Seven-Coordinate Co^{II}, Fe^{II} and Six-Coordinate Ni^{II} Amide-Appended Macrocyclic Complexes as ParaCEST Agents in Biological Media

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Additional experimental methods

The mass susceptibility of solute (χ_g) is typically calculated by obtaining the observed frequency shift of the reference (Δf) in Hz, the spectrometer frequency (f) in Hz, the mass of the substance per cm^3 of solution (m), and the mass susceptibility of solvent D_2O (χ_0= -0.6466 x 10^{-6} cm^3/g).[1] The last term is neglected here due to the minimal contribution to mass susceptibility of solute. The molar susceptibility (χ_m) is the product of χ_g multiplied by the molecular weight of the complex.[2,3]

Eq.S1 $\chi_g = (-3\Delta f)/(4\pi fm) + \chi_0 + [\chi_0 (d_0-d_s)]/m$

Eq. S2 $\mu_{eff} = 2.84 (\chi_m T)^{1/2}$

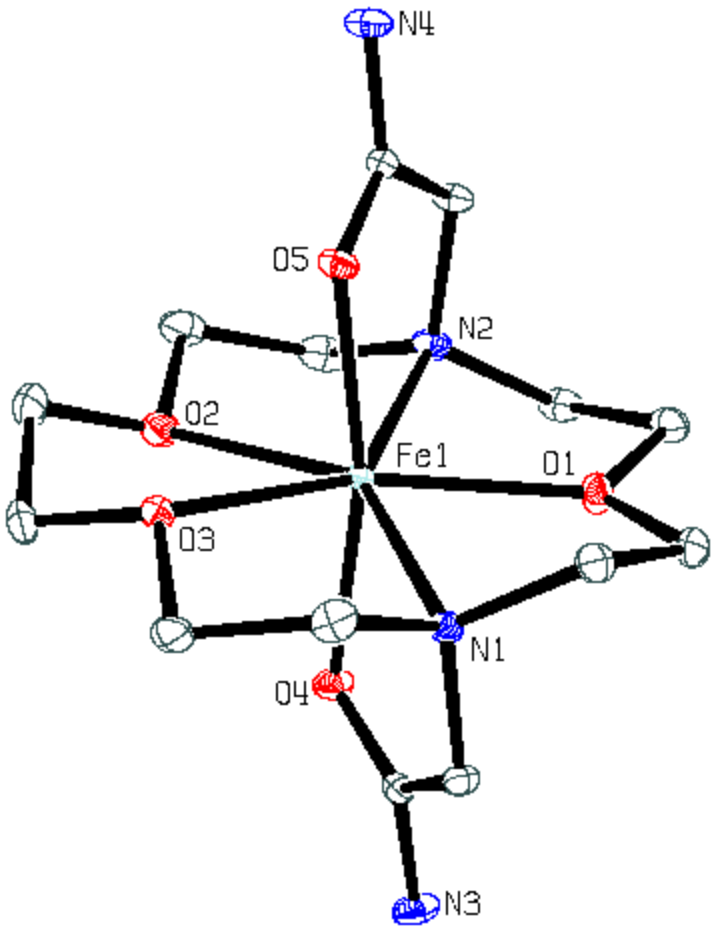

Figure S1. Ortep diagram (50% ellipsoids**)** of [Fe(**L**)]$(CF_3SO_3)_2$. For clarity, the H atoms, solvent, and counter ions were omitted in the structure.

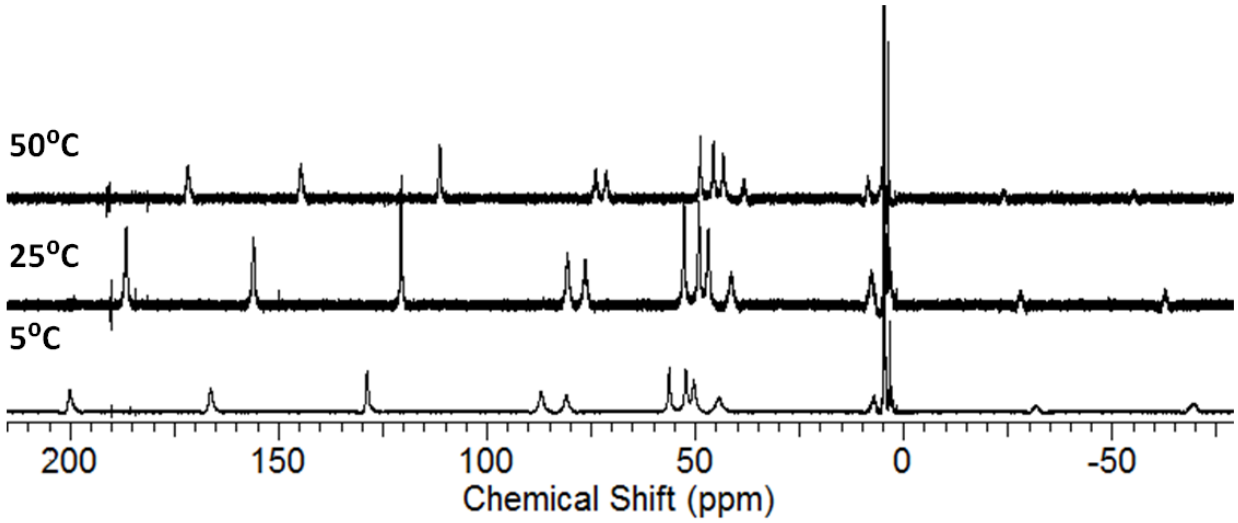

Figure S2. ^{1}H NMR spectra of 10 mM [Fe(**L**)]$^{2+}$at varying temperatures in D_2O.

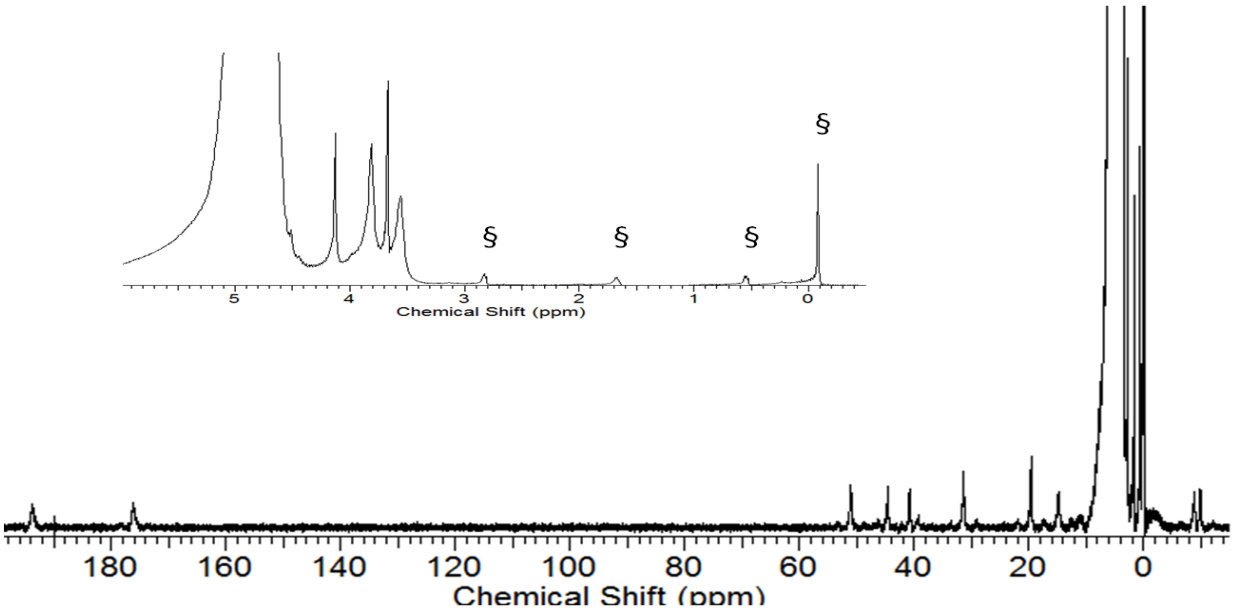

Figure S3. ^{1}H NMR spectra of 9.8 mM [Ni(**L**)]$^{2+}$, 100 mM NaCl, 3 mM 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (§) at pD 4.0 after 12 hours of incubation at 37 °C. Peaks at 3.5- 4.0 ppm represent newly formed free ligand in the acidic solution. The percent dissociation of [Ni(**L**)]$^{2+}$ was calculated by integrating peaks paramagnetic peaks at 176 and 193 ppm verses standard. Inset represents diamagnetic region.

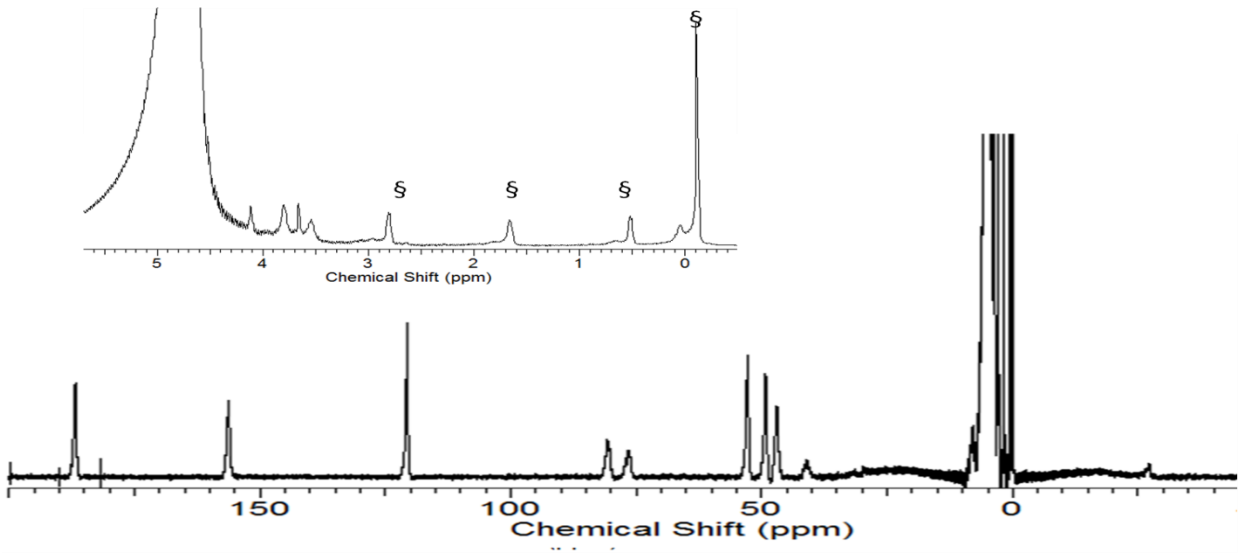

Figure S4. ^{1}H NMR spectra of 9.9 mM [Fe(**L**)]$^{2+}$, 100 mM NaCl, 5 mM 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (§) at pD 4.3 after 12 hours of incubation at 37°C. Inset represents diamagnetic region. Peaks at 3.5- 4.0 ppm represent newly formed free ligand in acidic solution.

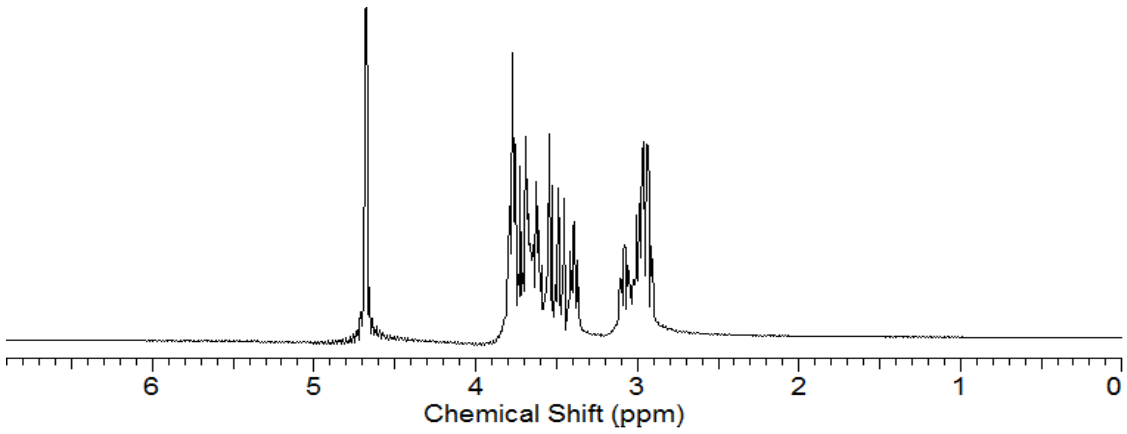

Figure S5. ^{1}H NMR spectrum of [Zn(**L**)]$^{2+}$ complex in D_2O

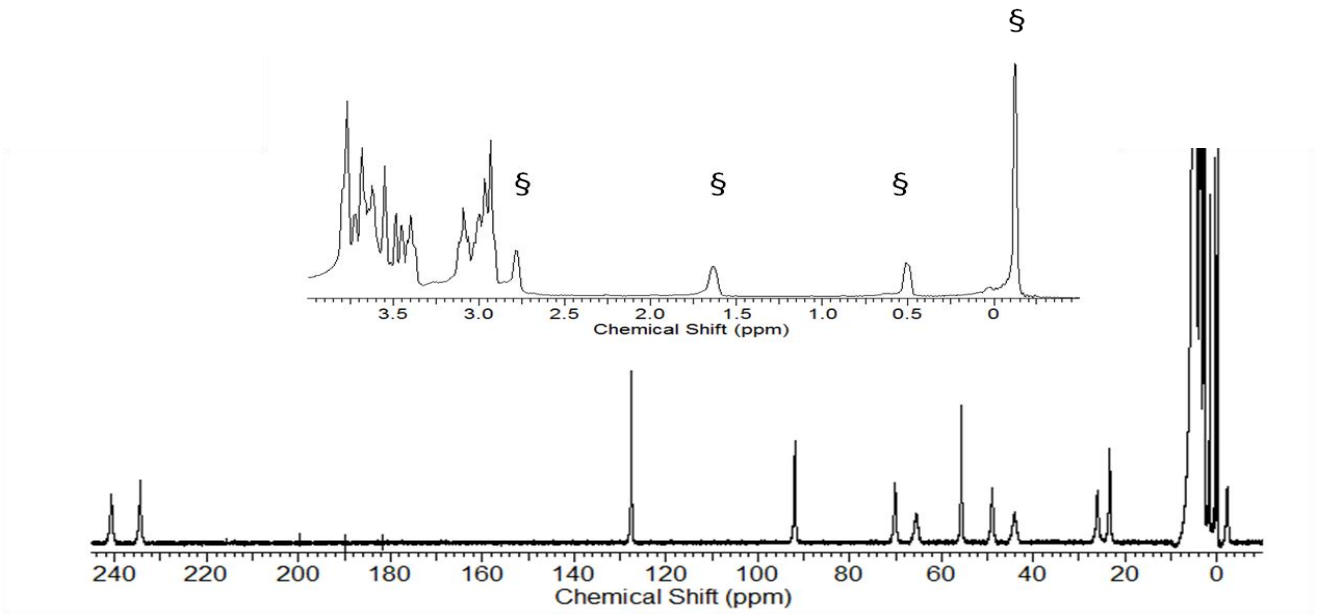

Figure S6. ^{1}H NMR spectra of 10 mM [Co(**L**)]$^{2+}$, 100 mM NaCl, 5mM 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (§) incubated with10 mM $ZnCl_2$ at pD 7.0 after 12 hours of incubation at 37°C. The percent dissociation of [Co(**L**)]$^{2+}$ was calculated by integrating peaks of the peaks at 234 and 241 ppm verses standard. Inset represents diamagnetic region.

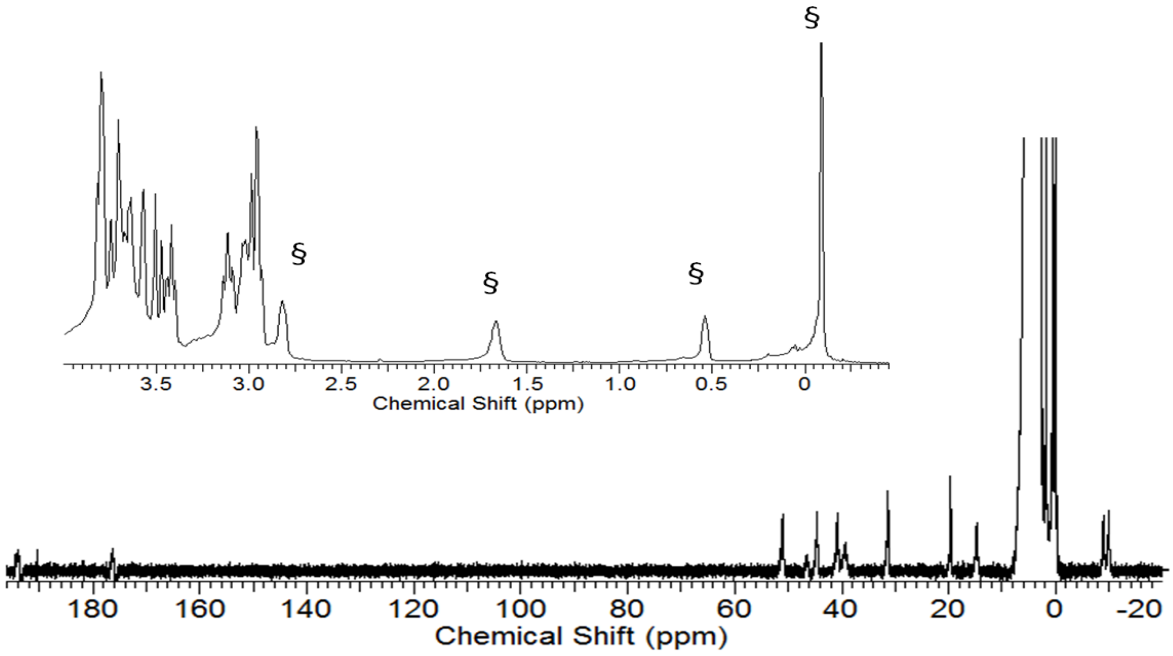

Figure S7. ^{1}H NMR spectra of 10 mM [Ni(**L**)]$^{2+}$, 100 mM NaCl , 5 mM 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (§), and 10 mM $ZnCl_2$ at pD 7.0 after 12 hours of incubation at 37°C. The percent dissociation of [Ni(**L**)]$^{2+}$ was calculated by integrating peaks of the peaks at 15 and 20 ppm verses standard. Inset represents diamagnetic region.

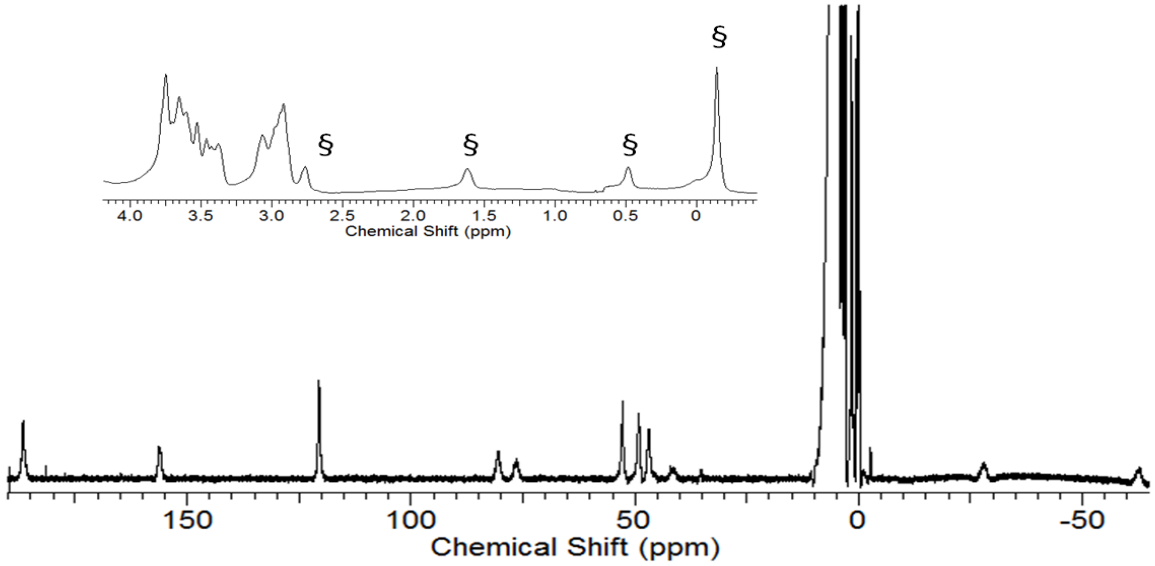

Figure S8. ^{1}H NMR spectra of 10 mM [Fe(**L**)]$^{2+}$, 100 mM NaCl , 5 mM 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (§), incubated with 10 mM $ZnCl_2$ at pD 7.0 after 12 hours of incubation at 37°C. Inset represents diamagnetic region.

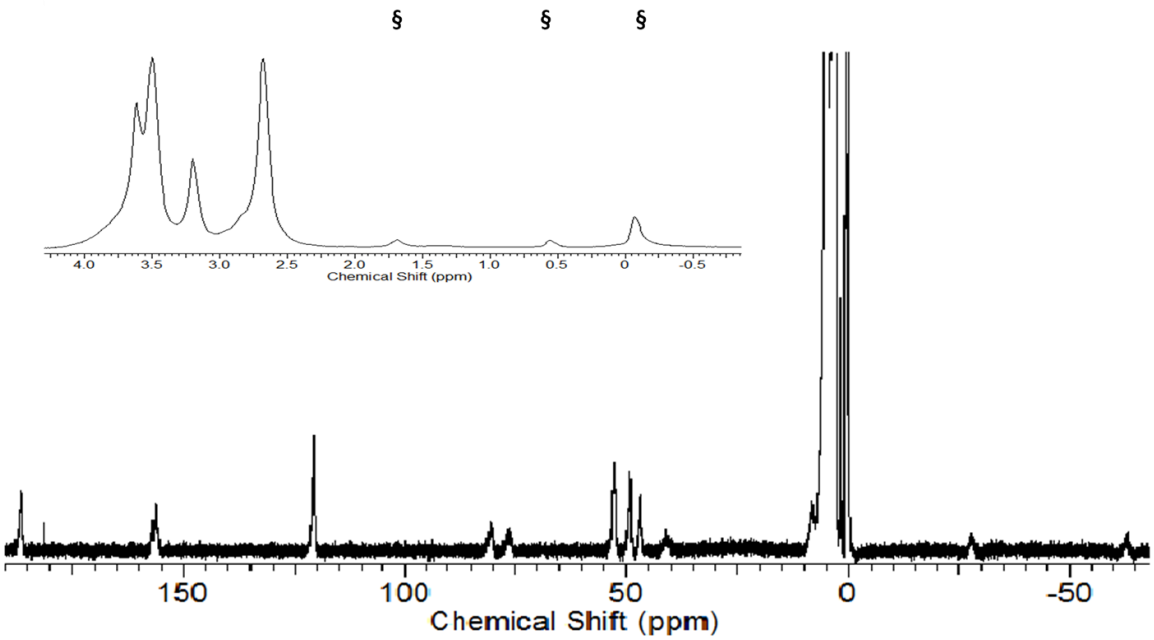

Figure S9. ^{1}H NMR spectra of 10 mM [Fe(**L**)]$^{2+}$, 100 mM NaCl, 0.4 mM Na_2HPO_4, 25 mM K_2CO_3, after 12 hours of incubation at 37°C. The 3 mM 3-(trimethylsilyl)-1-propanesulfonic acid sodium (§) salt was added as a reference. Initial spectrum showed no evidence for free ligand in solution. Inset represents diamagnetic region

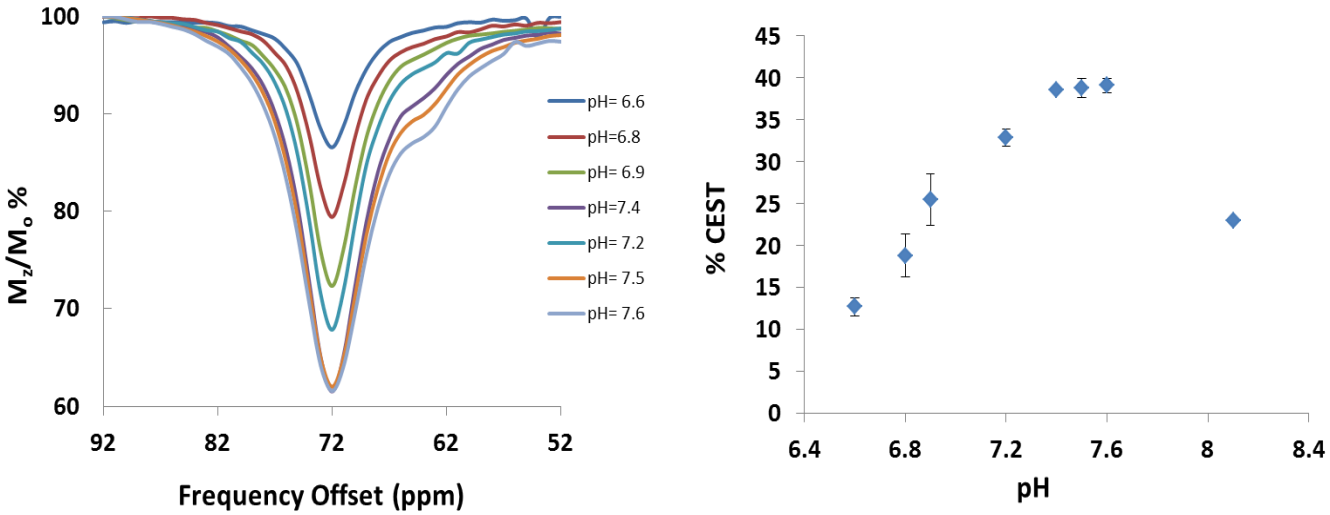

Figure S10. pH dependent CEST recorded at 11.7 T of solutions containing 10 mM $[Ni(\mathbf{L})]^{2+}$, 20 mM buffer pH 6.6-7.6, and 100 mM NaCl (left). Plot of the CEST effect for 10 mM $[Ni(\mathbf{L})]^{2+}$, 20 mM buffer pH 6.6-8.1 and 100 mM NaCl (right). RF presaturation pulse applied for 2 seconds B_1 =24 µT at 37 °C.

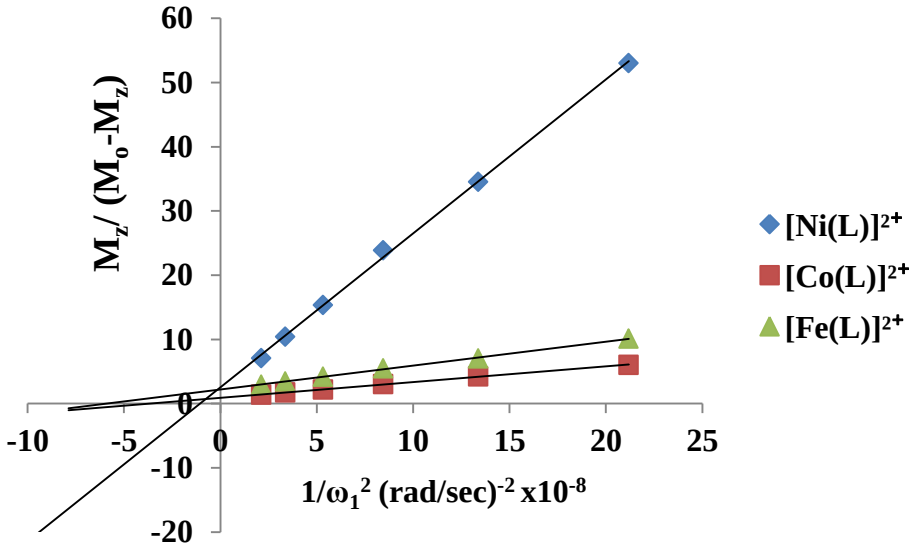

Figure S11. The plot of $M_z/(M_o-M_z)$ against the $1/\omega_1^2$ (rad/sec)$^{-2}$ x10^{-8} recorded at 11.7 T of 10 mM complex in egg white pH 7.3-7.5. RF presaturation pulse applied for 4 seconds with varying B_1 (8.2-24 µT)

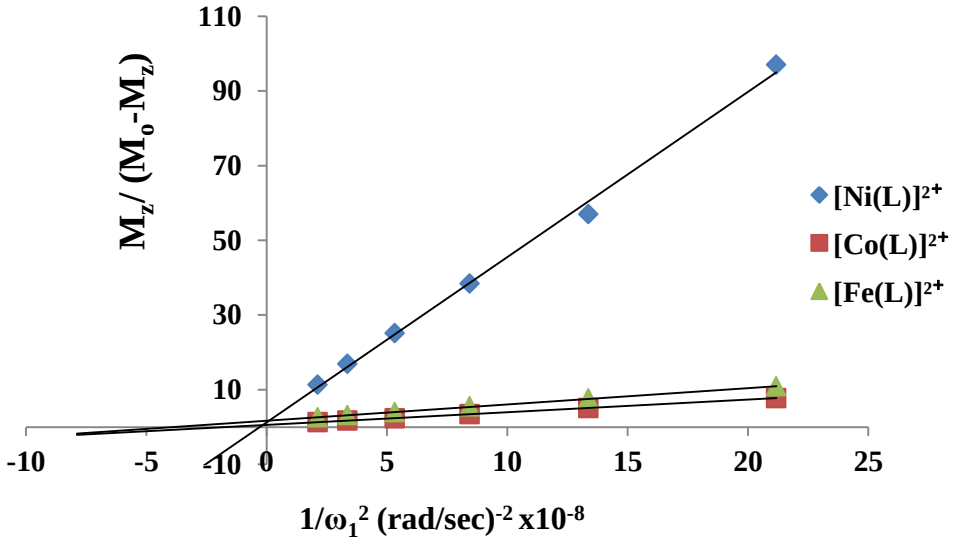

Figure S12. The plot of $M_z/(M_o-M_z)$ against the $1/\omega_1^2$ (rad/sec)$^{-2}$ x10^{-8} recorded at 11.7 T of 10 mM complex in rabbit serum pH7.3-7.5. RF presaturation pulse applied for 4 seconds with varying B_1 (8.2-24 µT)

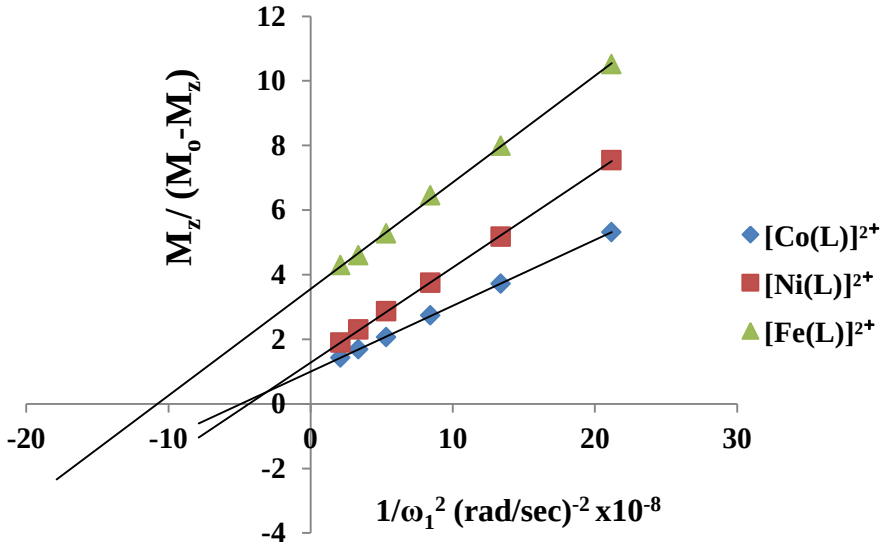

Figure S13. The plot of $M_z/(M_o-M_z)$ against the $1/\omega_1^2$ (rad/sec)$^{-2}$ x10^{-8} recorded at 11.7 T of 10 mM complex , 100 mM NaCl , 20 mM HEPES in 4 % agarose (w/w). RF presaturation pulse applied for 4 seconds with varying B_1 (8.2-24 µT)

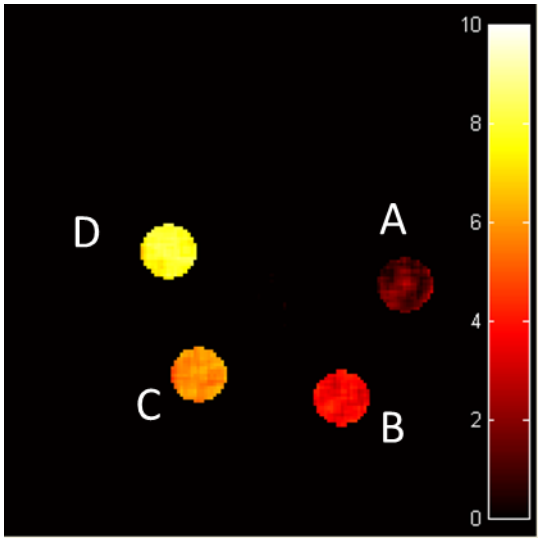

Figure S14. CEST phantom image of $[Fe(\mathbf{L})]^{2+}$ on a 4.7 T MRI scanner with B_1 =12μT. Samples contained A) 1 mM $[Fe(\mathbf{L})]^{2+}$, B) 2 mM $[Fe(\mathbf{L})]^{2+}$, C) 4 mM $[Fe(\mathbf{L})]^{2+}$, D) 8 mM $[Fe(\mathbf{L})]^{2+}$ in 20 mM HEPES pH 7.3-7.4 and 100 mM NaCl. The scale represents the loss of water signal due to the presaturation pulse.

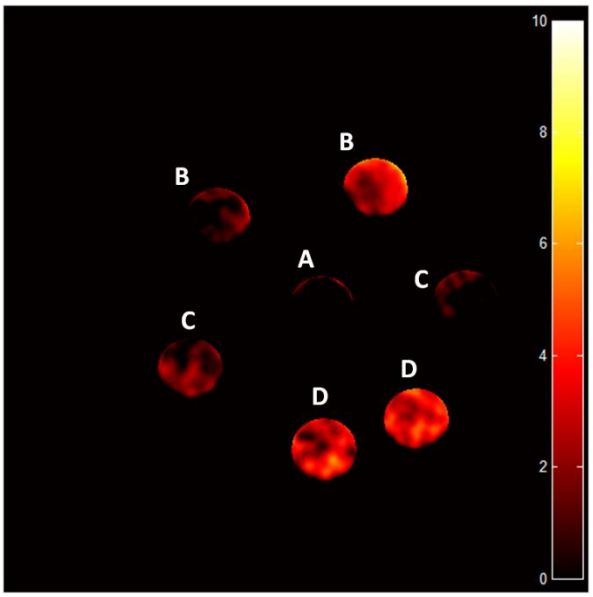

Figure S15. CEST images of phantoms on a MRI 4.7 T scanner with B_1 =12 μT. Sample A consisted of 20 mM HEPES pH 7.4 and 100 mM NaCl. Solutions contained 4 mM $[Fe(\mathbf{L})]^{2+}$ in B) 20 mM HEPES pH 7.4 and 100 mM NaCl, C) rabbit serum D) 20 mM HEPES pH 7.4 and 100 mM NaCl in 4 % agarose pH 7.3-7.4 at 37 ºC.

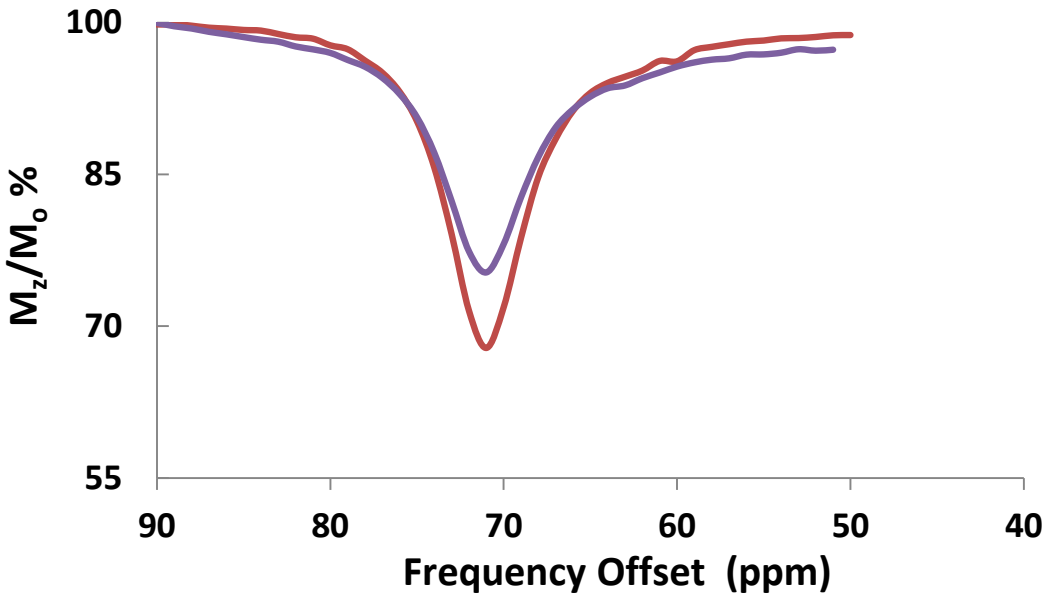

Figure S16. Overlaid CEST spectra of a solution containing 10 mM [Ni(**L**)]$^{2+}$, 100 mM NaCl, 20 mM HEPES pH 7.2 (red) and 10 mM [Ni(**L**)]$^{2+}$ in albumin from porcine albumin (purple) pH 7.2. RF presaturation pulse applied for 2 seconds B_1 =24 μT at 37 °C.

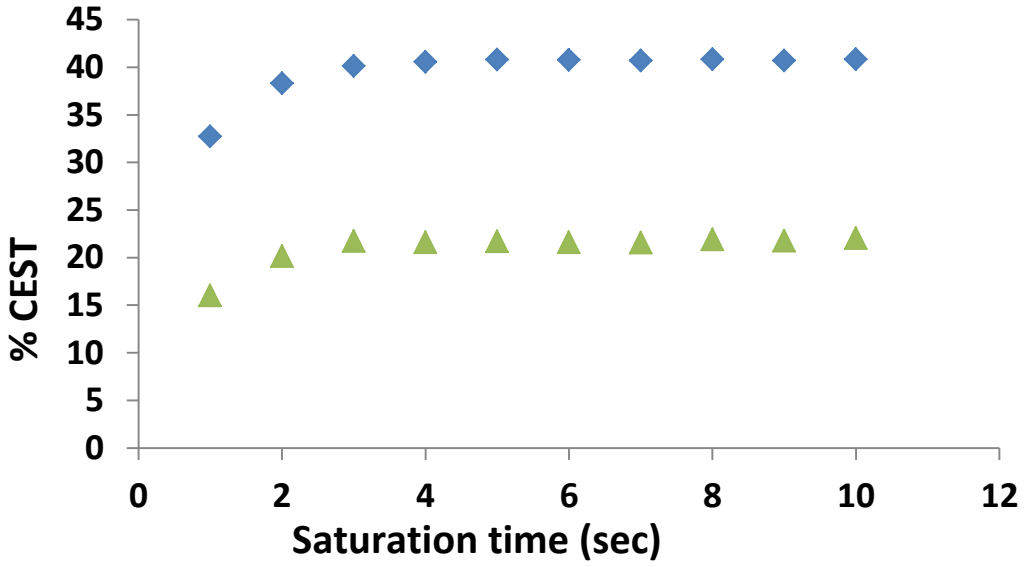

Figure S17. The CEST effect recorded at 11.7 T of a solution containing 10 mM [Fe(**L**)]$^{2+}$ (Δ) or 10 mM [Ni(**L**)]$^{2+}$ (◊), 100 mM NaCl, 20 mM HEPES pH 7.4, RF presaturation pulse applied as noted (1-10 sec) B_1 =24 μT at 37 °C.

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for [Fe(**L**)]$(CF_3SO_3)_2$.

Atom	*x*	*y*	*z*	U(eq)
Fe1	7473.8(2)	5487.4(2)	4708.5(2)	7.43(4)
S2	9760.3(2)	10402.6(3)	3080.2(2)	11.90(6)
S1	5037.7(2)	9321.8(3)	3620.8(2)	11.45(6)
F1	5126.2(6)	9394.3(10)	2190.1(5)	22.15(19)
F3	6300.1(6)	10229.7(10)	2777.8(5)	22.20(19)
O2	7647.8(7)	4926.8(10)	5918.4(5)	14.38(18)
O1	7616.7(7)	7163.3(10)	3911.8(5)	12.75(17)
O5	6097.6(6)	5672.7(9)	4905.6(5)	10.80(17)
F5	9630.0(6)	7995.1(9)	3753.9(5)	23.31(19)
O4	8848.3(6)	4959(1)	4684.8(5)	11.95(17)
N1	7576.4(7)	4529.4(11)	3578.2(6)	9.22(18)
O3	7134.2(6)	3211.6(9)	4857.9(5)	12.08(17)
O9	9166.8(7)	11030.9(11)	3587.3(6)	19.9(2)
F6	10887.9(6)	8291.5(10)	3225.1(5)	25.0(2)
F4	10640.6(7)	9368.2(11)	4224.8(5)	31.4(2)
O6	5465.3(7)	7980.4(10)	3628.0(5)	16.59(19)
O7	4061.7(7)	9334.1(12)	3541.4(6)	20.8(2)
F2	5048.7(7)	11397.1(10)	2708.1(5)	28.1(2)
O8	5423.5(7)	10279.3(10)	4163.8(5)	15.69(19)
O10	9296.9(7)	9727.6(11)	2466.6(5)	17.8(2)
N2	7418.0(7)	7553.2(12)	5319.5(6)	10.87(19)
O11	10545.2(7)	11202.9(11)	2905.8(6)	21.0(2)
N3	10042.3(7)	4690.2(13)	3976.2(6)	14.7(2)
N4	4965.4(7)	6948.5(12)	5344.5(6)	13.4(2)
C14	5817.2(8)	6771.6(13)	5183.9(6)	9.1(2)
C2	7104.1(9)	5494.2(14)	3060.5(7)	13.1(2)
C1	7490.3(9)	6940.6(14)	3144.2(7)	14.6(2)
C12	9166.2(8)	4701.7(13)	4075.4(7)	9.8(2)
C13	6457.1(8)	7971.6(13)	5350.1(7)	11.2(2)
C6	7215.6(11)	3656.0(16)	6117.4(8)	19.8(3)
C16	10252.0(9)	8937.8(15)	3594.9(7)	16.1(3)
C11	8547.0(8)	4368.1(13)	3421.8(6)	10.2(2)
C9	7946.9(9)	8586.5(14)	4919.9(8)	13.9(2)
C15	5390.5(10)	10126.0(14)	2778.3(7)	15.5(2)
C10	7650.5(9)	8593.7(13)	4125.4(8)	14.3(2)
C4	7365.7(9)	2363.1(14)	4251.4(8)	14.9(2)
C7	7464.7(9)	6048.5(15)	6400.0(7)	16.5(3)
C8	7834.0(9)	7342.9(15)	6060.7(7)	16.1(3)
C3	7103.3(9)	3176.8(14)	3574.4(7)	13.8(2)
C5	7427.9(11)	2617.7(15)	5542.2(8)	18.9(3)

U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for [Fe(**L**)]$(CF_3SO_3)_2$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	6.78(7)	7.53(8)	8.00(7)	-0.45(6)	0.56(5)	1.12(6)
S2	11.08(13)	11.34(14)	13.49(13)	-0.86(11)	2.82(10)	0.41(11)
S1	11.71(13)	11.31(14)	11.31(13)	-0.88(10)	0.38(10)	1.07(11)
F1	26.0(5)	28.4(5)	11.8(4)	-2.3(3)	-2.8(3)	-3.0(4)
F3	18.5(4)	28.7(5)	19.5(4)	3.0(4)	2.9(3)	-6.9(4)
O2	17.0(5)	16.7(5)	9.6(4)	0.0(3)	2.3(3)	5.1(4)
O1	18.5(5)	8.7(4)	11.2(4)	0.6(3)	2.0(3)	0.4(3)
O5	9.0(4)	8.8(4)	14.7(4)	-2.5(3)	0.9(3)	1.1(3)
F5	23.3(4)	17.6(4)	29.5(5)	8.5(4)	5.8(4)	3.4(4)
O4	8.5(4)	17.7(5)	9.6(4)	-1.4(3)	0.1(3)	2.0(3)
N1	7.1(4)	9.6(5)	10.9(4)	-0.3(4)	-0.1(3)	0.2(4)
O3	14.5(4)	9.1(4)	13.0(4)	1.2(3)	4.5(3)	3.1(3)
O9	22.7(5)	14.9(5)	23.0(5)	-1.0(4)	11.5(4)	4.8(4)
F6	19.9(4)	28.6(5)	26.9(5)	0.8(4)	6.4(4)	13.4(4)
F4	33.3(5)	40.0(6)	19.7(5)	-4.8(4)	-12.9(4)	7.1(5)
O6	22.5(5)	10.4(4)	16.6(4)	0.0(3)	-1.6(4)	2.7(4)
O7	12.2(4)	27.6(6)	22.6(5)	-1.5(4)	1.2(4)	-0.2(4)
F2	40.4(6)	15.8(4)	27.8(5)	8.2(4)	-2.4(4)	7.5(4)
O8	19.4(5)	13.6(5)	13.8(4)	-4.8(3)	-1.6(4)	2.9(4)
O10	17.5(5)	21.3(5)	14.3(4)	0.3(4)	-2.6(4)	-1.2(4)
N2	7.5(4)	12.0(5)	13.0(5)	-3.1(4)	-1.2(4)	0.6(4)
O11	19.2(5)	19.5(5)	24.9(5)	-2.4(4)	7.8(4)	-6.9(4)
N3	7.9(4)	24.9(6)	11.3(5)	-2.5(4)	1.0(4)	1.5(4)
N4	8.2(5)	11.0(5)	21.4(5)	-4.4(4)	3.5(4)	0.0(4)
C14	8.9(5)	9.1(5)	9.2(5)	0.3(4)	0.7(4)	0.8(4)
C2	11.4(5)	17.6(6)	10.1(5)	0.7(4)	-2.1(4)	2.2(5)
C1	17.8(6)	15.9(6)	10.2(5)	3.1(4)	2.2(4)	4.5(5)
C12	9.4(5)	9.4(5)	10.5(5)	0.7(4)	0.0(4)	2.1(4)
C13	8.1(5)	10.5(5)	14.9(5)	-3.8(4)	0.4(4)	0.8(4)
C6	27.0(7)	19.2(7)	13.6(6)	5.9(5)	7.0(5)	5.7(6)
C16	14.2(6)	19.9(7)	14.2(6)	-1.6(5)	-0.4(5)	4.2(5)
C11	9.1(5)	12.7(6)	8.8(5)	-1.4(4)	1.3(4)	1.1(4)
C9	9.3(5)	9.3(6)	23.2(6)	-4.5(5)	1.7(5)	-2.2(4)
C15	18.4(6)	13.0(6)	14.9(6)	1.4(5)	-1.4(5)	0.3(5)
C10	12.9(6)	7.5(5)	22.9(6)	0.6(5)	4.6(5)	-0.2(4)
C4	16.9(6)	8.3(6)	20.0(6)	-1.9(5)	6.3(5)	1.1(5)
C7	16.8(6)	23.6(7)	9.1(5)	-3.7(5)	-1.0(4)	7.5(5)
C8	12.7(6)	21.9(7)	13.3(6)	-8.3(5)	-4.0(4)	3.1(5)
C3	13.8(6)	12.5(6)	15.2(6)	-4.9(4)	1.6(4)	-3.6(5)
C5	26.2(7)	14.0(6)	17.1(6)	7.3(5)	6.2(5)	7.2(5)

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]c$

Table S3. Bond Lengths for [Fe(**L**)]$(CF_3SO_3)_2$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	O2	2.2952(9)	F5	C16	1.3331(17)
Fe1	O1	2.1978(9)	O4	C12	1.2593(15)
Fe1	O5	2.0866(9)	N1	C2	1.4832(16)
Fe1	O4	2.0938(9)	N1	C11	1.4815(16)
Fe1	N1	2.2873(11)	N1	C3	1.4785(17)
Fe1	O3	2.2690(9)	O3	C4	1.4370(16)
Fe1	N2	2.2896(11)	O3	C5	1.4332(16)
S2	O9	1.4412(10)	F6	C16	1.3371(16)
S2	O10	1.4487(10)	F4	C16	1.3368(16)
S2	O11	1.4395(11)	F2	C15	1.3288(16)
S2	C16	1.8320(14)	N2	C13	1.4778(16)
S1	O6	1.4382(10)	N2	C9	1.4806(17)
S1	O7	1.4415(11)	N2	C8	1.4854(16)
S1	O8	1.4576(10)	N3	C12	1.3139(16)
S1	C15	1.8296(14)	N4	C14	1.3152(16)
F1	C15	1.3359(16)	C14	C13	1.5156(17)
F3	C15	1.3461(17)	C2	C1	1.511(2)
O2	C6	1.4355(18)	C12	C11	1.5132(17)
O2	C7	1.4312(16)	C6	C5	1.500(2)
O1	C1	1.4332(16)	C9	C10	1.508(2)
O1	C10	1.4335(16)	C4	C3	1.508(2)
O5	C14	1.2544(15)	C7	C8	1.508(2)

Table S4 Bond Angles for [Fe(**L**)]$(CF_3SO_3)_2$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Fe1	O2	144.15(4)	C11	N1	C2	111.85(10)
O1	Fe1	N1	71.18(4)	C3	N1	Fe1	108.05(8)
O1	Fe1	O3	145.01(3)	C3	N1	C2	109.94(10)
O1	Fe1	N2	72.28(4)	C3	N1	C11	111.53(10)
O5	Fe1	O2	85.39(4)	C4	O3	Fe1	113.23(7)
O5	Fe1	O1	100.13(4)	C5	O3	Fe1	115.62(8)
O5	Fe1	O4	167.38(4)	C5	O3	C4	112.49(10)
O5	Fe1	N1	107.25(4)	C13	N2	Fe1	108.13(7)
O5	Fe1	O3	80.77(3)	C13	N2	C9	111.31(10)
O5	Fe1	N2	77.52(4)	C13	N2	C8	111.16(10)
O4	Fe1	O2	84.02(4)	C9	N2	Fe1	108.02(8)
O4	Fe1	O1	92.48(4)	C9	N2	C8	110.02(10)
O4	Fe1	N1	77.29(4)	C8	N2	Fe1	108.07(8)
O4	Fe1	O3	89.25(4)	O5	C14	N4	122.47(11)
O4	Fe1	N2	106.11(4)	O5	C14	C13	120.85(11)
N1	Fe1	O2	141.14(4)	N4	C14	C13	116.68(11)
N1	Fe1	N2	143.41(4)	N1	C2	C1	110.37(10)
O3	Fe1	O2	70.78(4)	O1	C1	C2	105.71(10)
O3	Fe1	N1	75.17(4)	O4	C12	N3	122.21(11)
O3	Fe1	N2	140.16(4)	O4	C12	C11	120.95(11)
N2	Fe1	O2	74.51(4)	N3	C12	C11	116.83(11)
O9	S2	O10	114.46(7)	N2	C13	C14	112.01(10)
O9	S2	C16	103.11(6)	O2	C6	C5	106.25(11)
O10	S2	C16	102.71(6)	F5	C16	S2	112.18(9)
O11	S2	O9	115.94(6)	F5	C16	F6	107.45(12)
O11	S2	O10	115.07(6)	F5	C16	F4	107.11(12)
O11	S2	C16	102.93(7)	F6	C16	S2	111.50(10)
O6	S1	O7	116.39(7)	F4	C16	S2	110.77(10)
O6	S1	O8	113.86(6)	F4	C16	F6	107.59(11)
O6	S1	C15	104.32(6)	N1	C11	C12	112.25(10)
O7	S1	O8	115.02(6)	N2	C9	C10	110.37(10)
O7	S1	C15	103.35(6)	F1	C15	S1	112.31(10)
O8	S1	C15	101.30(6)	F1	C15	F3	107.12(12)
C6	O2	Fe1	114.61(8)	F3	C15	S1	110.67(9)
C7	O2	Fe1	114.03(8)	F2	C15	S1	110.60(10)
C7	O2	C6	112.83(11)	F2	C15	F1	108.15(11)
C1	O1	Fe1	122.39(8)	F2	C15	F3	107.81(12)
C1	O1	C10	114.57(10)	O1	C10	C9	105.47(10)
C10	O1	Fe1	121.78(8)	O3	C4	C3	106.56(10)
C14	O5	Fe1	118.96(8)	O2	C7	C8	106.66(11)
C12	O4	Fe1	117.76(8)	N2	C8	C7	110.55(11)
C2	N1	Fe1	106.47(8)	N1	C3	C4	110.51(10)
C11	N1	Fe1	108.80(7)	O3	C5	C6	106.84(11)

Table S5. Torsion Angles for [Fe(**L**)]$(CF_3SO_3)_2$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Fe1	O2	C6	C5	44.11(13)	O8	S1	C15	F1	178.46(10)
Fe1	O2	C7	C8	-38.33(12)	O8	S1	C15	F3	58.80(11)
Fe1	O1	C1	C2	9.58(13)	O8	S1	C15	F2	-60.61(11)
Fe1	O1	C10	C9	22.17(13)	O10	S2	C16	F5	-54.54(11)
Fe1	O5	C14	N4	-177.88(9)	O10	S2	C16	F6	66.03(11)
Fe1	O5	C14	C13	2.26(15)	O10	S2	C16	F4	-174.19(10)
Fe1	O4	C12	N3	163.26(10)	N2	C9	C10	O1	-47.03(13)
Fe1	O4	C12	C11	-17.65(15)	O11	S2	C16	F5	-174.37(10)
Fe1	N1	C2	C1	54.36(11)	O11	S2	C16	F6	-53.80(11)
Fe1	N1	C11	C12	7.23(12)	O11	S2	C16	F4	65.99(11)
Fe1	N1	C3	C4	-45.38(11)	N3	C12	C11	N1	-175.04(11)
Fe1	O3	C4	C3	-40.99(12)	N4	C14	C13	N2	166.09(11)
Fe1	O3	C5	C6	43.08(14)	C2	N1	C11	C12	124.56(11)
Fe1	N2	C13	C14	16.80(12)	C2	N1	C3	C4	-161.19(11)
Fe1	N2	C9	C10	50.68(11)	C1	O1	C10	C9	-170.37(10)
Fe1	N2	C8	C7	-47.34(12)	C13	N2	C9	C10	-67.89(13)
O2	C6	C5	O3	-55.14(15)	C13	N2	C8	C7	71.17(13)
O2	C7	C8	N2	57.28(13)	C6	O2	C7	C8	-171.36(11)
O5	C14	C13	N2	-14.05(16)	C11	N1	C2	C1	-64.36(13)
O4	C12	C11	N1	5.82(17)	C11	N1	C3	C4	74.16(13)
N1	C2	C1	O1	-41.98(13)	C9	N2	C13	C14	135.30(11)
O3	C4	C3	N1	57.93(13)	C9	N2	C8	C7	-165.07(11)
O9	S2	C16	F5	64.68(11)	C10	O1	C1	C2	-157.80(10)
O9	S2	C16	F6	-174.74(10)	C4	O3	C5	C6	175.31(11)
O9	S2	C16	F4	-54.96(11)	C7	O2	C6	C5	176.86(11)
O6	S1	C15	F1	59.99(11)	C8	N2	C13	C14	-101.67(12)
O6	S1	C15	F3	-59.67(11)	C8	N2	C9	C10	168.44(10)
O6	S1	C15	F2	-179.08(9)	C3	N1	C2	C1	171.17(10)
O7	S1	C15	F1	-62.15(11)	C3	N1	C11	C12	-111.86(12)
O7	S1	C15	F3	178.18(10)	C5	O3	C4	C3	-174.39(11)
O7	S1	C15	F2	58.77(11)					

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for [Fe(**L**)](CF_3SO_3)$_2$.

Atom	*x*	*y*	*z*	U(eq)
H3A	10420	4862	4334	18
H3B	10238	4511	3553	18
H4A	4577	6297	5259	16
H4B	4797	7716	5535	16
H2A	6462	5510	3151	16
H2B	7174	5172	2567	16
H1A	8064	7011	2909	17
H1B	7074	7620	2930	17
H13A	6333	8711	5002	13
H13B	6349	8329	5831	13
H6A	6565	3787	6137	24
H6B	7449	3344	6590	24
H11A	8690	4978	3024	12
H11B	8655	3421	3269	12
H9A	8587	8363	4971	17
H9B	7859	9501	5125	17
H10A	7059	9022	4055	17
H10B	8081	9100	3843	17
H4C	7038	1491	4257	18
H4D	8011	2166	4271	18
H7A	7759	5889	6874	20
H7B	6817	6137	6458	20
H8A	7706	8139	6362	19
H8B	8487	7264	6033	19
H3C	7260	2651	3148	17
H3D	6453	3327	3549	17
H5A	8074	2431	5551	23
H5B	7111	1753	5623	23

Table S7. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for [Co(**L**)]Cl_2•$2H_2O$.

Atom	*x*	*y*	*z*	U(eq)
Co1	-3775.1(3)	-3775.1(3)	-5000	8.97(7)
Cl1	-9256.4(6)	-9361.9(6)	-6009.3(2)	14.02(8)
O3	-2400.6(18)	-5285.0(17)	-4635.9(3)	13.2(2)
O2	-4578.0(17)	-6550.4(17)	-5212.9(3)	13.1(2)
O4	-5274(2)	-7960(2)	-3924.2(4)	18.9(3)
O1	-1602.5(18)	-1602.5(18)	-5000	22.6(4)
N2	-1214(2)	-5331(2)	-4100.1(4)	14.3(3)
C6	-2721(2)	-2977(2)	-5738.8(4)	12.6(3)
N1	-1993(2)	-4134(2)	-5458.8(4)	11.1(3)
C2	-106(2)	-3602(3)	-5366.6(5)	16.4(3)
C7	-2167(2)	-4564(2)	-4348.5(4)	10.5(3)
C4	-3902(3)	-6816(3)	-5556.4(5)	18.0(4)
C5	-6458(2)	-7004(3)	-5179.3(5)	16.6(4)
C1	-59(3)	-1706(3)	-5217.4(5)	17.8(4)
C3	-2005(3)	-6073(2)	-5561.4(5)	16.3(3)

U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor

Table S8. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for [Co(**L**)]Cl_2•$2H_2O$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	10.37(9)	10.37(9)	6.16(14)	-0.24(8)	0.24(8)	3.12(10)
Cl1	12.76(18)	15.20(18)	14.11(19)	0.89(15)	0.80(14)	3.18(13)
O3	15.7(6)	13.2(6)	10.7(6)	-0.6(5)	-2.0(5)	4.7(4)
O2	13.3(6)	14.4(6)	11.6(6)	-2.4(5)	-0.3(5)	0.0(4)
O4	18.6(7)	17.6(7)	20.6(7)	-3.5(6)	-2.2(5)	1.3(5)
O1	21.7(6)	21.7(6)	24.5(10)	-12.6(7)	12.6(7)	-9.1(7)
N2	17.6(7)	13.5(6)	11.7(7)	1.0(5)	-2.1(6)	4.2(6)
C6	12.7(7)	15.6(7)	9.4(7)	-0.1(6)	0.7(6)	3.2(6)
N1	11.2(6)	13.2(7)	8.8(6)	-1.3(5)	-0.3(5)	3.5(5)
C2	9.4(7)	26.0(9)	13.7(9)	-2.9(7)	-0.3(6)	3.5(7)
C7	9.5(7)	11.3(7)	10.6(8)	1.6(6)	0.5(6)	0.2(5)
C4	26.5(9)	15.3(8)	12.2(8)	-5.4(6)	3.0(7)	-2.1(7)
C5	15.4(8)	16.4(8)	18.0(9)	-1.4(7)	-2.0(7)	-2.4(6)
C1	14.6(8)	26.8(9)	12.0(9)	-2.2(7)	2.6(6)	-5.6(7)
C3	21.7(8)	13.1(8)	14.3(8)	-3.2(6)	5.2(7)	5.8(7)

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Table S9. Bond Lengths for [Co(**L**)]Cl_2•2H_2O

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	O3	2.0631(12)	O1	C1	1.417(2)
Co1	$O3^1$	2.0631(12)	N2	C7	1.320(2)
Co1	$O2^1$	2.2799(13)	C6	N1	1.482(2)
Co1	O2	2.2800(13)	C6	$C7^1$	1.518(2)
Co1	O1	2.2595(19)	N1	C2	1.485(2)
Co1	N1	2.2287(14)	N1	C3	1.481(2)
Co1	$N1^1$	2.2288(14)	C2	C1	1.511(3)
O3	C7	1.249(2)	C7	$C6^1$	1.518(2)
O2	C4	1.438(2)	C4	C3	1.498(3)
O2	C5	1.428(2)	C5	$C5^1$	1.505(4)
O1	$C1^1$	1.417(2)			

^{1}+Y,+X,-1-Z

Table S10. Bond Angles for [Co(**L**)]Cl_2•2H_2O.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O3^1$	Co1	O3	176.09(8)	C4	O2	Co1	111.65(11)
O3	Co1	O2	83.91(5)	C5	O2	Co1	115.26(10)
O3	Co1	$O2^1$	92.89(5)	C5	O2	C4	112.81(14)
$O3^1$	Co1	O2	92.88(5)	$C1^1$	O1	Co1	121.90(10)
$O3^1$	Co1	$O2^1$	83.91(5)	C1	O1	Co1	121.90(10)
O3	Co1	O1	91.96(4)	C1	O1	$C1^1$	116.2(2)
$O3^1$	Co1	O1	91.96(4)	N1	C6	$C7^1$	112.56(14)
$O3^1$	Co1	N1	79.97(5)	C6	N1	Co1	107.89(10)
O3	Co1	N1	101.36(5)	C6	N1	C2	111.34(15)
$O3^1$	Co1	$N1^1$	101.36(5)	C2	N1	Co1	108.98(11)
O3	Co1	$N1^1$	79.96(5)	C3	N1	Co1	109.01(11)
$O2^1$	Co1	O2	70.61(6)	C3	N1	C6	110.68(14)
O1	Co1	O2	144.69(3)	C3	N1	C2	108.89(14)
O1	Co1	$O2^1$	144.70(3)	N1	C2	C1	110.91(15)
N1	Co1	O2	75.88(5)	O3	C7	N2	123.08(16)
$N1^1$	Co1	O2	141.82(5)	O3	C7	$C6^1$	121.68(15)
N1	Co1	$O2^1$	141.82(5)	N2	C7	$C6^1$	115.25(15)
$N1^1$	Co1	$O2^1$	75.88(5)	O2	C4	C3	106.53(15)
N1	Co1	O1	70.60(4)	O2	C5	$C5^1$	106.29(12)
$N1^1$	Co1	O1	70.60(4)	O1	C1	C2	105.06(15)
N1	Co1	$N1^1$	141.19(8)	N1	C3	C4	110.68(15)
C7	O3	Co1	116.90(11)				

^{1}+Y,+X,-1-Z

Table S11. Torsion Angles for[Co(**L**)]Cl_2•$2H_2O$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Co1	O3	C7	N2	-175.62(13)	N1	C2	C1	O1	40.8(2)
Co1	O3	C7	$C6^1$	4.5(2)	C2	N1	C3	C4	163.37(16)
Co1	O2	C4	C3	41.47(16)	$C7^1$	C6	N1	Co1	-9.09(17)
Co1	O2	C5	$C5^1$	-43.90(19)	$C7^1$	C6	N1	C2	-128.63(15)
Co1	O1	C1	C2	-10.36(17)	$C7^1$	C6	N1	C3	110.10(16)
Co1	N1	C2	C1	-54.03(17)	C4	O2	C5	$C5^1$	-173.76(16)
Co1	N1	C3	C4	44.59(17)	C5	O2	C4	C3	173.15(14)
O2	C4	C3	N1	-57.72(19)	$C1^1$	O1	C1	C2	169.63(17)
C6	N1	C2	C1	64.86(19)	C3	N1	C2	C1	-172.84(15)
C6	N1	C3	C4	-73.92(18)					

^{1}+Y,+X,-1-Z

Table S12. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for [Co(**L**)]Cl_2•$2H_2O$.

Atom	*x*	*y*	*z*	U(eq)
H2A	-719	-6377	-4133	17
H2B	-1087	-4786	-3906	17
H6A	-2830	-3699	-5947	15
H6B	-1869	-1999	-5785	15
H2C	655	-3650	-5570	20
H2D	377	-4457	-5200	20
H4A	-4659	-6177	-5721	22
H4B	-3898	-8099	-5614	22
H5A	-6639	-8299	-5213	20
H5B	-7176	-6351	-5348	20
H1A	1050	-1514	-5087	21
H1B	-128	-800	-5398	21
H3A	-1248	-6767	-5405	20
H3B	-1501	-6194	-5791	20
H4C	-5300(40)	-7050(40)	-3837(7)	23(7)
H4D	-6350(40)	-8320(40)	-3928(8)	36(8)

TableS13. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for [Ni(**L**)]$(CF_3SO_3)_2 \bullet H_2O$.

Atom	*x*	*y*	*z*	U(eq)
Ni1	1906.7(2)	6367.6(2)	3991.3(2)	8.78(6)
S1	7104.6(4)	5236.6(2)	3902.2(2)	12.25(9)
S2	2416.4(19)	3293.6(12)	4290(2)	13.2(3)
O4	3357(1)	6420.0(5)	4592.7(6)	13.2(2)
O3	2968.7(10)	6742.4(5)	3152.1(6)	12.6(2)
O5	616.4(10)	6444.7(5)	3290.3(6)	11.2(2)
O6	6472.7(11)	5672.9(5)	3531.1(6)	16.9(3)
O2	2137.5(10)	7458.4(6)	3959.6(6)	14.7(2)
O1	1206.5(11)	5694.0(5)	4427.4(6)	17.3(3)
O7	6638.4(11)	5104.5(6)	4504.5(6)	17.9(3)
O8	8345.2(11)	5278.6(6)	3936.6(7)	24.6(3)
O12	3381.4(11)	3117.0(6)	6437.2(7)	18.5(3)
F2	7214.8(13)	4143.3(5)	3737.9(6)	34.7(3)
O10	1503(3)	2878(2)	4277(4)	23.6(8)
N2	2776.6(12)	5657.5(6)	3626.2(7)	10.7(3)
N1	638.0(12)	6746.6(6)	4557.5(6)	9.8(3)
O11	3580(5)	3071.1(19)	4412(3)	24.7(7)
C13	-498.2(14)	6685.3(7)	4169.6(8)	11.0(3)
F1	7212.1(15)	4620.6(6)	2861.6(6)	44.1(4)
O9	2201(4)	3814.4(18)	4621(4)	26.5(8)
F3	5637.1(13)	4522.8(6)	3317.2(8)	45.3(4)
C8	3199.4(15)	5768.6(7)	2987.6(8)	13.2(3)
C12	4074.3(14)	6032.4(7)	4536.6(8)	11.7(3)
N4	-1238.4(12)	6697.1(6)	3042.6(7)	13.8(3)
C14	-343.4(14)	6604.0(7)	3463.5(8)	9.9(3)
F4	3219(3)	3891.0(8)	3363.1(10)	44.0(6)
N3	5122.1(13)	6037.8(7)	4841.7(7)	16.7(3)
C10	1328.1(15)	5133.8(7)	4191.8(8)	14.3(3)
C3	845.3(14)	7346.0(7)	4744.5(8)	12.0(3)
C7	3793.7(14)	6334.0(7)	2982.7(8)	13.0(3)
C4	1103.5(14)	7692.3(7)	4166.9(8)	13.4(3)
F5	1385(3)	3747.2(10)	3229.3(12)	68.1(9)
C2	709.9(15)	6391.1(7)	5151.2(8)	12.8(3)
C5	2457.5(16)	7672.6(7)	3365.5(9)	16.3(3)
F6	2573(3)	3068.7(10)	3067.1(10)	64.1(9)
C11	3749.3(14)	5523.8(7)	4116.6(8)	12.5(3)

C1	573.2(15)	5772.7(7)	4979.1(8)	13.8(3)
C6	3427.0(15)	7301.7(7)	3188.2(9)	15.3(3)
C9	1898.0(15)	5199.2(7)	3567.7(8)	14.3(3)
C15	6773.0(19)	4599.5(8)	3428.5(10)	23.4(4)
C16	2397(3)	3512.2(12)	3442.8(14)	33.6(7)
F4A	3720(20)	3777(7)	3466(9)	44.0(6)
F5A	2060(20)	3672(9)	3080(12)	68.1(9)
F6A	3200(30)	2952(9)	3204(9)	64.1(9)
C16A	2890(30)	3419(11)	3467(13)	33.6(7)
O10A	1520(20)	2955(13)	4115(18)	23.6(8)
O11A	3410(30)	3103(15)	4516(19)	24.7(7)
O9A	2160(30)	3828(15)	4454(18)	26.5(8)
S2A	2442(14)	3329(7)	4187(10)	13.2(3)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Table S14. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for [Ni(**L**)]$(CF_3SO_3)_2 \bullet H_2O$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	7.22(10)	11.8(1)	7.44(10)	0.45(7)	1.44(7)	0.81(7)
S1	13.26(19)	12.11(18)	11.60(19)	0.47(14)	2.25(14)	2.22(14)
S2	12.7(2)	13.5(4)	13.9(8)	-3.3(5)	3.5(4)	1.5(2)
O4	11.5(5)	16.1(6)	11.6(6)	-1.8(4)	-0.1(4)	3.9(4)
O3	9.9(5)	13.6(6)	14.9(6)	0.0(4)	3.6(4)	0.2(4)
O5	8.1(5)	16.2(6)	9.6(5)	0.1(4)	2.1(4)	1.2(4)
O6	21.6(6)	14.1(6)	15.3(6)	2.8(5)	3.5(5)	5.7(5)
O2	12.3(6)	22.7(6)	9.8(6)	1.9(5)	4.6(4)	2.7(5)
O1	24.7(7)	12.2(6)	17.6(6)	0.9(5)	14.8(5)	0.3(5)
O7	22.5(7)	19.7(6)	12.2(6)	2.3(5)	4.7(5)	3.3(5)
O8	14.6(6)	26.1(7)	33.6(8)	1.5(6)	3.9(6)	3.0(5)
O12	17.3(6)	14.2(6)	24.6(7)	-2.9(5)	4.5(5)	0.2(5)
F2	59.2(9)	13.8(6)	29.3(7)	0.4(5)	-5.5(6)	9.3(6)
O10	18.1(7)	19.4(12)	35(2)	-7.7(13)	12.6(11)	-4.1(8)
N2	9.6(6)	14.4(7)	8.4(6)	-0.2(5)	2.5(5)	0.1(5)
N1	9.3(6)	12.9(6)	7.0(6)	0.7(5)	0.1(5)	1.1(5)
O11	13.0(14)	23.4(9)	37.4(19)	-3.6(11)	0.7(11)	8.0(9)
C13	8.5(7)	16.0(8)	8.7(7)	-0.5(6)	1.7(5)	1.5(6)
F1	86.0(12)	30.9(7)	16.7(6)	-5.4(5)	11.6(7)	19.7(7)
O9	23.6(8)	23.5(8)	34(2)	-17.8(15)	9.3(15)	0.1(6)
F3	39.4(8)	33.7(8)	58.3(10)	-16.1(7)	-18.9(7)	-5.2(6)
C8	14.7(8)	17.0(8)	8.7(7)	-1.9(6)	5.6(6)	2.4(6)
C12	11.0(7)	16.6(8)	7.9(7)	1.3(6)	2.8(6)	0.7(6)
N4	9.5(6)	22.0(8)	9.8(6)	-1.1(5)	0.7(5)	2.0(5)
C14	9.6(7)	10.9(7)	9.3(7)	0.4(5)	2.0(6)	-1.0(5)
F4	70.9(17)	23.8(9)	40.4(10)	10.8(7)	22.1(11)	-2.5(9)
N3	11.3(7)	23.1(8)	15.0(7)	-4.6(6)	-2.3(5)	5.3(6)
C10	15.1(8)	10.9(7)	17.5(8)	0.4(6)	5.0(6)	-0.4(6)
C3	10.9(7)	14.6(8)	10.7(7)	-3.6(6)	1.9(6)	1.5(6)
C7	9.1(7)	19.5(8)	11.2(7)	1.0(6)	5.5(6)	2.7(6)
C4	12.8(7)	13.4(8)	14.3(8)	-2.3(6)	1.9(6)	1.8(6)
F5	67.0(19)	58.8(13)	69.2(15)	26.0(11)	-42.7(14)	-1.3(12)
C2	12.4(7)	19.6(8)	6.8(7)	1.4(6)	2.6(6)	3.3(6)
C5	19.4(8)	15.4(8)	14.9(8)	3.5(6)	6.3(7)	-0.5(6)
F6	139(3)	37.8(12)	17.6(9)	-9.1(8)	16.3(12)	-17.1(14)
C11	10.0(7)	16.3(8)	11.2(7)	-0.5(6)	1.7(6)	3.9(6)
C1	13.1(8)	18.7(8)	10.5(7)	4.3(6)	5.5(6)	2.2(6)
C6	15.4(8)	15.6(8)	15.8(8)	1.9(6)	6.8(6)	-4.0(6)
C9	14.2(8)	13.0(8)	16.2(8)	-2.8(6)	3.4(6)	-0.9(6)
C15	34.4(11)	16.4(9)	18.1(9)	-1.5(7)	-3.8(8)	7.2(8)
C16	56(2)	20.9(13)	22.6(12)	2.9(10)	-6.1(15)	-0.2(13)
F4A	70.9(17)	23.8(9)	40.4(10)	10.8(7)	22.1(11)	-2.5(9)
F5A	67.0(19)	58.8(13)	69.2(15)	26.0(11)	-42.7(14)	-1.3(12)

F6A	139(3)	37.8(12)	17.6(9)	-9.1(8)	16.3(12)	-17.1(14)
C16A	56(2)	20.9(13)	22.6(12)	2.9(10)	-6.1(15)	-0.2(13)
O10A	18.1(7)	19.4(12)	35(2)	-7.7(13)	12.6(11)	-4.1(8)
O11A	13.0(14)	23.4(9)	37.4(19)	-3.6(11)	0.7(11)	8.0(9)
O9A	23.6(8)	23.5(8)	34(2)	-17.8(15)	9.3(15)	0.1(6)
S2A	12.7(2)	13.5(4)	13.9(8)	-3.3(5)	3.5(4)	1.5(2)

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Table S15. Bond Lengths for[Ni(**L**)]$(CF_3SO_3)_2$•H_2O.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	O4	2.0042(12)	N2	C9	1.487(2)
Ni1	O3	2.4006(12)	N1	C13	1.487(2)
Ni1	O5	1.9980(12)	N1	C3	1.486(2)
Ni1	O1	2.0421(12)	N1	C2	1.491(2)
Ni1	N2	2.1381(14)	C13	C14	1.510(2)
Ni1	N1	2.1653(14)	F1	C15	1.329(2)
S1	O6	1.4478(13)	F3	C15	1.329(3)
S1	O7	1.4456(13)	C8	C7	1.507(2)
S1	O8	1.4379(14)	C12	N3	1.317(2)
S1	C15	1.824(2)	C12	C11	1.516(2)
S2	O10	1.446(4)	N4	C14	1.313(2)
S2	O11	1.449(5)	F4	C16	1.332(4)
S2	O9	1.446(5)	C10	C9	1.520(2)
S2	C16	1.836(6)	C3	C4	1.509(2)
O4	C12	1.252(2)	F5	C16	1.337(4)
O3	C7	1.428(2)	C2	C1	1.513(2)
O3	C6	1.427(2)	C5	C6	1.501(2)
O5	C14	1.2602(19)	F6	C16	1.337(4)
O2	C4	1.425(2)	F4A	C16A	1.28(3)
O2	C5	1.418(2)	F5A	C16A	1.34(3)
O1	C10	1.427(2)	F6A	C16A	1.30(3)
O1	C1	1.433(2)	C16A	S2A	1.65(4)
F2	C15	1.335(2)	O10A	S2A	1.39(3)
N2	C8	1.483(2)	O11A	S2A	1.37(4)
N2	C11	1.483(2)	O9A	S2A	1.36(4)

Table S16. Bond Angles for [Ni(**L**)]$(CF_3SO_3)_2$•H_2O.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Ni1	O3	88.47(5)	C3	N1	C13	110.42(12)
O4	Ni1	O1	96.69(5)	C3	N1	C2	109.14(13)
O4	Ni1	N2	82.77(5)	C2	N1	Ni1	103.23(9)
O4	Ni1	N1	102.01(5)	N1	C13	C14	111.13(13)
O5	Ni1	O4	167.87(5)	N2	C8	C7	110.72(13)
O5	Ni1	O3	80.53(4)	O4	C12	N3	122.63(16)
O5	Ni1	O1	95.40(5)	O4	C12	C11	120.37(15)
O5	Ni1	N2	99.13(5)	N3	C12	C11	116.99(15)
O5	Ni1	N1	81.87(5)	O5	C14	C13	120.40(14)
O1	Ni1	O3	149.94(5)	O5	C14	N4	121.61(15)
O1	Ni1	N2	76.34(5)	N4	C14	C13	117.98(14)
O1	Ni1	N1	76.29(5)	O1	C10	C9	105.31(13)
N2	Ni1	O3	74.97(5)	N1	C3	C4	110.52(13)
N2	Ni1	N1	152.58(5)	O3	C7	C8	106.44(13)
N1	Ni1	O3	131.63(5)	O2	C4	C3	105.42(13)
O6	S1	C15	103.42(8)	N1	C2	C1	110.76(13)
O7	S1	O6	113.91(8)	O2	C5	C6	105.58(14)
O7	S1	C15	102.27(9)	N2	C11	C12	111.05(13)
O8	S1	O6	115.55(8)	O1	C1	C2	105.40(13)
O8	S1	O7	115.23(8)	O3	C6	C5	105.82(13)
O8	S1	C15	104.08(9)	N2	C9	C10	110.77(13)
O10	S2	O11	115.1(3)	F2	C15	S1	110.93(13)
O10	S2	O9	115.6(2)	F1	C15	S1	111.70(15)
O10	S2	C16	103.4(2)	F1	C15	F2	107.26(16)
O11	S2	C16	101.4(5)	F3	C15	S1	111.26(14)
O9	S2	O11	115.3(3)	F3	C15	F2	107.61(18)
O9	S2	C16	103.25(19)	F3	C15	F1	107.88(17)
C12	O4	Ni1	115.00(11)	F4	C16	S2	111.4(2)
C7	O3	Ni1	109.31(9)	F4	C16	F5	107.1(2)
C6	O3	Ni1	121.29(10)	F4	C16	F6	107.8(3)
C6	O3	C7	112.77(12)	F5	C16	S2	111.6(3)
C14	O5	Ni1	116.10(10)	F5	C16	F6	108.1(3)
C5	O2	C4	114.96(13)	F6	C16	S2	110.6(2)
C10	O1	Ni1	121.20(10)	F4A	C16A	F5A	102(2)
C10	O1	C1	118.13(13)	F4A	C16A	F6A	109(3)
C1	O1	Ni1	120.67(10)	F4A	C16A	S2A	113(2)
C8	N2	Ni1	112.70(10)	F5A	C16A	S2A	110(2)
C8	N2	C9	109.78(13)	F6A	C16A	F5A	110(2)
C11	N2	Ni1	106.11(10)	F6A	C16A	S2A	113(2)
C11	N2	C8	111.13(13)	O10A	S2A	C16A	106.9(17)
C11	N2	C9	111.82(13)	O11A	S2A	C16A	101(2)
C9	N2	Ni1	105.13(10)	O11A	S2A	O10A	113(2)
C13	N1	Ni1	106.09(9)	O9A	S2A	C16A	111.6(18)

C13	N1	C2	111.86(13)	O9A	S2A	O10A	113(2)
C3	N1	Ni1	115.93(10)	O9A	S2A	O11A	111(2)

Table S17. Torsion Angles for [Ni(**L**)]$(CF_3SO_3)_2$•H_2O.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Ni1	O4	C12	N3	172.09(13)	O11	S2	C16	F4	-58.9(3)
Ni1	O4	C12	C11	-9.21(19)	O11	S2	C16	F5	-178.6(3)
Ni1	O3	C7	C8	39.97(14)	O11	S2	C16	F6	61.0(3)
Ni1	O3	C6	C5	-47.85(17)	C13	N1	C3	C4	-72.12(16)
Ni1	O5	C14	C13	-4.38(19)	C13	N1	C2	C1	60.83(17)
Ni1	O5	C14	N4	176.53(12)	O9	S2	C16	F4	60.8(3)
Ni1	O1	C10	C9	-6.58(18)	O9	S2	C16	F5	-58.9(3)
Ni1	O1	C1	C2	-6.26(17)	O9	S2	C16	F6	-179.3(3)
Ni1	N2	C8	C7	45.75(16)	C8	N2	C11	C12	100.67(15)
Ni1	N2	C11	C12	-22.17(15)	C8	N2	C9	C10	-171.99(13)
Ni1	N2	C9	C10	-50.52(15)	N3	C12	C11	N2	-158.65(15)
Ni1	N1	C13	C14	-21.81(15)	C10	O1	C1	C2	173.99(14)
Ni1	N1	C3	C4	48.55(16)	C3	N1	C13	C14	104.56(15)
Ni1	N1	C2	C1	-52.82(14)	C3	N1	C2	C1	-176.68(13)
O4	C12	C11	N2	22.6(2)	C7	O3	C6	C5	179.71(13)
O6	S1	C15	F2	-174.49(15)	C4	O2	C5	C6	-170.34(14)
O6	S1	C15	F1	65.90(16)	C2	N1	C13	C14	-133.67(14)
O6	S1	C15	F3	-54.72(16)	C2	N1	C3	C4	164.53(13)
O2	C5	C6	O3	58.34(17)	C5	O2	C4	C3	171.90(14)
O1	C10	C9	N2	37.84(18)	C11	N2	C8	C7	-73.21(17)
O7	S1	C15	F2	-55.91(17)	C11	N2	C9	C10	64.19(17)
O7	S1	C15	F1	-175.53(14)	C1	O1	C10	C9	173.16(14)
O7	S1	C15	F3	63.85(16)	C6	O3	C7	C8	178.04(13)
O8	S1	C15	F2	64.37(17)	C9	N2	C8	C7	162.56(13)
O8	S1	C15	F1	-55.24(16)	C9	N2	C11	C12	-136.27(14)
O8	S1	C15	F3	-175.86(14)	F4A	C16A	S2A	O10A	178(2)
O10	S2	C16	F4	-178.4(2)	F4A	C16A	S2A	O11A	-64(3)
O10	S2	C16	F5	61.9(3)	F4A	C16A	S2A	O9A	53(3)
O10	S2	C16	F6	-58.5(3)	F5A	C16A	S2A	O10A	65(3)
N2	C8	C7	O3	-57.12(17)	F5A	C16A	S2A	O11A	-176(2)
N1	C13	C14	O5	19.2(2)	F5A	C16A	S2A	O9A	-59(3)
N1	C13	C14	N4	-161.72(14)	F6A	C16A	S2A	O10A	-58(3)
N1	C3	C4	O2	-61.99(17)	F6A	C16A	S2A	O11A	60(3)
N1	C2	C1	O1	39.87(17)	F6A	C16A	S2A	O9A	178(3)

Table S18. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for [Ni(**L**)]$(CF_3SO_3)_2$•H_2O.

Atom	*x*	*y*	*z*	U(eq)
H13A	-963	7020	4222	13
H13B	-908	6364	4325	13
H8A	2552	5762	2657	16
H8B	3737	5474	2890	16
H4A	-1178	6649	2638	17
H4B	-1885	6806	3172	17
H3A	5337	6315	5091	20
H3B	5591	5764	4791	20
H10A	578	4953	4112	17
H10B	1809	4909	4501	17
H3C	1493	7369	5074	14
H3D	166	7497	4923	14
H7A	4473	6339	3293	16
H7B	4033	6414	2558	16
H4C	473	7666	3827	16
H4D	1217	8086	4285	16
H2A	107	6502	5418	15
H2B	1452	6450	5398	15
H5A	2714	8061	3414	20
H5B	1809	7656	3036	20
H11A	4415	5404	3902	15
H11B	3528	5215	4385	15
H1A	887	5537	5335	17
H1B	-237	5678	4877	17
H6A	3679	7415	2776	18
H6B	4081	7324	3514	18
H9A	2266	4847	3467	17
H9B	1313	5285	3218	17
H12A	3420(30)	2861(10)	6153(12)	46(8)
H12B	3490(20)	3425(8)	6274(12)	30(7)

Table S19. Atomic Occupancy for [Ni(**L**)]$(CF_3SO_3)_2$•H_2O.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
S2	0.87(3)	O10	0.87(3)	O11	0.87(3)
O9	0.87(3)	F4	0.889(5)	F5	0.889(5)
F6	0.889(5)	C16	0.889(5)	F4A	0.111(5)
F5A	0.111(5)	F6A	0.111(5)	C16A	0.111(5)
O10A	0.13(3)	O11A	0.13(3)	O9A	0.13(3)

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