259	506	1953	33
H39B	436	-56	2605	33
H39C	1427	634	2358	33
H41A	4578	4042	2402	24
H41B	3918	4392	1578	24
H42A	3155	2847	726	24
H42B	4856	2988	1079	24
H44A	249	3898	1462	27
H44B	1250	3511	812	27
H45	7484	-510	4612	32
H46A	5048	1001	2602	25
H46B	6332	1706	3251	25
H47	-1050	761	-1003	29
H49	-282	3264	5064	26
H51A	-1659	2044	2011	38
H51B	-2055	2750	1456	38
H51C	-590	2925	2183	38
H52A	5483	3324	3798	20
H52B	5802	2829	4551	20
H53A	7016	1719	7244	57

H53B	6705	2594	6902	57
H53C	8262	2232	7002	57
H54	-2293	1489	31	25
H56	1559	7149	643	42
H57A	3454	3114	4804	24
H57B	4391	4051	4974	24
H58	-236	6879	1330	42
H59A	4452	5854	358	61
H59B	3647	6651	48	61
H59C	3279	5615	-544	61
H60	-492	5434	1593	31
H61A	3384	844	1331	20
H61B	3719	1207	563	20

Co(TMPC)

Table S29. Crystal data and structure refinement for Co(TMPC).

Identification code	Co(TMPC)
Empirical formula	$C_{36}H_{60}Cl_2CoN_8O_6$
Formula weight	830.75
Temperature/K	90.0
Crystal system	monoclinic
Space group	C2/c
a/Å	11.3586(7)
b/Å	14.8399(10)
c/Å	24.1643(16)
α/°	90.00
β/°	98.4869(10)
γ/°	90.00
Volume/Å^3	4028.5(5)
Z	4
ρ_{calc}g/cm^3	1.370
μ/mm^{-1}	0.613
F(000)	1764.0
Crystal size/mm^3	0.3 × 0.22 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.4 to 67.58
Index ranges	$-17 \leq h \leq 17$, $-23 \leq k \leq 23$, $-37 \leq l \leq 37$
Reflections collected	54363
Independent reflections	8083 [R_{int} = 0.0278, R_{sigma} = 0.0164]
Data/restraints/parameters	8083/0/263
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.0298, wR_2 = 0.0792
Final R indexes [all data]	R_1 = 0.0325, wR_2 = 0.0811
Largest diff. peak/hole / e Å^{-3}	0.75/-0.33

Table S30. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Co(TMPC). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Co1	5000	7551.43(10)	7500	6.86(4)
N1	5611.1(6)	6529.1(5)	6952.8(3)	8.74(11)
N2	3829.4(7)	8572.6(5)	5300.5(3)	10.71(12)
N3	6456.1(6)	8230.5(5)	7189.8(3)	8.05(11)
N4	3991.3(6)	8245.2(5)	6672.9(3)	8.04(11)
C1	7328.4(7)	7506.8(5)	7128.2(4)	10.22(13)
C2	6691.5(7)	6731.5(5)	6814.1(3)	9.32(12)
C3	7184.9(8)	6276.3(6)	6402.7(4)	12.27(14)
C4	6541.0(8)	5571.1(6)	6126.2(4)	13.84(14)
C5	5452.8(8)	5332.5(6)	6280.3(4)	12.74(14)
C6	4999.6(7)	5826.3(5)	6693.3(3)	10.13(13)
C7	3821.3(8)	5581.1(6)	6861.8(4)	13.54(14)
C8	6071.5(7)	8650.6(6)	6632.6(3)	9.90(13)
C9	4812.3(7)	9001.2(5)	6601.4(3)	9.58(13)
C10	3734.3(7)	7693.9(5)	6147.9(3)	9.34(12)
C11	3119.1(7)	8200.3(5)	5640.9(3)	9.19(12)
C12	1882.7(7)	8272.2(6)	5538.2(3)	11.48(13)
C13	1364.2(8)	8791.7(6)	5085.8(4)	14.03(14)
C14	2096.3(8)	9201.4(6)	4750.3(4)	14.96(15)
C15	3326.5(8)	9058.3(6)	4857.8(3)	12.76(14)
C16	4123.3(9)	9430.8(7)	4469.7(4)	19.35(17)
C17	2857.2(7)	8600.1(5)	6817.7(3)	9.68(13)
C18	2997.0(7)	8932.6(5)	7415.9(3)	9.77(13)
O2	6217.6(7)	7859.0(7)	5336.1(3)	24.64(16)
O1	8615.8(8)	8424.1(6)	5561.3(4)	26.74(17)
O4	5000	10810.3(8)	7500	35.1(3)
O3	0	8734.1(8)	7500	21.6(2)
Cl1	161.1(2)	7271.96(19)	6540.32(10)	20.92(5)

Table S31. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Co(TMPC). 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}
Co1	6.47(6)	5.87(6)	8.40(7)	0	1.56(5)	0
N1	8.0(3)	7.9(3)	10.0(3)	0.2(2)	0.5(2)	-0.2(2)
N2	13.1(3)	10.5(3)	8.4(3)	0.2(2)	0.8(2)	-1.6(2)
N3	8.3(3)	8.1(3)	7.7(3)	-0.5(2)	0.7(2)	-0.5(2)
N4	8.1(3)	7.4(3)	8.4(3)	-0.2(2)	0.5(2)	-0.4(2)
C1	7.3(3)	10.6(3)	12.7(3)	-2.5(2)	1.4(2)	-0.5(2)
C2	8.6(3)	8.7(3)	10.5(3)	-0.8(2)	1.1(2)	0.3(2)
C3	12.0(3)	12.0(3)	13.1(3)	-2.3(3)	2.9(3)	1.6(3)
C4	15.9(4)	12.0(3)	13.4(3)	-3.1(3)	1.5(3)	3.0(3)
C5	15.0(3)	8.6(3)	13.5(3)	-2.0(2)	-1.4(3)	0.6(3)
C6	10.9(3)	7.4(3)	11.1(3)	1.0(2)	-1.5(2)	-0.4(2)
C7	12.9(3)	13.1(3)	14.0(3)	1.2(3)	-0.2(3)	-4.7(3)
C8	9.8(3)	11.7(3)	8.2(3)	1.1(2)	0.9(2)	-2.1(2)
C9	11.0(3)	7.8(3)	9.5(3)	1.0(2)	0.2(2)	-1.8(2)
C10	11.1(3)	7.9(3)	8.5(3)	0.2(2)	-0.3(2)	-0.2(2)
C11	11.0(3)	8.0(3)	8.1(3)	-0.2(2)	-0.2(2)	-1.0(2)
C12	11.3(3)	12.6(3)	10.1(3)	-0.6(2)	-0.1(2)	-1.0(3)
C13	13.1(3)	15.3(4)	12.4(3)	-0.7(3)	-2.7(3)	1.4(3)
C14	18.9(4)	13.7(3)	10.9(3)	2.1(3)	-2.5(3)	0.8(3)
C15	17.7(4)	11.2(3)	8.9(3)	0.6(2)	0.1(3)	-2.3(3)
C16	24.4(4)	21.7(4)	12.1(4)	3.9(3)	3.1(3)	-5.7(3)
C17	8.0(3)	11.0(3)	9.6(3)	0.8(2)	-0.2(2)	2.2(2)
C18	10.3(3)	9.2(3)	9.5(3)	1.0(2)	0.4(2)	3.3(2)
O2	15.7(3)	38.0(5)	19.9(3)	-6.8(3)	1.6(3)	4.6(3)
O1	20.4(4)	29.3(4)	30.2(4)	1.5(3)	2.8(3)	-1.4(3)
O4	68(1)	12.3(5)	23.1(6)	0	1.1(6)	0
O3	16.3(4)	15.8(4)	32.0(6)	0	1.3(4)	0
Cl1	16.76(10)	28.77(12)	17.89(10)	-1.33(8)	4.75(8)	-8.54(8)

Table S32. Bond Lengths for Co(TMPC).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	N1	2.1915(7)	C1	C2	1.5037(11)
Co1	N1[1]	2.1915(7)	C2	C3	1.3868(11)
Co1	N3	2.1631(7)	C3	C4	1.3901(12)
Co1	N3[1]	2.1631(7)	C4	C5	1.3884(13)
Co1	N4	2.3857(7)	C5	C6	1.3963(12)
Co1	N4[1]	2.3857(7)	C6	C7	1.5001(12)
N1	C2	1.3528(10)	C8	C9	1.5133(12)
N1	C6	1.3546(10)	C10	C11	1.5170(11)
N2	C11	1.3522(11)	C11	C12	1.3937(11)
N2	C15	1.3452(11)	C12	C13	1.3951(12)
N3	C1	1.4835(11)	C13	C14	1.3846(13)
N3	C8	1.4894(10)	C14	C15	1.3993(13)
N3	C18[1]	1.4848(10)	C15	C16	1.5015(13)
N4	C9	1.4852(10)	C17	C18	1.5135(11)
N4	C10	1.5017(10)	C18	N3[1]	1.4849(10)
N4	C17	1.4805(10)			

[1]1-X,+Y,3/2-Z

Table S33. Bond Angles for Co(TMPC).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1[1]	Co1	N1	92.37(4)	C17	N4	Co1	106.42(5)
N1	Co1	N4[1]	130.43(2)	C17	N4	C9	110.00(6)
N1[1]	Co1	N4[1]	87.08(2)	C17	N4	C10	109.03(6)
N1	Co1	N4	87.08(2)	N3	C1	C2	109.02(6)
N1[1]	Co1	N4	130.43(2)	N1	C2	C1	115.55(7)
N3[1]	Co1	N1[1]	77.70(3)	N1	C2	C3	123.15(7)
N3[1]	Co1	N1	149.10(3)	C3	C2	C1	121.29(7)
N3	Co1	N1	77.70(3)	C2	C3	C4	118.14(8)
N3	Co1	N1[1]	149.10(3)	C5	C4	C3	119.29(8)
N3[1]	Co1	N3	124.47(4)	C4	C5	C6	119.64(8)
N3[1]	Co1	N4[1]	78.80(2)	N1	C6	C5	121.13(8)
N3	Co1	N4[1]	78.00(2)	N1	C6	C7	118.56(7)
N3	Co1	N4	78.81(2)	C5	C6	C7	120.30(7)
N3[1]	Co1	N4	78.00(2)	N3	C8	C9	109.76(6)
N4	Co1	N4[1]	128.86(3)	N4	C9	C8	109.85(6)
C2	N1	Co1	112.05(5)	N4	C10	C11	114.91(6)
C2	N1	C6	118.57(7)	N2	C11	C10	116.65(7)
C6	N1	Co1	128.75(6)	N2	C11	C12	122.44(7)
C15	N2	C11	118.76(8)	C12	C11	C10	120.91(7)
C1	N3	Co1	104.69(5)	C11	C12	C13	118.66(8)
C1	N3	C8	108.88(6)	C14	C13	C12	118.74(8)
C1	N3	C18[1]	110.48(6)	C13	C14	C15	119.62(8)
C8	N3	Co1	111.77(5)	N2	C15	C14	121.61(8)
C18[1]	N3	Co1	111.92(5)	N2	C15	C16	118.01(8)
C18[1]	N3	C8	109.00(6)	C14	C15	C16	120.37(8)
C9	N4	Co1	101.03(4)	N4	C17	C18	111.67(6)
C9	N4	C10	111.12(6)	N3[1]	C18	C17	111.05(6)
C10	N4	Co1	118.82(5)				

[1]1-X,+Y,3/2-Z

Table S34. Torsion Angles for Co(TMPC).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Co1	N1	C2	C1	9.58(8)	$N4^1$	Co1	N1	C6	141.46(6)
Co1	N1	C2	C3	-169.06(7)	N4	Co1	N1	C6	-77.10(7)
Co1	N1	C6	C5	168.41(6)	N4	Co1	N3	C1	-123.45(5)
Co1	N1	C6	C7	-12.07(11)	$N4^1$	Co1	N3	C1	102.44(5)
Co1	N3	C1	C2	49.03(7)	N4	Co1	N3	C8	-5.74(5)
Co1	N3	C8	C9	35.30(7)	$N4^1$	Co1	N3	C8	-139.85(5)
Co1	N4	C9	C8	50.38(6)	$N4^1$	Co1	N3	$C18^1$	-17.26(5)
Co1	N4	C10	C11	-178.49(5)	N4	Co1	N3	$C18^1$	116.85(5)
Co1	N4	C17	C18	34.62(7)	$N4^1$	Co1	N4	C9	40.55(4)
$N1^1$	Co1	N1	C2	-136.10(6)	$N4^1$	Co1	N4	C10	162.30(6)
$N1^1$	Co1	N1	C6	53.27(6)	$N4^1$	Co1	N4	C17	-74.33(5)
N1	Co1	N3	C1	-34.02(5)	N4	C10	C11	N2	93.07(9)
$N1^1$	Co1	N3	C1	39.61(7)	N4	C10	C11	C12	-86.87(9)
$N1^1$	Co1	N3	C8	157.32(5)	N4	C17	C18	$N3^1$	-52.60(9)
N1	Co1	N3	C8	83.69(5)	C1	N3	C8	C9	150.47(6)
$N1^1$	Co1	N3	$C18^1$	-80.09(7)	C1	C2	C3	C4	-179.45(8)
N1	Co1	N3	$C18^1$	-153.72(5)	C2	N1	C6	C5	-1.69(12)
N1	Co1	N4	C9	-101.91(5)	C2	N1	C6	C7	177.83(7)
$N1^1$	Co1	N4	C9	167.46(4)	C2	C3	C4	C5	-1.76(13)
$N1^1$	Co1	N4	C10	-70.79(6)	C3	C4	C5	C6	2.62(13)
N1	Co1	N4	C10	19.84(6)	C4	C5	C6	N1	-0.90(12)
$N1^1$	Co1	N4	C17	52.58(6)	C4	C5	C6	C7	179.59(8)
N1	Co1	N4	C17	143.22(5)	C6	N1	C2	C1	-178.74(7)
N1	C2	C3	C4	-0.89(13)	C6	N1	C2	C3	2.62(12)
N2	C11	C12	C13	-3.85(12)	C8	N3	C1	C2	-70.64(8)
$N3^1$	Co1	N1	C2	154.13(5)	C9	N4	C10	C11	-61.96(9)
N3	Co1	N1	C2	14.35(5)	C9	N4	C17	C18	-74.01(8)
N3	Co1	N1	C6	-156.28(7)	C10	N4	C9	C8	-76.62(8)
$N3^1$	Co1	N1	C6	-16.49(10)	C10	N4	C17	C18	163.91(6)
$N3^1$	Co1	N3	C1	169.69(5)	C10	C11	C12	C13	176.09(8)
$N3^1$	Co1	N3	C8	-72.60(5)	C11	N2	C15	C14	1.41(12)
$N3^1$	Co1	N3	$C18^1$	49.99(5)	C11	N2	C15	C16	-177.25(8)
N3	Co1	N4	C9	-23.87(5)	C11	C12	C13	C14	1.22(13)
$N3^1$	Co1	N4	C9	105.32(5)	C12	C13	C14	C15	2.48(13)
$N3^1$	Co1	N4	C10	-132.93(6)	C13	C14	C15	N2	-3.92(13)
N3	Co1	N4	C10	97.88(6)	C13	C14	C15	C16	174.70(9)

N3	Co1	N4	C17	-138.75(5)	C15	N2	C11	C10	-177.42(7)
N3[1]	Co1	N4	C17	-9.56(5)	C15	N2	C11	C12	2.52(12)
N3	C1	C2	N1	-40.53(9)	C17	N4	C9	C8	162.55(6)
N3	C1	C2	C3	138.14(8)	C17	N4	C10	C11	59.44(8)
N3	C8	C9	N4	-60.89(8)	C18[1]	N3	C1	C2	169.69(6)
N4	Co1	N1	C2	93.52(6)	C18[1]	N3	C8	C9	-88.94(7)
N4[1]	Co1	N1	C2	-47.92(7)					

[1]1-X,+Y,3/2-Z

Table S35. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Co(TMPC).

Atom	*x*	*y*	*z*	U(eq)
H1A	7711	7303	7502	12
H1B	7956	7739	6922	12
H3	7942	6442	6312	15
H4	6842	5256	5835	17
H5	5019	4836	6106	15
H7A	3951	5216	7203	20
H7B	3353	5236	6561	20
H7C	3390	6132	6932	20
H8A	6108	8199	6334	12
H8B	6614	9153	6575	12
H9A	4777	9456	6898	11
H9B	4565	9295	6235	11
H10A	3229	7176	6221	11
H10B	4495	7449	6058	11
H12	1403	7973	5771	14
H13	525	8863	5009	17
H14	1765	9577	4449	18
H16A	4956	9319	4626	29
H16B	3991	10081	4426	29
H16C	3943	9136	4104	29
H17A	2247	8119	6765	12
H17B	2577	9102	6562	12
H18A	3503	9479	7454	12
H18B	2207	9098	7511	12
H2A	6185(18)	7512(12)	5080(9)	37
H2B	5547(17)	8044(13)	5305(8)	37
H1C	7915(18)	8340(13)	5535(8)	40
H1D	8923(17)	8119(14)	5851(8)	40
H4A	4852(19)	11105(14)	7757(8)	47(6)
H3A	32(15)	8381(11)	7225(7)	27(4)