Supporting Information

A single H-bond triggers the formation of a cleft around Et_3NH^+ through bond rearrangement and rotations of arms in both Co(III) and Fe(III) complexes

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A. Synthesis and characterization data of the ligand.

$H_2L^{L\text{-}Trp}$. At room temperature, L-Tryptophan (3.0 g, 14.7 mmol) and $LiOH.H_2O$ (0.616 g, 14.7 mmol) were dissolved in 30 mL of methanol and stirred for 10 min, giving a colorless solution. The methanolic solution of *o*-vanillin was added to this solution, and immediately it became yellow-colored. The solution was stirred for 45 min, and then solid $NaBH_4$ (0.667 g, 17.6 mmol) was slowly added to the solution with constant stirring. The yellow-colored solution became colorless within a few minutes, and the reaction mixture was stirred for another 30 min. Then, the solvent was removed using a rotary evaporator, which gave a sticky mass. That sticky solid was dissolved in 10 mL water and acidified with dilute HCl to pH 6-5. White-colored solid precipitated out and was filtered, washed with water and cold ethanol, and dried under a vacuum desiccator.

Yield: 92 %. ^{1}H NMR (CD_3OD, 500 MHz) δ 7.55 (d, 1H, J = 8 Hz, H^{12}), δ 7.38 (d, 1H, J = 8 Hz, H^{15}), δ 7.19 (s, 1H, H^{17}), δ 7.13 (t, 1H, J = 7.5 Hz, H^{14}), δ 6.99 (t, 1H, J = 8 Hz, H^{13}), δ 6.85 (d, 1H, J = 8 Hz, H^3), δ 6.68 (t, 1H, J = 8 Hz, H^4), δ 6.48 (d, 1H, J = 8 Hz, H^5), δ 4.04 (d, 1H, J = 13 Hz, H^7), δ 3.88 (d, 1H, J = 13 Hz, H^{7a}), δ 3.86 (dd, 1H, J = 4.5, 8 Hz, H^8), δ 3.77 (s, 3H, H^{-OCH3}), δ 3.56 (dd, J = 4.5/8, 14.5 Hz 1H, H^9), δ 3.14 (dd, 1H, J = 4.5/8,14.5 Hz, H^{9a}); FTIR (KBr, cm^{-1}): $\upsilon(COO^-)_{asym}$ 1607; $\upsilon(COO^-)_{sym}$ 1400; υ(C-O) 1243; υ(C-H)o/p-ring H 750. m/z (ESI-MS) $\{M+H\}^+$, $\{(H_2L^{L\text{-}Trp})+H\}^+$; calcd: 341.15, found: 341.15.

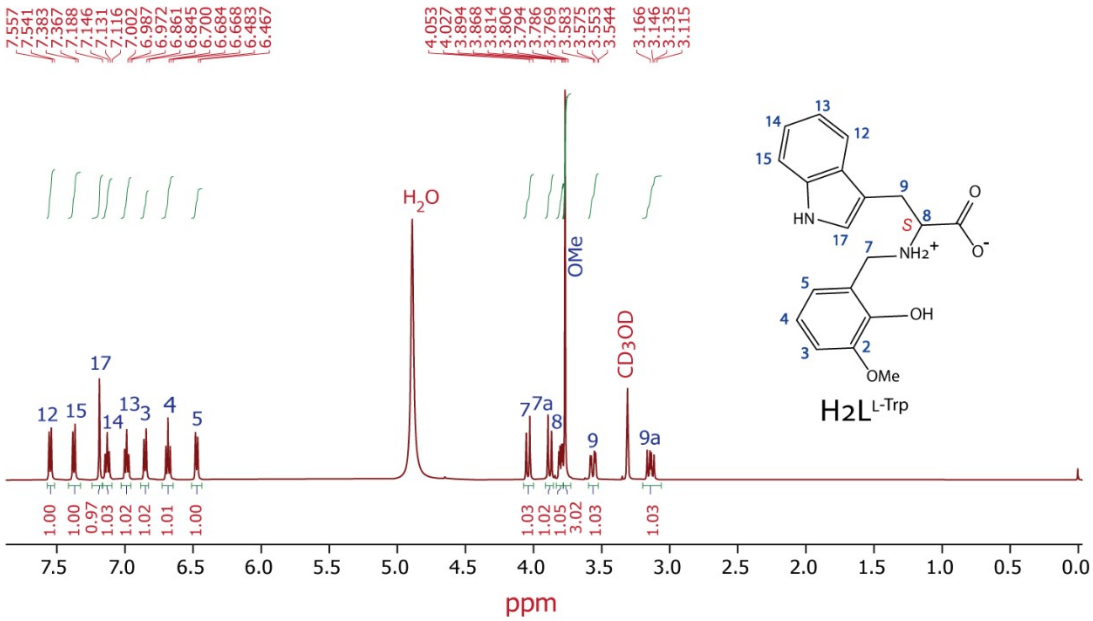


Figure S1. ^{1}H NMR (500 MHz, CD_3OD) of $\mathbf{H_2L^{L\text{-}Trp}}$.

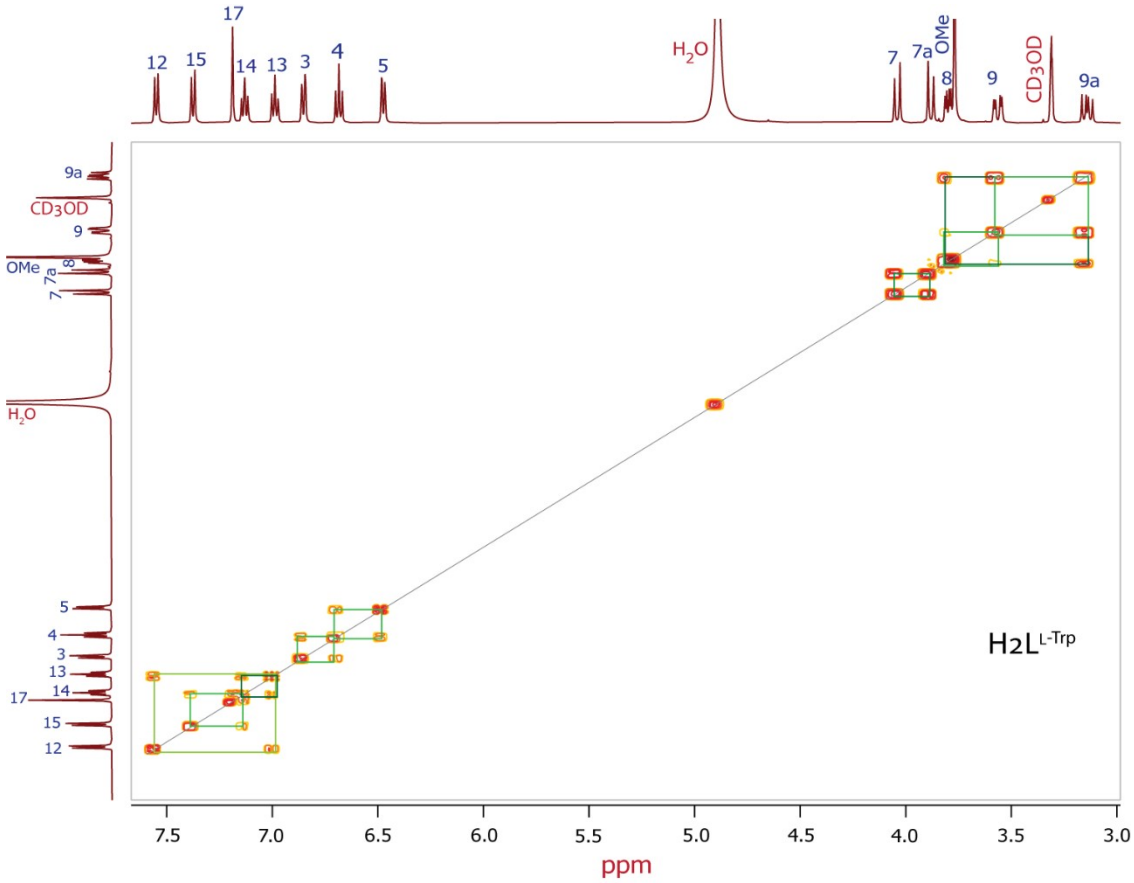


Figure S2. ^{1}H-^{1}H COSY NMR (500 MHz, CD_3OD) of $\mathbf{H_2L^{L\text{-}Trp}}$.

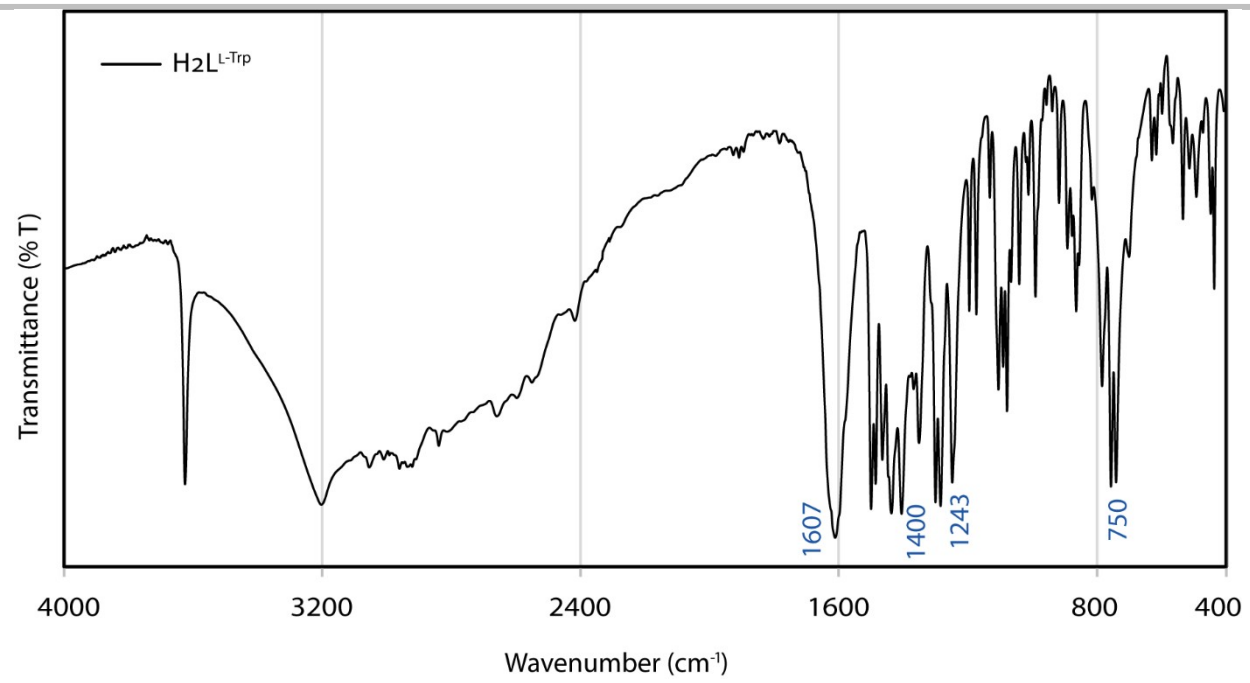


Figure S3. FTIR spectrum of $\mathbf{H_2L^{L\text{-}Trp}}$.

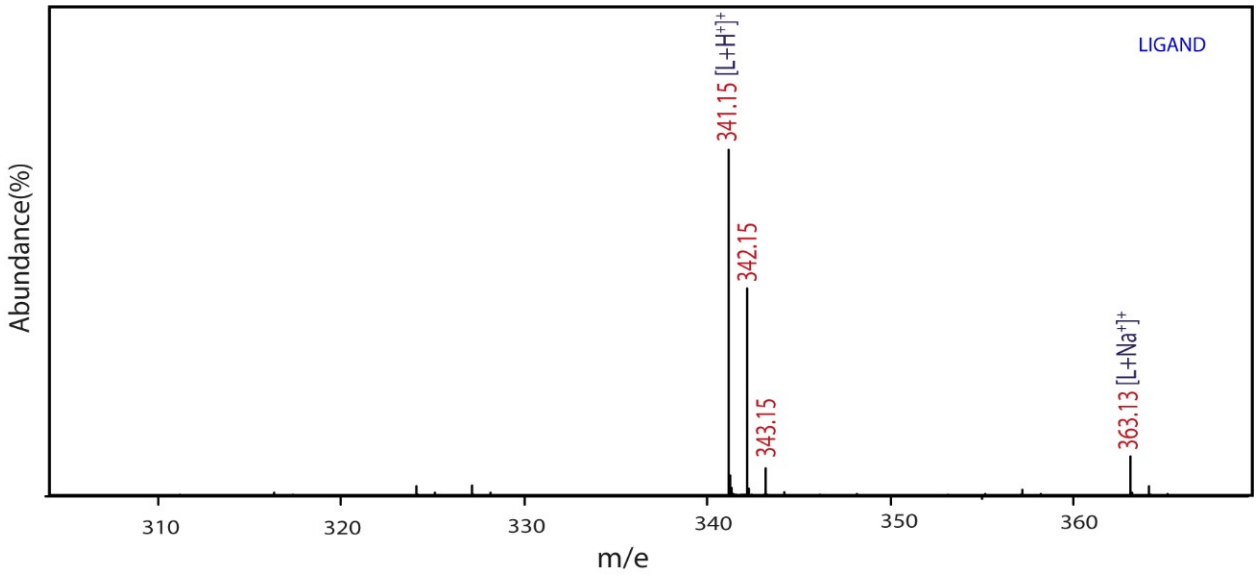


Figure S4. ESI-MS (+ve) spectrum of $H_2L^{L\text{-}Trp}$ in MeOH.

B. Synthesis and characterization data of the complexes.

$(NEt_4)[Co(L^{L\text{-}Trp})_2]$ (1). Solid $Co(ClO_4)_2.6H_2O$ (0.269 g, 0.735 mmol) was added to the methanolic solution (10 mL) of $H_2L^{L\text{-}Trp}$ (0.500 g, 1.47 mmol) and the reaction mixture was stirred for 15 min. The colour of the reaction mixture became pink. After 15 min., tetraethyl ammonium hydroxide solution (2.16 g, 14.7 mmol, 20 wt% in water) was slowly added to the reaction mixture, and the colour of the reaction mixture gradually changed from pink to reddish brown. The reaction mixture was stirred again for 6 h. at room temperature. Then, the solvent was evaporated using a rotary evaporator to reduce the volume of the reaction mixture, and DMF was added to it in a proportion of 3:1 (methanol: DMF) and was kept in a 50 mL beaker. Diamond-shaped reddish-brown coloured crystals were obtained after 8-10 days of slow evaporation. Crystals were washed with ethyl acetate and diethyl ether and dried under a vacuum. Yield: 72%.

^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.87 (s, 2H, $H^{NH\ indole}$), δ 7.82 (d, 2H, J = 8 Hz, H^{12}), δ 7.30 (d, 2H, J = 8 Hz, H^{15}), δ 7.20 (s, 2H, H^{17}), δ 7.04 (t, 2H, J = 7 Hz, H^{14}), δ 6.98 (t, 2H, J = 8 Hz, H^{13}), δ 6.55 (d, 2H, J = 7.5 Hz, H^5), δ 6.17 (d, 2H, J = 7.5 Hz, H^3), δ 6.03 (t, 2H, J = 7.5 Hz, H^4), δ 5.48 (t, 2H, J =11 Hz, $H^{NH\ LIGAND}$), δ 4.10 (dd, 2H, J = 4.5, 5.5 Hz, H^8), δ 4.17 (t, 2H, J = 12 Hz, H^7), δ 3.86 (d, 2H, J = 10.5 Hz, H^{7a}), δ 3.79 (dd, J = 4.5/5.5, 16 Hz 2H, H^9), δ 3.40 (dd, 2H, J = 4.5/5.5,16 Hz, H^{9a}), δ 3.18 (q, 8H, J = 7 Hz, H^{CH2}), δ 2.45 (s, 6H, H^{-OCH3}), δ 1.13 (t, 12H, J = 7 Hz, H^{CH3}); ^{1}H-^{1}H-COSY was also performed. Anal. Calcd for $(NEt_4)[Co(L^{L\text{-}Trp})_2]$: C, 63.80; H, 6.52; N, 8.09. Found: C, 63.887; H, 6.83; N, 8.122. IR (KBr, cm^{-1}): $\upsilon(COO^-)_{asym}$ 1646; $\upsilon(COO^-)_{sym}$ 1450; υ(C-O) 1284; υ(C-H)o/p-ring H 757; υ(M-O) 527; υ(M-N) 426. m/z (ESI-MS) $\{M+H\}^+$, $\{[(NEt_4)[Co(L^{L\text{-}Trp})_2]+H\}^+$; calcd: 866.35, found: 866.35.

$(Et_3NH)[Co(L^{L\text{-}Trp})_2]$ (2). Solid $Co(ClO_4)_2.6H_2O$ (0.269 g, 0.735 mmol) was added to the methanolic solution (10 mL) of $H_2L^{L\text{-}Trp}$ (0.500 g, 1.47 mmol) and the reaction mixture was stirred for 15 min. The colour of the reaction mixture became pink. After 15 min., methanolic solution (10 mL) of triethyl amine (0.298 g, 2.95 mmol) was slowly added to the reaction mixture, and the colour of the reaction mixture gradually changed from pink to light purple to reddish brown. The reaction mixture was stirred again for 6 h. at room temperature and evaporated using a rotary evaporator to reduce the volume. Acetonitrile was

added to it in a proportion of 1:3 (methanol: acetonitrile). Block-shaped dark brown coloured crystals were obtained after 3-4 days of slow evaporation. Crystals were washed with ethyl acetate and diethyl ether and dried under a vacuum. Yield: 75%.

^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.93 (s, 2H, $H^{NH\ indole}$), δ 8.95 (s, 1H, $H^{NH\ TEA}$), δ 7.83 (d, 2H, J = 7.5 Hz, H^{12}), δ 7.34 (d, 2H, J = 8 Hz, H^{15}), δ 7.21 (s, 2H, H^{17}), δ 7.08 (t, 2H, J = 7.5 Hz, H^{14}), δ 7.03 (t, 2H, J = 7.5 Hz, H^{13}), δ 6.62 (d, 2H, J = 7.5 Hz, H^5), δ 6.48 (d, 2H, J = 7 Hz, H^3), δ 6.24 (t, 2H, J = 8 Hz, H^4), δ 5.55 (t, 2H, J =11.5 Hz, $H^{NH\ LIGAND}$), δ 4.50 (dd, 2H, J = 4.5, 5.5 Hz, H^8), δ 4.11 (t, 2H, J = 11.5 Hz, H^7), δ 3.75-3.65 (m, 4H, $H^{7a,9}$), δ 3.54 (s, 6H, H^{-OCH3}), δ 3.39 (dd, 2H, J = 4.5/5.5,16 Hz, H^{9a}), δ 2.93 (q, 6H, J = 7 Hz, H^{CH2}), δ 1.06 (t, 9H, J = 7 Hz, H^{CH3}); ^{1}H-^{1}H-COSY was also performed. Anal. Calcd for $(Et_3NH)[Co(L^{L\text{-}Trp})_2]$: C, 63.07; H, 6.25; N, 8.36. Found: C, 62.708; H, 6.143; N, 8.034. IR (KBr, cm^{-1}): $\upsilon(COO^-)_{asym}$ 1615,1596; $\upsilon(COO^-)_{sym}$ 1458; υ(C-O) 1281; υ(C-H)o/p-ring H 744; υ(M-O) 532; υ(M-N) 431. m/z (ESI-MS) $\{M+H\}^+$, $\{[(Et_3NH)[Co(L^{L\text{-}Trp})_2]+H\}^+$; calcd: 838.32, found: 838.32.

$(Et_3NH)[Co(L^{L\text{-}Trp})_2]$ (3). Complex **1** (0.100 g, 0.115 mmol) was dissolved in 8 mL methanol, and methanolic solution (2 mL) of triethylammonium perchlorate (0.070 g, 0.374 mmol) was added to it and kept for stirring. After 10 min stirring, some solid precipitation appeared. Then filtered, filtrate was collected in a 25 mL beaker and kept for slow evaporation of the solvent at room temperature. Orange-red colored crystalline solids were obtained after 3 days. The crystals were filtered, washed with acetonitrile and diethyl ether, and dried in a vacuum. Yield: 0.084 g.

^{1}H NMR (d_6-DMSO, 500 MHz) δ 10.86 (s, 2H, $H^{NH\ indole}$), δ 8.83 (s, 1H, $H^{NH\ TEA}$), δ 7.82 (d, 2H, J = 8 Hz, H^{12}), δ 7.30 (d, 2H, J = 8 Hz, H^{15}), δ 7.20 (s, 2H, H^{17}), δ 7.04 (t, 2H, J = 7 Hz, H^{14}), δ 6.98 (t, 2H, J = 8 Hz, H^{13}), δ 6.54 (d, 2H, J = 7.5 Hz, H^5), δ 6.17 (d, 2H, J = 7.5 Hz, H^3), δ 6.03 (t, 2H, J = 7.5 Hz, H^4), δ 5.48 (t, 2H, J =11 Hz, $H^{NH\ LIGAND}$), δ 4.10 (dd, , J = 4.5,5.5 Hz, 2H, H^8), δ 4.18 (t, 2H, J = 12 Hz, H^7), δ 3.85 (d, 2H, J = 11 Hz, H^{7a}), δ 3.79 (dd, J = 4.5/5.5, 16 Hz 2H, H^9), δ 3.40 (dd, 2H, J = 4.5/5.5,16 Hz, H^{9a}), δ 3.08 (q, 6H, J = 7 Hz, H^{CH2}), δ 2.46 (s, 6H, H^{-OCH3}), δ 1.16 (t, 9H, J = 7 Hz, H^{CH3}); ^{1}H-^{1}H-COSY was also performed. Anal. Calcd for $(Et_3NH)[Co(L^{L\text{-}Trp})_2]$: C, 63.07; H, 6.25; N, 8.36. Found: C, 62.276; H, 6.203; N, 8.299. IR (KBr, cm^{-1}): $\upsilon(COO^-)_{asym}$ 1657; $\upsilon(COO^-)_{sym}$ 1456; υ(C-O) 1282; υ(C-H)o/p-ring H

754; υ(M-O) 540; υ(M-N) 430. m/z (ESI-MS) $\{M+H\}^+$, $\{(Et_3NH)[Co(L^{L\text{-}Trp})_2]+H\}^+$; calcd: 838.32, found: 838.32.

$(NEt_4)[Fe(L^{L\text{-}Trp})_2]$ (4). Solid $Fe(ClO_4)_2.7H_2O$ (0.269 g, 0.735 mmol) was added to the methanolic solution (10 mL) $H_2L^{L\text{-}Trp}$ (0.500 g, 1.47 mmol) and the reaction mixture was stirred for 15 min. The colour of the reaction mixture became bluish-purple. After 15 min., tetraethyl ammonium hydroxide solution (0.298 g, 2.94 mmol, 20 wt% in water) was slowly added to the reaction mixture and the colour of the reaction mixture gradually changed from bluish-purple to red. The reaction mixture was stirred again for 3 h. at room temperature. Then, the solvent was evaporated using a rotary evaporator to reduce the volume of the reaction mixture, and acetonitrile was added to it in a proportion of 3:1 (methanol: acetonitrile) and was kept in a 50 mL beaker. Diamond-shaped dark red coloured crystals were obtained after 8-9 days of slow evaporation. Crystals were washed with ethyl acetate and diethyl ether dried under vacuum. Yield: 65%.

Anal. Calcd for $(NEt_4)[Fe(L^{L\text{-}Trp})_2]$: C, 64.03; H, 6.54; N, 8.12. Found: C, 63.803; H, 7.183; N, 8.159. IR (KBr, cm^{-1}): $\upsilon(COO^-)_{asym}$ 1639; $\upsilon(COO^-)_{sym}$ 1453; υ(C-O) 1283; υ(C-H)o/p-ring H 757; υ(M-O) 579; υ(M-N) 426. μ_{eff} (solid, 292K); 5.75 μB/Fe. m/z (ESI-MS) $\{M+2H\}^+$, $\{[Fe(L^{L\text{-}Trp})_2]^- +2H\}^+$; calcd: 734.21, found: 734.20.

$(Et_3NH)[Fe(L^{L\text{-}Trp})_2].(Et_3NHClO_4)$ (5). Method 1 Directly from the ligand: The ligand $H_2L^{L\text{-}Trp}$ (0.500 g, 1.47 mmol) was dissolved in 10 mL MeOH in a 100 mL round bottom flask, and solid $Fe(ClO_4)_2.7H_2O$ (0.270 g, 0.735 mmol) was added into it. The colour of the solution became blue-violet and the reaction mixture was stirred for 15 min. Then, a methanolic solution (10 mL) of triethyl amine (0.446 g, 4.41 mmol) was slowly added to the reaction mixture, and the colour of the reaction mixture gradually changed from blue-violet to red-violet. The resulting red-violet solution was stirred for another 3 h. at room temperature. Solid crystalline red-violet coloured solid appeared, which was filtered off, and washed with ethyl acetate and diethyl ether. The solid was dried in a vacuum desiccator. The solid was redissolved in

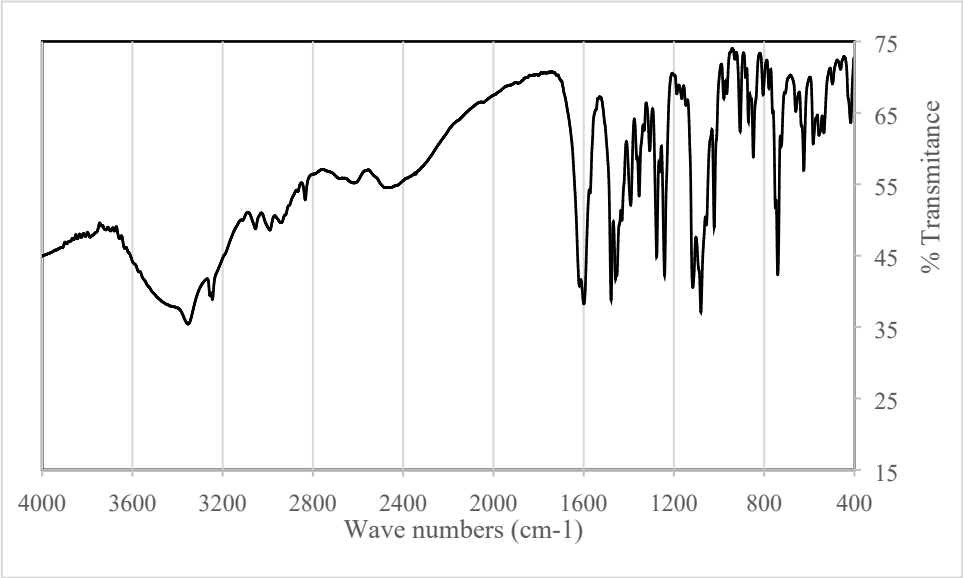
methanol along with a few drops of DMF, and it was kept in a 25 mL beaker for slow evaporation of the solvent. Block-shaped red crystals were obtained after 3 days. Yield: 74%.

Method 2, Synthesis from Complex 4: Complex **4** (0.100 g, 0.116 mmol) was dissolved in 10 mL methanol, and methanolic solution (5 mL) of triethylammonium perchlorate (0.070 g, 0.347 mmol) was added to it and kept for stirring. After 15 min stirring, the red-colored solution was kept in a 25 mL conical flask, which, upon slow evaporation at room temperature, gave block-shaped red crystals of **5** after 6 days. Yield: 0.073 g

Anal. Calcd for $(Et_3NH)[Fe(L^{L\text{-}Trp})_2]$. Et_3NHClO_4: C, 57.94; H, 6.61; N, 8.11. Found: C, 57.804; H, 6.581; N, 8.088. IR (KBr, cm^{-1}): $\upsilon(COO^-)_{asym}$ 1600; $\upsilon(COO^-)_{sym}$ 1458; υ(C-O) 1276; υ(C-H)o/p-ring H 740; υ(M-O) 583; υ(M-N) 417. μ_{eff} (solid, 292K); 5.8 μB/Fe. m/z (ESI-MS) $\{M+H\}^+$, $\{(HNEt_3)[Fe(L^{L\text{-}Trp})_2]+H\}^+$; calcd: 835.33, found: 835.27.

FTIR of 5 from Method 1 and Method 2 are identical (Figure S4A). The Crystal Structure of 5 from both methods was solved. Structural data of crystals from method 2 has been used in the manuscript. The structural parameters of the crystals and an ORTEP diagram from method 1 are in Figure S4B.

Note. For elemental analysis, the crystalline samples were powdered and dried under a vacuum desiccator for several days before analysis. Thus, the number and type of solvent molecules in the crystal structure and isolated product differ. We used the formula weight of the bulk for solution concentration and magnetic moment calculation.



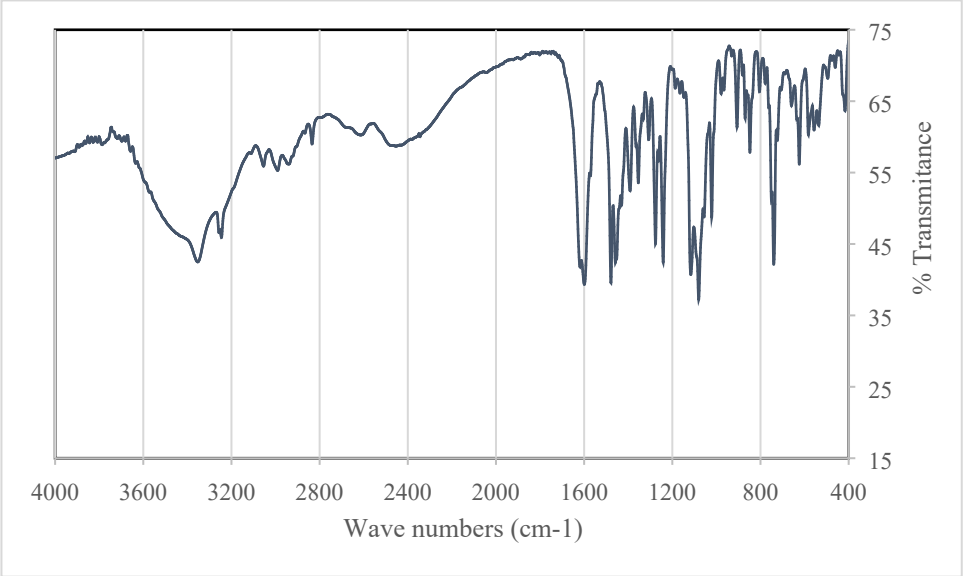


Figure S4a. FTIR of **5** obtained from Method **1** (Top) and Method **2** (Bottom).

Crystal Parameter for the crystals of 5 isolated from Method 1: Space group, $P2_1$, *a* 9.760(6) Å, *b* 19.804 (13) Å, *c* 27.476 Å, $\alpha = \gamma = 90°$, β 93.32(3), Volume 5301.611(6) $Å^3$, Z/ρ 4/1.298, μ 0.399, Coll reflns 11205, Indep Refln 6967, FLACK param. 0.00(2), GOF 1.031, *R*1 0.0679, *wR*2 0.1366, *R*1 (all data) 0.1293, *wR*2(all data) 0.1574. The parameters of crystals from Method 2 (used in the manuscript) are in Table S3.

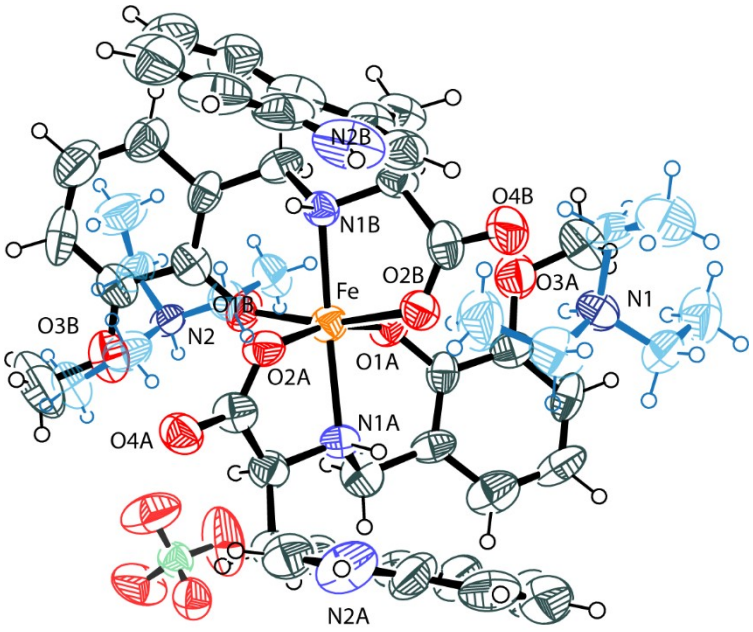


Figure S4b. ORTEP figure of **5** with 40% ellipsoid probability, obtained from Method 1.

C. NMR plots of the Co(III) complexes.

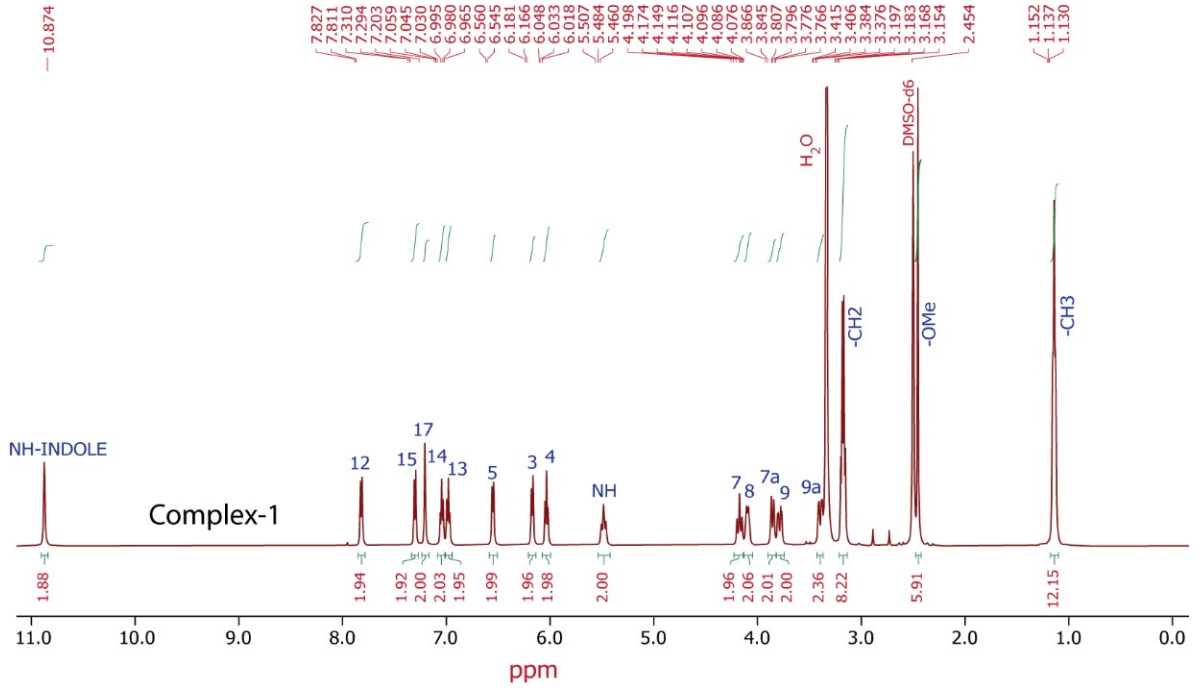


Figure S5. ^{1}H NMR (500 MHz, d_6-DMSO) of **1**.

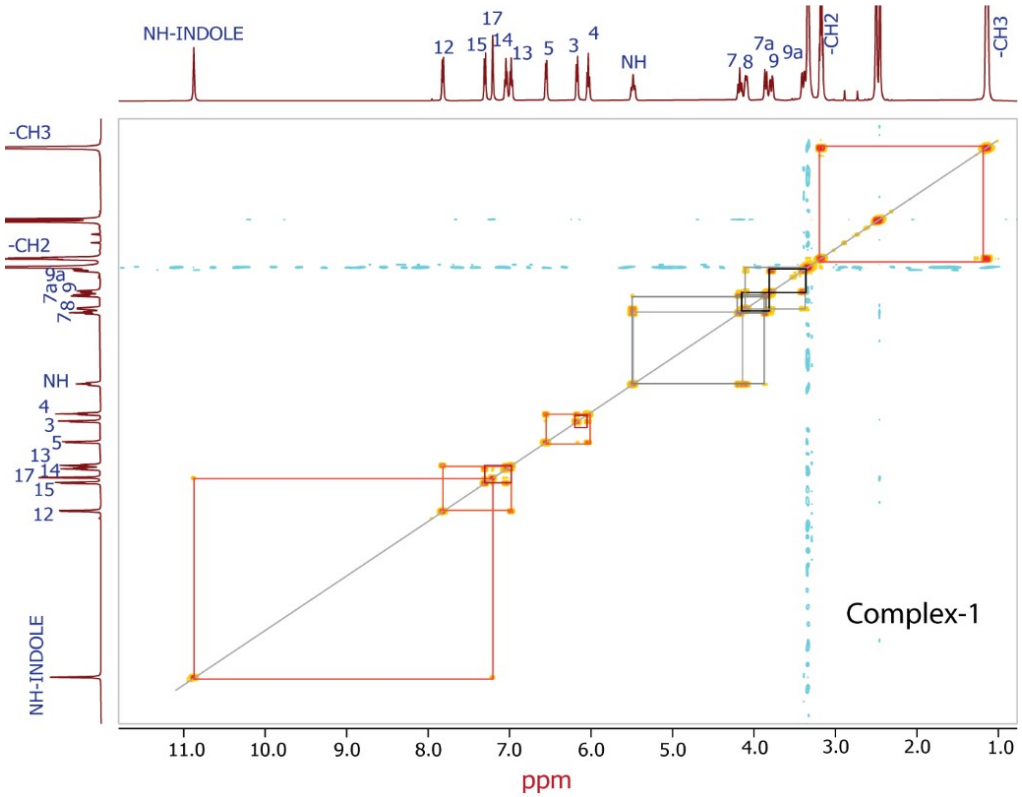


Figure S6. ^{1}H-^{1}H COSY NMR (500 MHz, d_6-DMSO) of **1**.

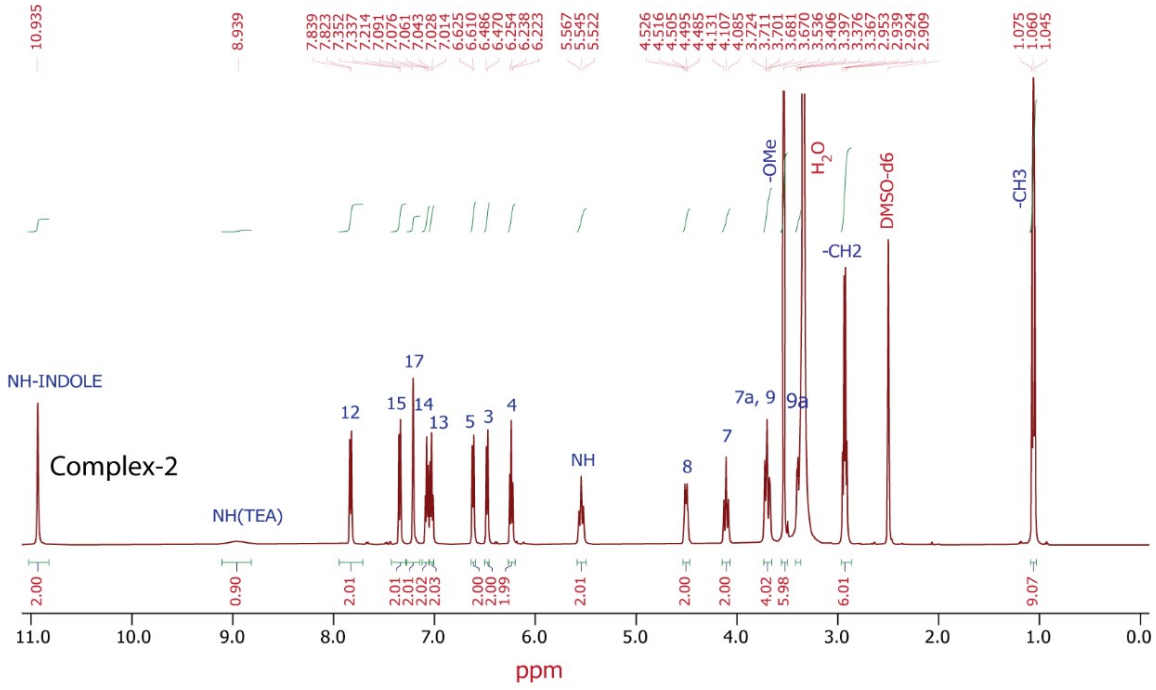


Figure S7. ^{1}H NMR (500 MHz, d_6-DMSO) of **2**.

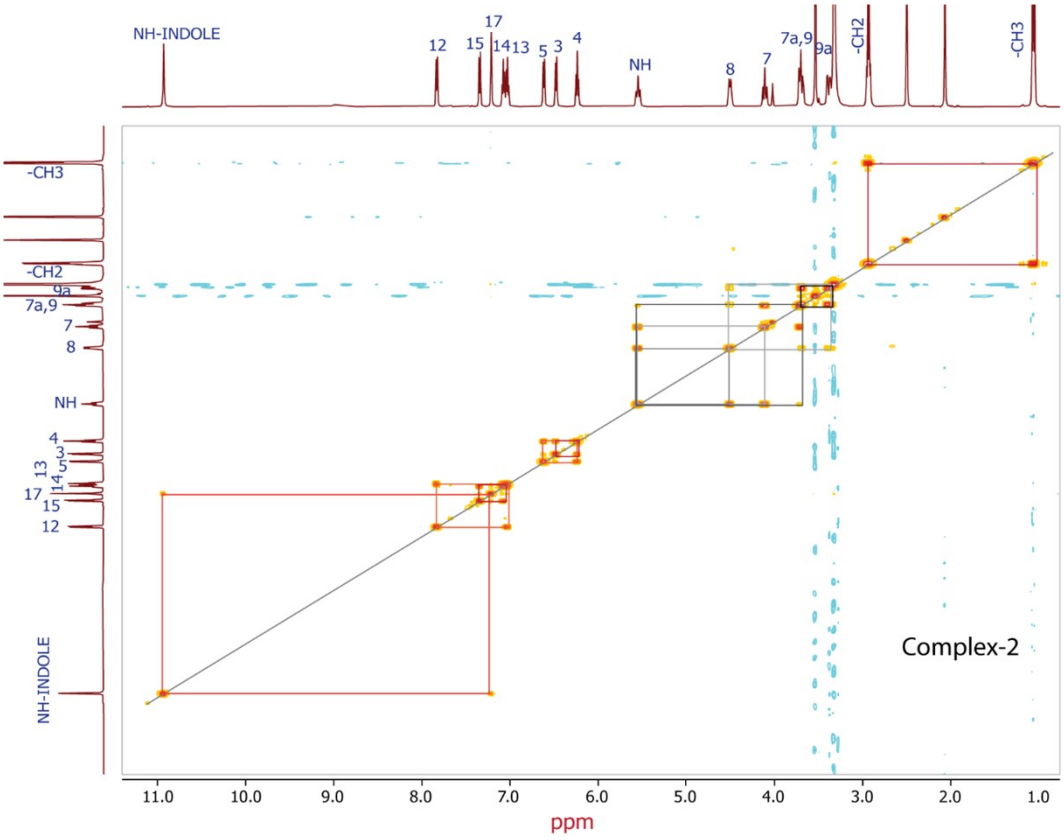


Figure S8. ^{1}H-^{1}H COSY NMR (500 MHz, d_6-DMSO) of **2**.

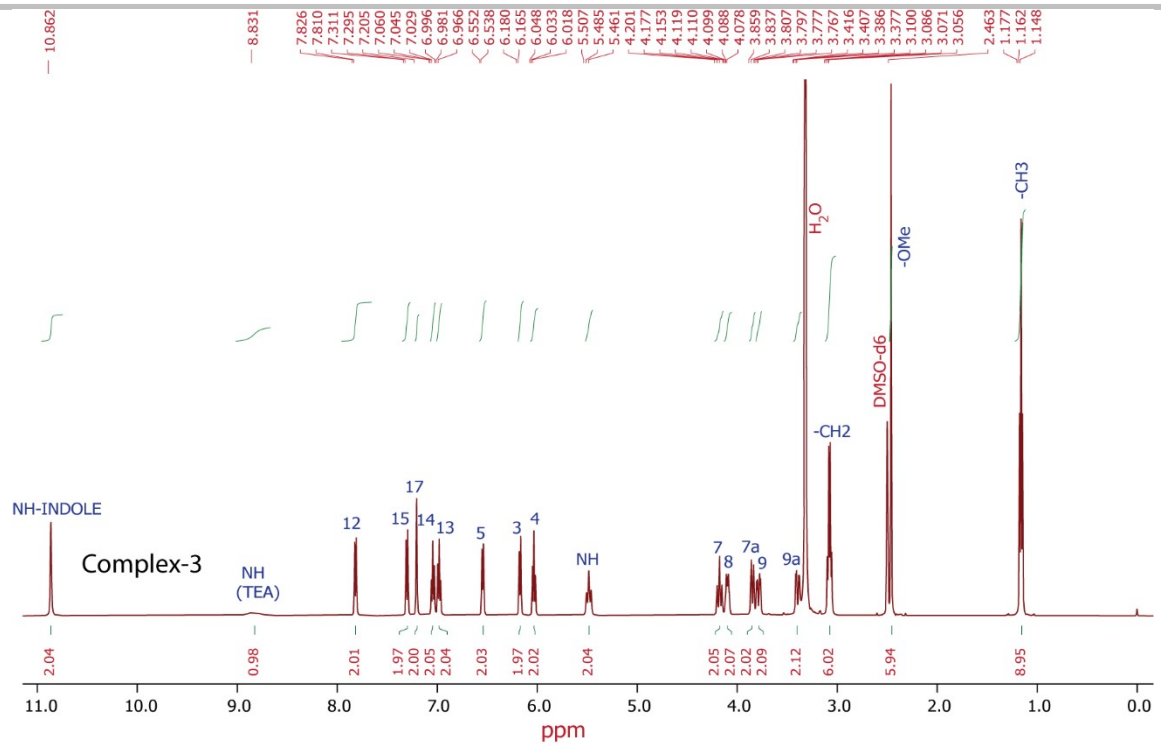


Figure S9. ^{1}H NMR (500 MHz, d_6-DMSO) of **3**.

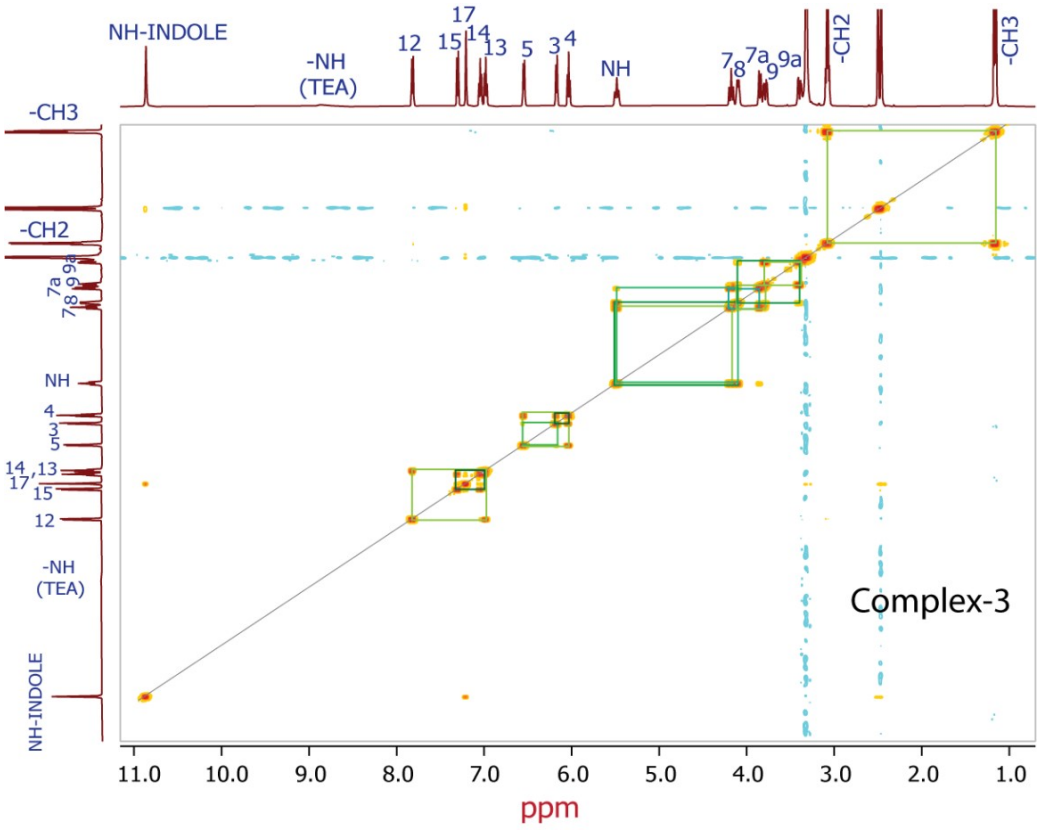


Figure S10. ^{1}H-^{1}H COSY NMR (500 MHz, d_6-DMSO) of **3**.

The solution-state structural difference among 1, 2, and 3

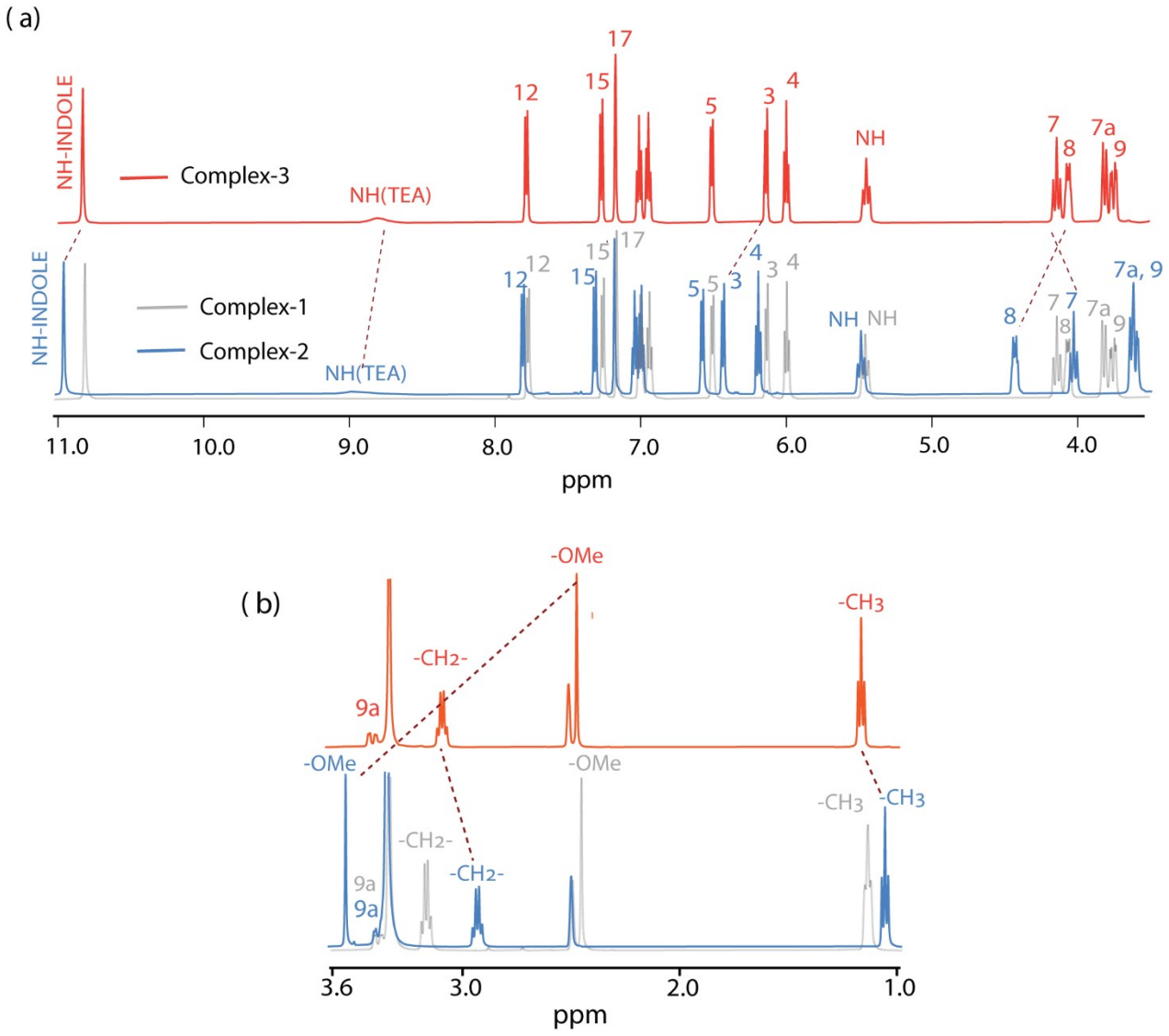


Figure S11. Stacked partial ^{1}H NMR spectra (500 MHz, d_6-DMSO) of **1**, **2**, and **3** - (a) and (b) showing different ^{1}H NMR signal positions of the similar type of protons belonging to their anionic Co(III) complex units and their respective counter ions.

D. ^{1}H NMR plots of the transformations in solution.

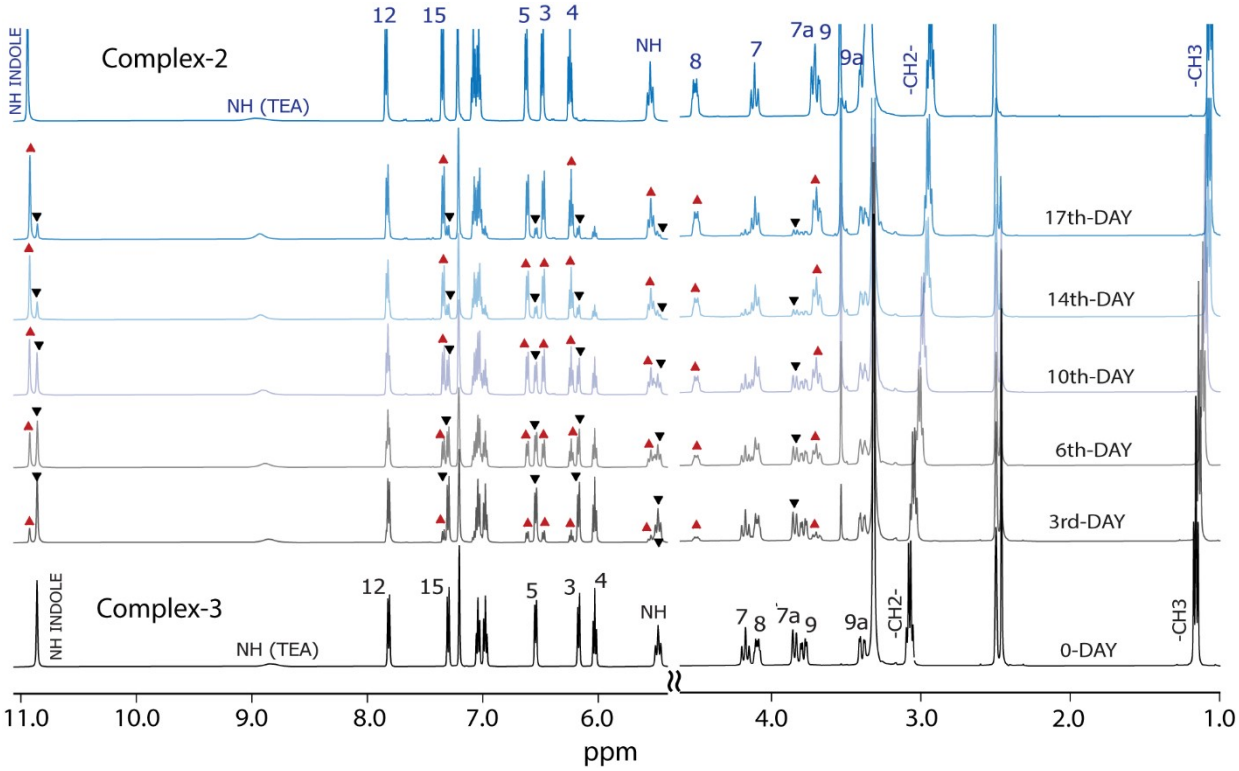


Figure S12. Partial stacked ^{1}H NMR spectra (500 MHz, d_6-DMSO) slowing structural transformation of **3** to **2 at room temperature**.

Protons	NH (Indole)	NH (TEA)	H13	H5	H3	H4	NH (com)	H7	H7a	H8	OMe
δ of **3** (ppm)	10.86	8.83	6.98	6.55	6.17	6.03	5.48	4.18	3.85	4.10	2.46
δ of **2** (ppm)	10.93	8.95	7.03	6.62	6.48	6.24	5.55	4.11	3.71	4.50	3.54
Δδ (ppm)	-0.07	-0.12	-0.05	-0.07	-0.31	-0.21	-0.07	+0.07	+0.14	-0.40	-1.08

Table S1. Chemical shift differences of the similar types of protons in **2** and **3**, respectively.

Note: (-)ve Δδ values indicating downfield shifting and (+) Δδ values indicating upfield shifting of the ^{1}H NMR signals.

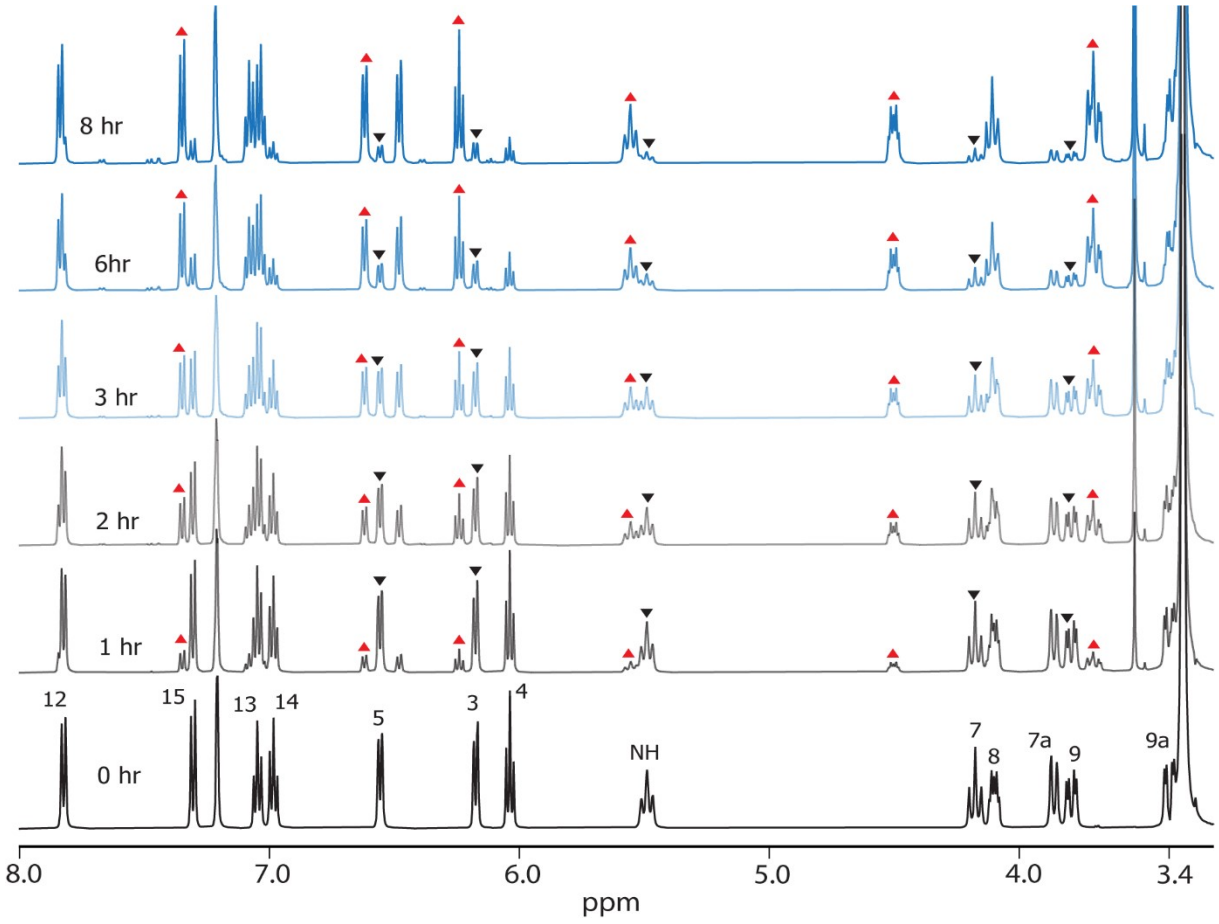


Figure S13. Partial stacked ^{1}H NMR spectra (500 MHz, d_6-DMSO) of **3**, showing that the structural transformation became faster **at 60˚C**.

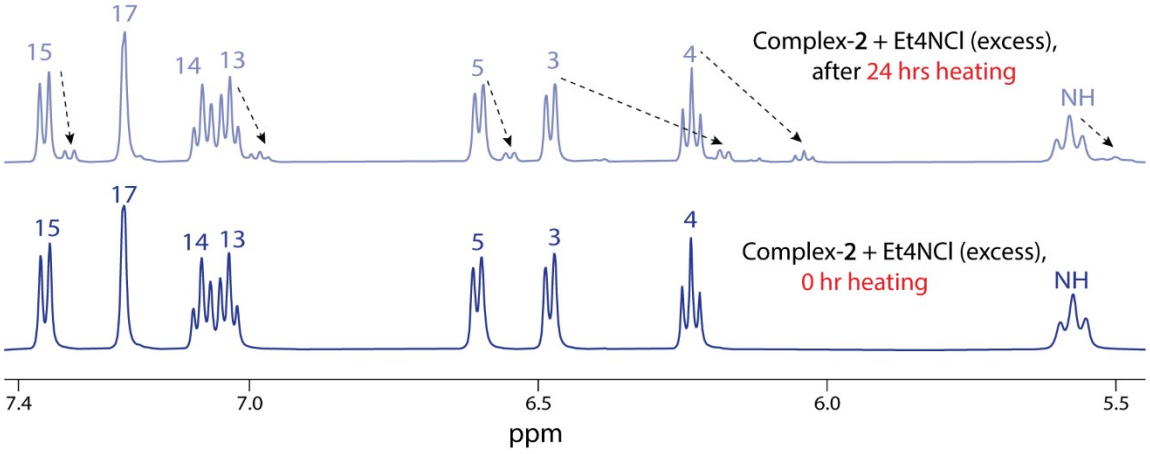


Figure S13a. ^{1}H NMR spectra (**partial**) of **3** with excess Et_4NCl before and after heating at 60˚C for 24 hrs. Spectra were recorded in d6-DMSO using a 500 MHz NMR instrument.

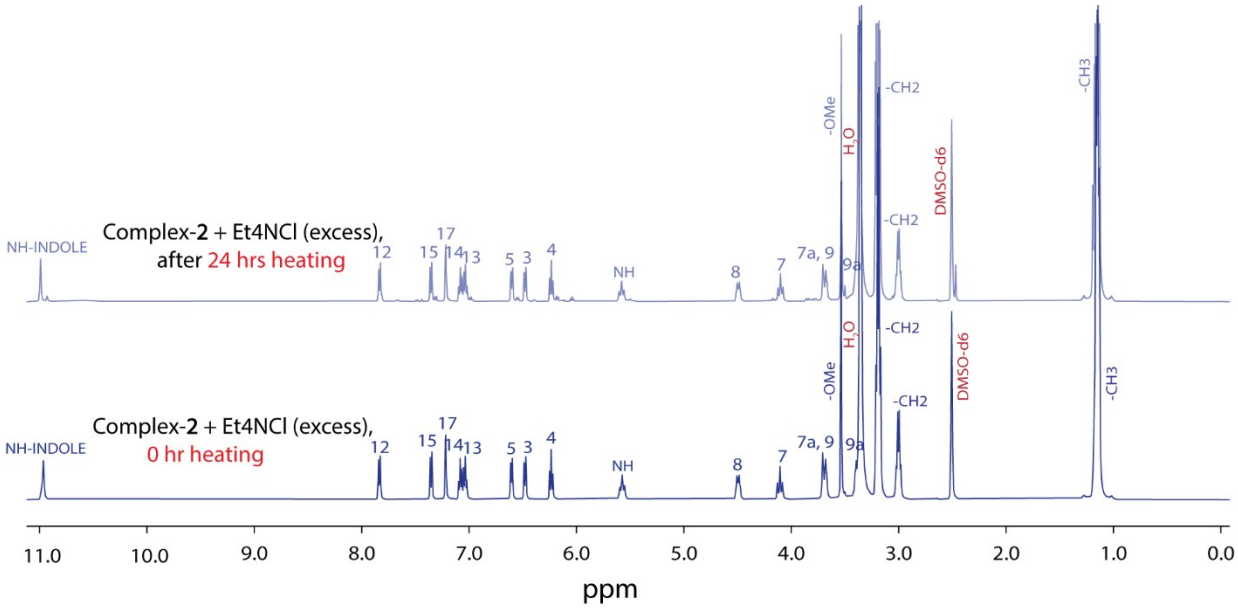


Figure S13b. ^{1}H NMR spectra **(Full)** of **3** with excess Et_4NCl before and after heating at 60˚C for 24 hrs. Spectra were recorded in d6-DMSO using a 500 MHz NMR instrument.

E. UV-visible and CD data

Table S2. Electronic spectroscopic data for complex **1-6** (In DMF).

Complexes	λ_{max}/nm (ε/$M^{-1}cm^{-1}$)
Co(III)-complexes	
1	690(96), 518(377) (sh), 390(2205)
2	680(280), 525(323) (sh), 378(3860)
3	690(103), 518(389) (sh), 390(2310)
Fe(III)-complexes	
4	471(3110), 329(5397) (sh)
5	475(3095), 332(4718) (sh)

Note: UV-visible spectra of Co(III)-complexes **1**, **2**, and **3** in DMF are in the manuscript Figure 3.

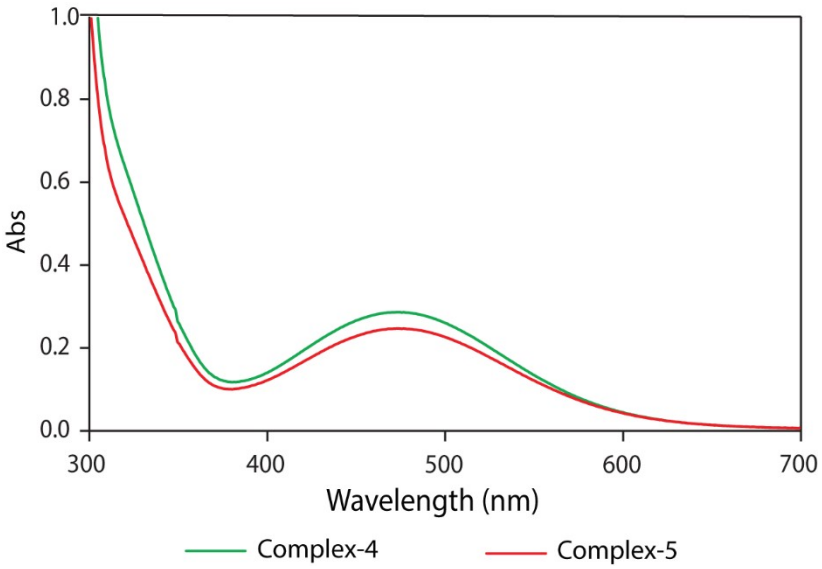


Figure S14. UV-visible spectra of Fe(III)-complexes (**4** and **5**) in DMF at a concentration of 0.1 mM.

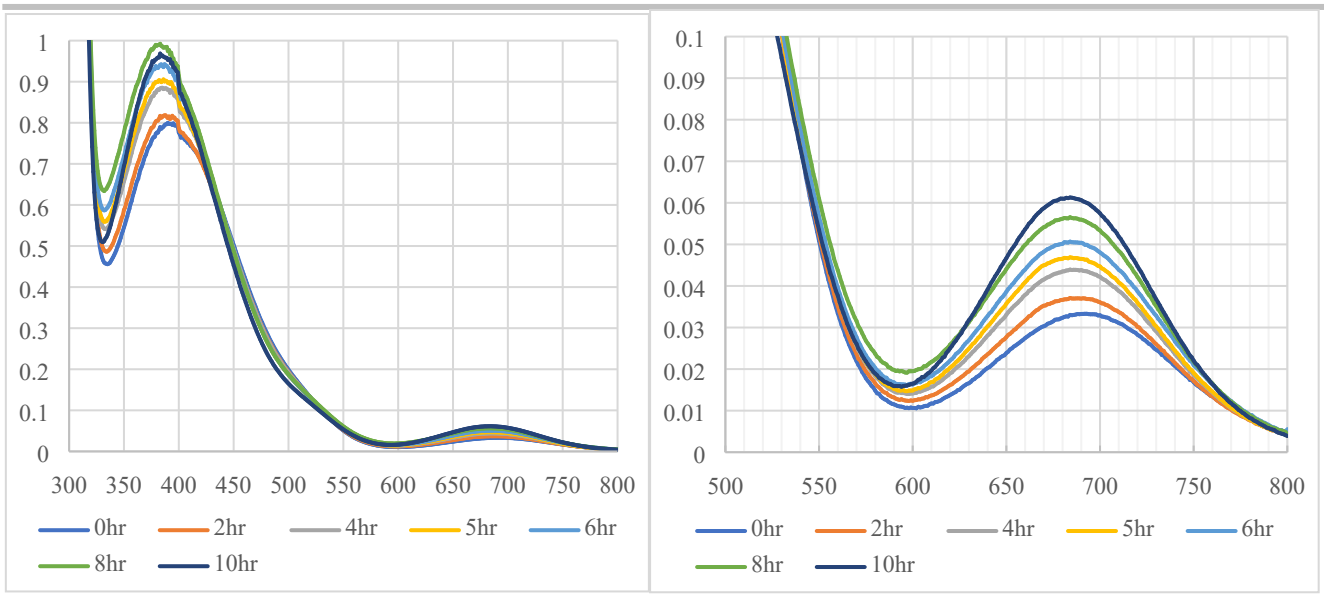


Figure S14a. Spectral change upon heating **3** at 60 °C in DMF.

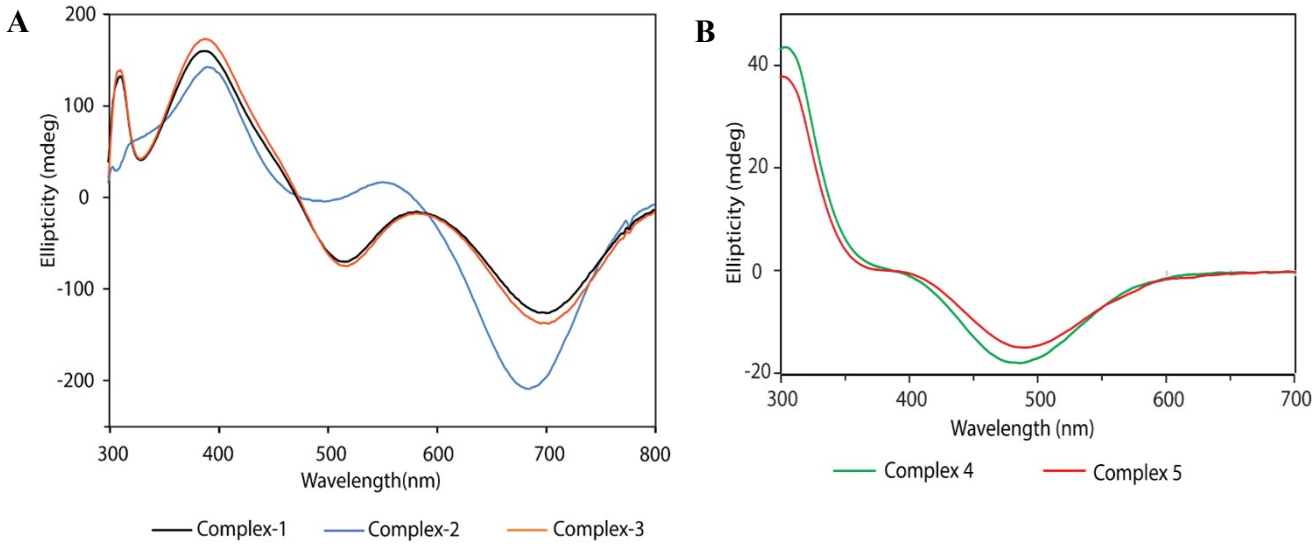


Figure S15. (A) CD spectra of Co(III) complexes (**1-3**), and **(B)** CD spectra of Fe(III) complexes (**4** and **5**) in DMF. Concentrations used: For **1-3**, 3 mM in DMF; For **4** and **5**, 1 mM in DMF. Path length used for all, 1mm.

F. Single Crystal X-ray Structure data

Complexes	**1**	**2**	**4**	**5**
Empirical Formula	$C_{46}H_{60}CoN_5O_{10}$	$C_{47}H_{55}CoN_6O_{10}$	$C_{46}H_{56}FeN_5O_{10}$	C_{50} H_{65} Cl Fe N_6 O_{12}
Formula Weight	901.92	922.90	894.80	1033.38
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	tetragonal	orthorhombic	tetragonal	monoclinic
Space group	$P4_32_12$	$P2_1\ 2_1\ 2_1$	$P4_32_12$	$P2_1$
a, Å	12.1822(4)	37.955(11)	12.1909(7)	9.7580(10)
b, Å	12.1822(4)	9.606(3)	12.1909(7)	19.6919(19)
c, Å	30.3583(16)	13.538(4)	30.773(3)	27.323(3)
α, deg	90	90	90	90
β, deg	90	90	90	93.402(3)
γ, deg	90	90	90	90
Volume, Å^3	4505.4(4)	4936(2)	4573.4(6)	5240.9(9)
Z/ρ	4/1.330	4/1.242	4/ 1.300	4/ 1.310
μ	0.444	0.407	0.392	0.404
Coll reflns	4427	8693	4039	18351
Indep refln	3911	5916	3516	11787
FLACK para.	0.010(5)	0.099(6)	0.009(6)	0.124(7)
GOF	1.121	1.179	1.147	1.176
R1[a]	0.0340	0.0565	0.0450	0.0904
wR2[a]	0.0876	0.1358	0.1176	0.1350
R1[b]	0.0434	0.1076	0.0570	0.1530
wR2[b]	0.0969	0.1763	0.1353	0.1585

Table S3. Crystallographic data and refinement parameters of **1**, **2**, **4**, and **5**.

[a] $I > 2\sigma$. [b] All data

Crystallography. The crystal of the complexes obtained during synthesis was used for X-ray analysis. The crystals were mounted on glass fibre. All geometric and intensity data were collected at room temperature using a Bruker SMART APEX CCD diffractometer equipped with a fine

focus 1.75 kW sealed tube Mo-Kα (λ= 0.71073 Å) X-ray source, with increasing ω (width of 0.3° per frame) at a scan speed of either 3 or 5 s/frame. The SMART software was used for data acquisition and the SAINT software for data extraction. Absorption corrections were done using a multi-scan. The structure solution and refinement were performed on the WinGX environment using the SHELXS97 SHELXL97 programs. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located from the Fourier maps and refined isotropically wherever possible. Thus, some C-H bonds will not be ideal and may vary. Some hydrogen atoms attached to the solvent molecules could not be located or fixed, so the molecular weight may not match. A perspective view of the complex was obtained by ORTEP. The structures were deposited to the CCDC with CCDC numbers of the structures 2351541-2351544 for **1**, **2**, **4**, and **5**, respectively.

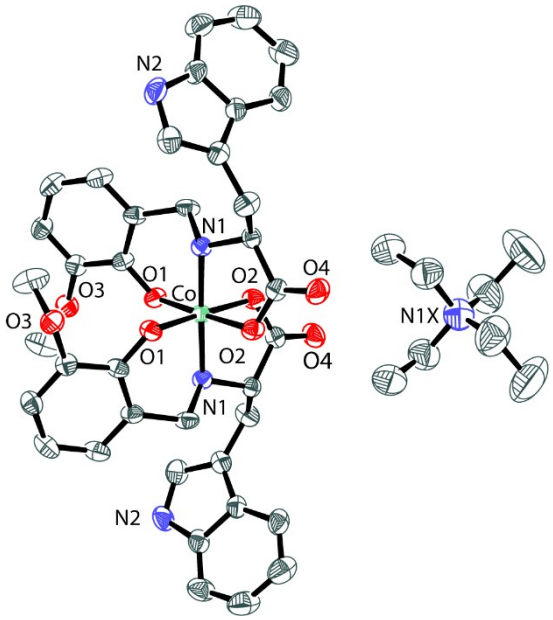


Figure S16. ORTEP figure **1** with 40 % ellipsoid probability.

Table S4. Bond lengths (Å) and angles (o) of complex **1**.

Co1	-O1	1.9088(19)	C10	-C17	1.364(5)
Co1	-O2	1.910(2)	C11	-C16	1.418(5)
Co1	-N1	1.940(3)	C11	-C12	1.394(5)
Co1	-O1_a	1.9088(19)	C12	-C13	1.375(7)
Co1	-O2_a	1.910(2)	C13	-C14	1.384(8)
Co1	-N1_a	1.940(3)	C14	-C15	1.372(7)
O1	-C1	1.331(3)	C15	-C16	1.389(6)
O2	-C18	1.288(4)	N1X	-C2X_b	1.501(8)
O3	-C2	1.388(4)	N1X	-C2X	1.501(8)
O3	-C19	1.402(6)	N1X	-C3X	1.523(7)
O4	-C18	1.235(4)	N1X	-C3X_b	1.523(7)
N1	-C7	1.482(4)	N1	-C8	1.483(4)
N2	-C16	1.364(5)	N2	-C17	1.360(5)
C1	-C2	1.400(5)	C1	-C6	1.407(5)
N1	-H1	0.77(4)	C2	-C3	1.378(5)
N2	-H2	0.8600	C3	-C4	1.375(5)
C4	-C5	1.380(5)	C5	-C6	1.387(5)
C6	-C7	1.495(5)	C8	-C9	1.547(4)
C8	-C18	1.529(5)	C9	-C10	1.503(5)
C10	-C11	1.426(5)	C1X	-C2X	1.579(11)
C3X	-C4X	1.530(9)			

Angles

O1	-Co1	-O2	175.44(9)	C16	-N2	-H2	126.00
O1	-Co1	-N1	95.35(10)	C17	-N2	-H2	126.00
O1	-Co1	-O1_a	96.16(9)	C1	-C2	-C3	121.4(3)
O1	-Co1	-O2_a	88.40(9)	O3	-C2	-C1	118.0(3)
O1	-Co1	-N1_a	85.65(10)	O3	-C2	-C3	120.3(3)
O2	-Co1	-N1	84.98(10)	C2	-C3	-C4	120.6(3)
O1_a	-Co1	-O2	88.40(9)	C3	-C4	-C5	119.3(3)
O2	-Co1	-O2_a	87.04(9)	C4	-C5	-C6	120.7(3)
O2	-Co1	-N1_a	93.94(10)	C1	-C6	-C7	117.8(3)

O1_a	-Co1	-N1	85.65(10)	C5	-C6	-C7	121.6(3)
O2_a	-Co1	-N1	93.94(10)	C1	-C6	-C5	120.6(3)
N1	-Co1	-N1_a	178.51(10)	N1	-C7	-C6	109.9(3)
O1_a	-Co1	-O2_a	175.44(9)	N1	-C8	-C9	112.5(3)
O1_a	-Co1	-N1_a	95.35(10)	N1	-C8	-C18	108.8(2)
O2_a	-Co1	-N1_a	84.98(10)	C9	-C8	-C18	110.2(3)
Co1	-O1	-C1	121.08(16)	C8	-C9	-C10	115.4(3)
Co1	-O2	-C18	114.1(2)	C9	-C10	-C17	127.3(3)
C2	-O3	-C19	115.3(3)	C9	-C10	-C11	127.2(3)
Co1	-N1	-C7	112.4(2)	C11	-C10	-C17	105.5(3)
Co1	-N1	-C8	109.18(19)	C10	-C11	-C12	134.7(3)
C7	-N1	-C8	114.2(2)	C10	-C11	-C16	107.3(3)
C16	-N2	-C17	108.7(3)	C12	-C11	-C16	118.0(3)
O1	-C1	-C2	120.5(3)	C11	-C12	-C13	119.6(4)
O1	-C1	-C6	122.3(3)	C12	-C13	-C14	120.8(4)
C2	-C1	-C6	117.2(3)	C13	-C14	-C15	122.2(5)
Co1	-N1	-H1	103(3)	C14	-C15	-C16	116.8(4)
C7	-N1	-H1	110(3)	N2	-C16	-C15	130.2(4)
C8	-N1	-H1	107(3)	C11	-C16	-C15	122.6(4)

Table S5 Non-covalent interactions in Complex **1.**

Atoms	**D-H (Å)**	**H…A (Å)**	**D…A(Å)**	**DHA(°)**
O1X-H1XD…O4	0.85	2.07	2.897(5)	163
N2-H2…O1	0.86	2.38	3.198(4)	160
N2-H2…O2	0.86	2.52	3.113(4)	127
O1X-H1HE…O1	0.85	2.57	3.233(6)	136
O1X-H1XE…O3	0.85	2.16	2.926(6)	151
N1-H1…O1	0.77(4)	2.28(4)	2.616(3)	107
C13-H13…O3	0.93	2.37	3.303(5)	176
C19-H19B…O4	0.96	2.59	3.475(5)	154

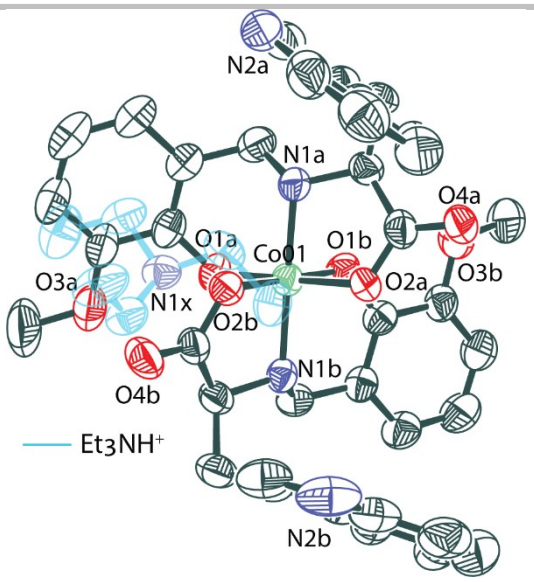


Figure S17. ORTEP figure of **2** with 40 % ellipsoid probability.

Table S6. Bond lengths (Å) and angles (o) of complex **2**.

Co01	-O1A	1.908(5)	C1B	-C2B	1.427(11)
Co01	-O1B	1.879(4)	N1B	-H1B	0.9800
Co01	-O2A	1.905(5)	C2A	-C3A	1.392(13)
Co01	-O2B	1.902(4)	N2A	-H2A	0.8600
Co01	-N1A	1.930(5)	N2B	-H2B	0.8600
Co01	-N1B	1.926(5)	C2B	-C3B	1.370(13)
O1A	-C1A	1.334(8)	C3A	-C4A	1.396(16)
O1B	-C1B	1.322(8)	C3B	-C4B	1.371(16)
O2A	-C18A	1.289(9)	C4A	-C5A	1.360(15)
O2B	-C18B	1.292(9)	C4B	-C5B	1.396(13)
O3A	-C2A	1.348(13)	C5A	-C6A	1.397(12)
O3A	-C19A	1.395(14)	C5B	-C6B	1.378(11)
O3B	-C2B	1.373(10)	C6A	-C7A	1.501(10)
O3B	-C19B	1.396(10)	C6B	-C7B	1.478(11)
O4A	-C18A	1.245(10)	C8A	-C9A	1.547(9)
O4B	-C18B	1.234(9)	C8A	-C18A	1.522(12)
N1A	-C7A	1.475(10)	C8B	-C9B	1.541(12)
N1A	-C8A	1.468(9)	C8B	-C18B	1.502(10)
N1B	-C7B	1.491(9)	C9A	-C10A	1.521(11)
N1B	-C8B	1.487(9)	C9B	-C10B	1.510(13)
N2A	-C16A	1.389(13)	C10A	-C11A	1.435(12)
N2A	-C17A	1.363(12)	C10A	-C17A	1.367(11)
N2B	-C16B	1.358(17)	C10B	-C17B	1.368(14)
N2B	-C17B	1.365(16)	C10B	-C11B	1.422(14)
C1A	-C2A	1.399(11)	C11A	-C16A	1.415(11)
C1A	-C6A	1.403(11)	C11A	-C12A	1.391(13)
N1A	-H1A	0.9800	C11B	-C16B	1.407(12)
C1B	-C6B	1.420(10)	C11B	-C12B	1.385(13)
C12A	-C13A	1.373(15)	C12B	-C13B	1.361(15)
C13A	-C14A	1.415(14)	C13B	-C14B	1.38(2)
C14A	-C15A	1.344(16)	C14B	-C15B	1.35(2)
C15A	-C16A	1.388(15)	C15B	-C16B	1.38(2)
N1X	-C5X	1.512(13)	C17B	-H17B	0.9300
N1X	-C1X	1.477(13)	C19A	-H19F	0.9600
N1X	-C3X	1.507(12)	C19A	-H19D	0.9600

C3A	-H3A	0.9300	C19A	-H19E	0.9600
C3B	-H3B	0.9300	C19B	-H19A	0.9600
C4A	-H4A	0.9300	C19B	-H19B	0.9600
C4B	-H4B	0.9300	C19B	-H19C	0.9600
C5A	-H5A	0.9300	C1X	-C2X	1.510(16)
C5B	-H5B	0.9300	O1X	-C50	1.34(4)
C7A	-H7AA	0.9700	N1X	-H1X	0.9800
C7A	-H7AB	0.9700	C3X	-C4X	1.502(18)
C7B	-H7BA	0.9700	C5X	-C6X	1.471(18)
C7B	-H7BB	0.9700	O51	-C50	1.33(5)
C8A	-H8A	0.9800	C1X	-H1XB	0.9700
C8B	-H8B	0.9800	C1X	-H1XA	0.9700
C9A	-H9AB	0.9700	C2X	-H2XB	0.9600
C9A	-H9AA	0.9700	C2X	-H2XC	0.9600
C9B	-H9BA	0.9700	C2X	-H2XA	0.9600
C9B	-H9BB	0.9700	C3X	-H3XA	0.9700
C12A	-H12A	0.9300	C3X	-H3XB	0.9700
C4X	-H4XA	0.9600	C6X	-H6XB	0.9600
C4X	-H4XC	0.9600	N2X	-C7X	1.11(2)
C4X	-H4XB	0.9600	C7X	-C8X	1.437(19)
C5X	-H5XB	0.9700	C8X	-H8XA	0.9600
C5X	-H5XA	0.9700	C8X	-H8XB	0.9600
C6X	-H6XC	0.9600	C8X	-H8XC	0.9600
C6X	-H6XA	0.9600			

N2	-C16	-C11	107.3(3)	C10	-C9	-H9A	108.00
N2	-C17	-C10	111.2(3)	C10	-C9	-H9B	108.00
O2	-C18	-C8	116.7(3)	C11	-C12	-H12	120.00
O4	-C18	-C8	119.2(3)	C13	-C12	-H12	120.00
O2	-C18	-O4	124.1(3)	C12	-C13	-H13	120.00
C2X_b	-N1X	-C3X	110.8(5)	C14	-C13	-H13	120.00
C3X	-N1X	-C3X_b	109.2(4)	C15	-C14	-H14	119.00
C2X_b	-N1X	-C3X_b	105.1(3)	C13	-C14	-H14	119.00
C2X	-N1X	-C3X_b	110.8(5)	C14	-C15	-H15	122.00
C2X	-N1X	-C3X	105.1(3)	C16	-C15	-H15	122.00
C2X	-N1X	-C2X_b	115.9(5)	N2	-C17	-H17	124.00
C2	-C3	-H3	120.00	C10	-C17	-H17	124.00
C4	-C3	-H3	120.00	H19B	-C19	-H19C	110.00
C5	-C4	-H4	120.00	O3	-C19	-H19A	109.00
C3	-C4	-H4	120.00	O3	-C19	-H19B	109.00
C4	-C5	-H5	120.00	O3	-C19	-H19C	109.00
C6	-C5	-H5	120.00	H19A	-C19	-H19B	109.00
N1	-C7	-H7A	110.00	H19A	-C19	-H19C	109.00
H7A	-C7	-H7B	108.00	N1X	-C2X	-C1X	112.5(5)
C6	-C7	-H7B	110.00	N1X	-C3X	-C4X	114.4(5)
N1	-C7	-H7B	110.00	C2X	-C1X	-H1XA	110.00
C6	-C7	-H7A	110.00	C2X	-C1X	-H1XB	109.00
C9	-C8	-H8	108.00	C2X	-C1X	-H1XC	109.00
N1	-C8	-H8	108.00	H1XA	-C1X	-H1XB	109.00
C18	-C8	-H8	108.00	H1XA	-C1X	-H1XC	109.00
C8	-C9	-H9B	108.00	H1XB	-C1X	-H1XC	109.00
C8	-C9	-H9A	108.00	H1XD	-O1X	-H1XE	105.00
H9A	-C9	-H9B	107.00	N1X	-C2X	-H2XA	109.00
C1X	-C2X	-H2XA	109.00	H3XA	-C3X	-H3XB	108.00
C1X	-C2X	-H2XB	109.00	C3X	-C4X	-H4XB	109.00
H2XA	-C2X	-H2XB	108.00	C3X	-C4X	-H4XC	109.00
N1X	-C2X	-H2XB	109.00	C3X	-C4X	-H4XA	109.00
N1X	-C3X	-H3XA	109.00	H4XA	-C4X	-H4XC	110.00
C4X	-C3X	-H3XA	109.00	H4XB	-C4X	-H4XC	109.00
C4X	-C3X	-H3XB	109.00	H4XA	-C4X	-H4XB	110.00
N1X	-C3X	-H3XB	109.00				

Table S7. Non-covalent interactions in Complex **2**

Atoms	D-H (Å)	H…A (Å)	D…A(Å)	DHA(˚)
N1X-H1X…O2B	0.98	2.51	3.266(8)	133
N1X-H1X…O4B	0.98	1.76	2.720(9)	167
N2A-H2A…O4A	0.86	2.07	2.885(9)	158
N2B-H2B…O1A	0.86	2.24	3.074(10)	163
C8A-H8A…O1B	0.98	2.51	2.870(8)	102
C2X-H2XC…O2B	0.96	2.60	3.328(12)	133
C12A-H12A…O4A	0.93	2.52	3.307(10)	142

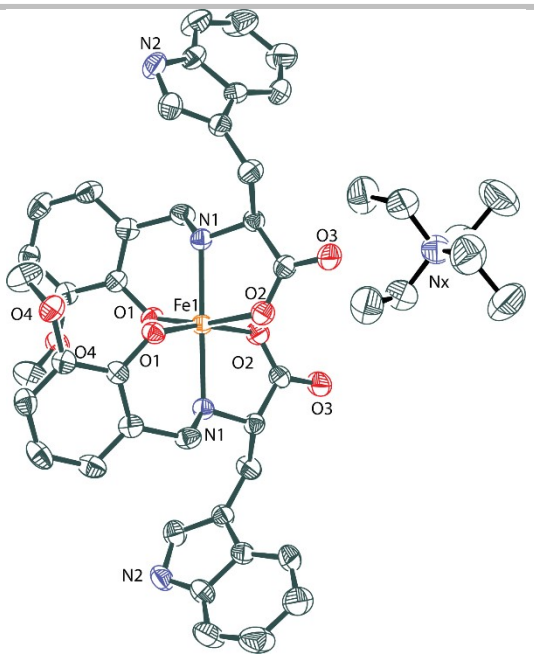


Figure S18. ORTEP figure of **4** with 40% ellipsoid probability.

Table S8. Bond lengths (Å) and angles (o) of complex **4**.

Fe1	-O1	1.943(3)	C10	-C17	1.363(7)
Fe1	-O2	2.020(4)	C11	-C16	1.418(7)
Fe1	-N1	2.160(4)	C11	-C12	1.391(8)
Fe1	-O1_a	1.943(3)	C12	-C13	1.372(9)
Fe1	-O2_a	2.020(4)	C13	-C14	1.401(11)
Fe1	-N1_a	2.160(4)	C14	-C15	1.372(10)
O1	-C1	1.335(4)	C15	-C16	1.393(8)
O2	-C18	1.278(6)	N1X	-C21_b	1.528(11)
O3	-C2	1.389(6)	N1X	-C21	1.527(11)
O3	-C19	1.419(7)	N1X	-C22	1.471(13)
O4	-C18	1.238(6)	N1X	-C22_b	1.470(13)
N1	-C7	1.486(6)	C3	-H3	0.9300
N1	-C8	1.485(6)	C4	-H4	0.9300
N2	-C16	1.364(7)	C5	-H5	0.9300
N2	-C17	1.357(7)	C7	-H7B	0.9700
C1	-C2	1.400(6)	C7	-H7A	0.9700
C1	-C6	1.407(6)	C8	-H8	0.9800
N1	-H1	0.77(5)	C9	-H9B	0.9700
C2	-C3	1.374(7)	C9	-H9A	0.9700
N2	-H2	0.91(5)	C12	-H12	0.9300
C3	-C4	1.379(7)	C13	-H13	0.9300
C4	-C5	1.376(8)	C14	-H14	0.9300
C5	-C6	1.388(7)	C15	-H15	0.9300
C6	-C7	1.502(7)	C17	-H17	0.9300
C8	-C9	1.543(6)	C19	-H19B	0.9600
C8	-C18	1.533(7)	C19	-H19C	0.9600
C9	-C10	1.497(7)	C19	-H19A	0.9600
C10	-C11	1.423(7)	C20	-C21	1.547(14)
C22	-C23	1.615(19)	C22	-H22A	0.9700
C20	-H20A	0.9600	C22	-H22B	0.9700
C20	-H20B	0.9600	C23	-H23A	0.9600
C20	-H20C	0.9600	C23	-H23B	0.9600
C21	-H21A	0.9700	C23	-H23C	0.9600
C21	-H21B	0.9700			

Angles

O1	-Fe1	-O2	165.08(15)	C16	-N2	-H2	124(3)
O1	-Fe1	-N1	89.59(13)	C17	-N2	-H2	127(3)
O1	-Fe1	-O1_a	100.55(15)	C1	-C2	-C3	121.9(4)
O1	-Fe1	-O2_a	88.20(14)	O3	-C2	-C1	117.5(4)
O1	-Fe1	-N1_a	90.84(13)	O3	-C2	-C3	120.4(4)
O2	-Fe1	-N1	78.12(14)	C2	-C3	-C4	119.4(5)
O1_a	-Fe1	-O2	88.20(14)	C3	-C4	-C5	120.3(5)
O2	-Fe1	-O2_a	85.99(14)	C4	-C5	-C6	120.9(5)
O2	-Fe1	-N1_a	101.37(14)	C1	-C6	-C7	117.8(4)
O1_a	-Fe1	-N1	90.84(13)	C5	-C6	-C7	122.5(4)
O2_a	-Fe1	-N1	101.37(14)	C1	-C6	-C5	119.6(4)
N1	-Fe1	-N1_a	179.32(14)	N1	-C7	-C6	110.8(4)
O1_a	-Fe1	-O2_a	165.08(15)	N1	-C8	-C9	112.7(4)
O1_a	-Fe1	-N1_a	89.59(13)	N1	-C8	-C18	110.0(3)
O2_a	-Fe1	-N1_a	78.12(14)	C9	-C8	-C18	109.9(4)
Fe1	-O1	-C1	125.2(2)	C8	-C9	-C10	115.0(4)
Fe1	-O2	-C18	118.9(3)	C9	-C10	-C17	127.5(5)
C2	-O3	-C19	115.2(4)	C9	-C10	-C11	126.9(5)
Fe1	-N1	-C7	111.4(3)	C11	-C10	-C17	105.6(4)
Fe1	-N1	-C8	109.7(3)	C10	-C11	-C12	133.9(5)
C7	-N1	-C8	114.8(3)	C10	-C11	-C16	107.0(4)
C16	-N2	-C17	108.1(4)	C12	-C11	-C16	119.1(5)
O1	-C1	-C2	120.7(4)	C11	-C12	-C13	119.5(6)
O1	-C1	-C6	121.5(4)	C12	-C13	-C14	120.8(6)
C2	-C1	-C6	117.9(4)	C13	-C14	-C15	121.3(7)
Fe1	-N1	-H1	104(3)	C14	-C15	-C16	118.1(6)
C7	-N1	-H1	109(4)	N2	-C16	-C15	131.1(5)
C8	-N1	-H1	108(4)	C11	-C16	-C15	121.2(5)
N2	-C16	-C11	107.7(4)	C10	-C9	-H9A	109.00
N2	-C17	-C10	111.6(4)	C10	-C9	-H9B	109.00
O2	-C18	-C8	117.0(4)	C11	-C12	-H12	120.00
O4	-C18	-C8	118.5(4)	C13	-C12	-H12	120.00
O2	-C18	-O4	124.5(5)	C12	-C13	-H13	120.00
C21_b	-N1X	-C22	111.2(8)	C14	-C13	-H13	120.00
C22	-N1X	-C22_b	118.0(9)	C15	-C14	-H14	119.00
C21_b	-N1X	-C22_b	104.2(6)	C13	-C14	-H14	119.00
C21	-N1X	-C22_b	111.3(8)	C14	-C15	-H15	121.00
C21	-N1X	-C22	104.2(6)	C16	-C15	-H15	121.00
C21	-N1X	-C21_b	107.6(7)	N2	-C17	-H17	124.00
C2	-C3	-H3	120.00	C10	-C17	-H17	124.00
C4	-C3	-H3	120.00	H19B	-C19	-H19C	109.00
C5	-C4	-H4	120.00	O3	-C19	-H19A	109.00
C3	-C4	-H4	120.00	O3	-C19	-H19B	109.00
C4	-C5	-H5	119.00	O3	-C19	-H19C	109.00
C6	-C5	-H5	120.00	H19A	-C19	-H19B	109.00
N1	-C7	-H7A	109.00	H19A	-C19	-H19C	110.00
H7A	-C7	-H7B	108.00	N1X	-C21	-C20	112.8(7)
C6	-C7	-H7B	109.00	N1X	-C22	-C23	109.2(9)
N1	-C7	-H7B	109.00	C21	-C20	-H20A	109.00
C6	-C7	-H7A	109.00	C21	-C20	-H20B	110.00
C9	-C8	-H8	108.00	C21	-C20	-H20C	109.00
N1	-C8	-H8	108.00	H20A	-C20	-H20B	109.00
C18	-C8	-H8	108.00	H20A	-C20	-H20C	109.00
C8	-C9	-H9B	109.00	H20B	-C20	-H20C	110.00
C8	-C9	-H9A	108.00	N1X	-C21	-H21A	109.00
H9A	-C9	-H9B	107.00	N1X	-C21	-H21B	109.00
C20	-C21	-H21A	109.00	H22A	-C22	-H22B	108.00
C20	-C21	-H21B	109.00	C22	-C23	-H23A	109.00
H21A	-C21	-H21B	108.00	C22	-C23	-H23B	109.00

N1X	-C22	-H22A	110.00	C22	-C23	-H23C	109.00
N1X	-C22	-H22B	110.00	H23A	-C23	-H23B	110.00
C23	-C22	-H22A	110.00	H23A	-C23	-H23C	110.00
C23	-C22	-H22B	110.00	H23B	-C23	-H23C	109.00

Table S9. Non-covalent interactions in Complex **4.**

Atoms	D-H (Å)	H…A (Å)	D…A(Å)	DHA(˚)
N2-H2…O1	0.91(5)	2.10(5)	2.998(6)	167(4)
C1-H1B…O3	0.96	2.58	3.449(7)	150
C17-H17…O4	0.93	2.37	3.294(7)	171

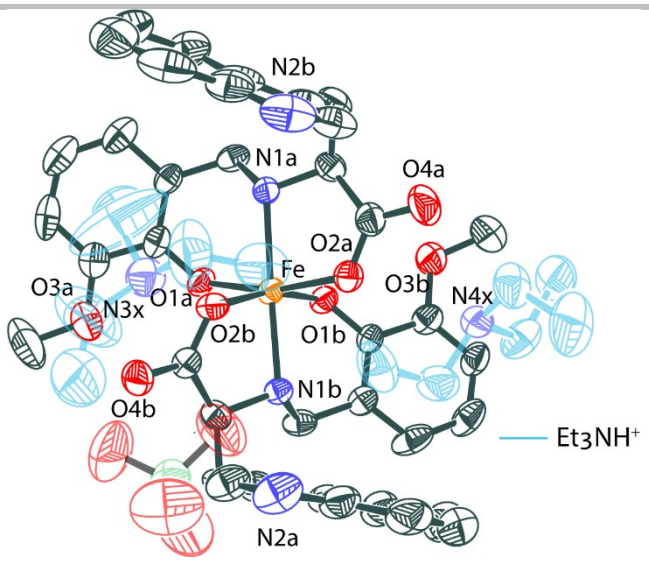


Figure S19. ORTEP figure of **5** with 40% ellipsoid probability.

Table S10. Bond lengths (Å) and angles (o) of complex **5**.

Fe1	-O1A	1.902(6)	N2B	-C17B	1.364(18)
Fe1	-O1B	1.937(7)	N2B	-C16B	1.353(18)
Fe1	-O2A	2.048(7)	C1A	-C6A	1.388(16)
Fe1	-O2B	2.054(7)	C1A	-C2A	1.436(17)
Fe1	-N1A	2.170(8)	N1A	-H1A	0.9800
Fe1	-N1B	2.157(8)	C1B	-C6B	1.393(14)
Fe2	-N1E	2.154(8)	C1B	-C2B	1.403(15)
Fe2	-N1F	2.170(8)	N1B	-H1B	0.9800
Fe2	-O1E	1.936(7)	O1E	-C1E	1.342(12)
Fe2	-O1F	1.891(6)	O1F	-C1F	1.329(12)
Fe2	-O2E	2.066(7)	C2A	-C3A	1.380(17)
Fe2	-O2F	2.037(6)	N2A	-H2A	0.8600
O1A	-C1A	1.313(12)	N2B	-H2B	0.8600
O1B	-C1B	1.327(12)	C2B	-C3B	1.378(15)
O2A	-C18A	1.268(16)	O2E	-C18E	1.268(16)
O2B	-C18B	1.279(14)	O2F	-C18F	1.273(14)
O3A	-C2A	1.363(16)	C3A	-C4A	1.37(2)
O3A	-C19A	1.41(2)	C3B	-C4B	1.33(2)
O3B	-C19B	1.388(16)	O3E	-C2E	1.381(14)
O3B	-C2B	1.384(14)	O3E	-C19E	1.419(17)
O4A	-C18A	1.233(16)	O3F	-C19F	1.32(2)
O4B	-C18B	1.238(14)	O3F	-C2F	1.368(17)
N1A	-C8A	1.466(13)	C4A	-C5A	1.36(2)
N1A	-C7A	1.480(13)	C4B	-C5B	1.37(2)
N1B	-C8B	1.496(13)	O4E	-C18E	1.251(15)
N1B	-C7B	1.491(12)	O4F	-C18F	1.228(14)
N2A	-C16A	1.34(3)	C5A	-C6A	1.410(15)
N2A	-C17A	1.36(2)	C5B	-C6B	1.388(15)
C6A	-C7A	1.481(15)	N1E	-C8E	1.490(13)
C6B	-C7B	1.504(15)	N1E	-C7E	1.486(14)
C8A	-C18A	1.513(16)	N1F	-C7F	1.480(12)
C8A	-C9A	1.529(16)	N1F	-C8F	1.479(12)
C8B	-C9B	1.528(15)	N2E	-C17E	1.371(19)
C8B	-C18B	1.511(15)	N2E	-C16E	1.37(2)
C9A	-C10A	1.472(18)	N2F	-C16F	1.345(19)
C9B	-C10B	1.481(16)	N2F	-C17F	1.342(19)
C10A	-C17A	1.37(2)	C3A	-H3A	0.9300
C10A	-C11A	1.41(2)	C3B	-H3B	0.9300

C10B	-C11B	1.420(16)	C4A	-H4A	0.9300
C10B	-C17B	1.362(18)	C4B	-H4B	0.9300
C11A	-C12A	1.41(2)	C5A	-H5A	0.9300
C11A	-C16A	1.434(19)	C5B	-H5B	0.9300
C11B	-C16B	1.41(2)	C7A	-H7AB	0.9700
C11B	-C12B	1.387(19)	C7A	-H7AA	0.9700
C12A	-C13A	1.36(2)	C7B	-H7BA	0.9700
C12B	-C13B	1.38(2)	C7B	-H7BB	0.9700
C13A	-C14A	1.43(3)	C8A	-H8A	0.9800
C13B	-C14B	1.37(3)	C8B	-H8B	0.9800
C14A	-C15A	1.37(3)	C9A	-H9AA	0.9700
C14B	-C15B	1.35(2)	C9A	-H9AB	0.9700
C15A	-C16A	1.37(3)	C9B	-H9BA	0.9700
C15B	-C16B	1.42(2)	C9B	-H9BB	0.9700
Cl1	-O3X	1.344(16)	C12A	-H12A	0.9300
Cl1	-O1X	1.432(14)	C12B	-H12B	0.9300
Cl1	-O2X	1.371(16)	C13A	-H13A	0.9300
Cl1	-O4X	1.351(15)	C13B	-H13B	0.9300
C14A	-H14A	0.9300	C6E	-C7E	1.487(16)
C14B	-H14B	0.9300	C6F	-C7F	1.478(13)
C15A	-H15A	0.9300	C8E	-C18E	1.547(16)
C15B	-H15B	0.9300	C8E	-C9E	1.545(14)
C17A	-H17A	0.9300	C8F	-C18F	1.530(14)
C17B	-H17B	0.9300	C8F	-C9F	1.539(15)
C19A	-H19F	0.9600	C9E	-C10E	1.489(17)
C19A	-H19D	0.9600	C9F	-C10F	1.494(16)
C19A	-H19E	0.9600	C10E	-C11E	1.422(18)
C19B	-H19A	0.9600	C10E	-C17E	1.38(2)
C19B	-H19B	0.9600	C10F	-C17F	1.364(19)
C19B	-H19C	0.9600	C10F	-C11F	1.418(15)
C1E	-C6E	1.398(15)	C11E	-C12E	1.42(2)
C1E	-C2E	1.389(15)	C11E	-C16E	1.40(2)
N1E	-H1E	0.9800	C11F	-C12F	1.380(15)
N1F	-H1F	0.9800	C11F	-C16F	1.417(16)
C1F	-C2F	1.381(17)	C12E	-C13E	1.37(2)
C1F	-C6F	1.415(16)	C12F	-C13F	1.404(18)
C2E	-C3E	1.397(16)	C13E	-C14E	1.38(3)
N2E	-H2E	0.8600	C13F	-C14F	1.39(2)
N2F	-H2F	0.8600	C14E	-C15E	1.36(3)
C2F	-C3F	1.397(16)	C14F	-C15F	1.33(2)
C3E	-C4E	1.39(2)	C15E	-C16E	1.40(3)
C3F	-C4F	1.39(2)	C15F	-C16F	1.39(2)
C4E	-C5E	1.37(2)	N1X	-C3X	1.498(16)
C4F	-C5F	1.36(2)	N1X	-C5X	1.495(17)
C5E	-C6E	1.387(16)	N1X	-C1X	1.479(16)
C5F	-C6F	1.396(14)	Cl2	-O7X	1.345(15)
Cl2	-O6X	1.444(11)	C17F	-H17F	0.9300
Cl2	-O5X	1.358(15)	C19E	-H19I	0.9600
Cl2	-O8X	1.375(13)	C19E	-H19G	0.9600
C3E	-H3E	0.9300	C19E	-H19H	0.9600
C3F	-H3F	0.9300	C19F	-H19K	0.9600
C4E	-H4E	0.9300	C19F	-H19L	0.9600
C4F	-H4F	0.9300	C19F	-H19J	0.9600
C5E	-H5E	0.9300	C1X	-C2X	1.48(2)
C5F	-H5F	0.9300	N1X	-H1X	0.9800
C7E	-H7EA	0.9700	C3X	-C4X	1.52(2)
C7E	-H7EB	0.9700	C5X	-C6X	1.54(2)
C7F	-H7FA	0.9700	C1X	-H1XA	0.9700
C7F	-H7FB	0.9700	C1X	-H1XB	0.9700
C8E	-H8E	0.9800	C2X	-H2XA	0.9600
C8F	-H8F	0.9800	C2X	-H2XB	0.9600
C9E	-H9EB	0.9700	C2X	-H2XC	0.9600

C9E	-H9EA	0.9700	N2X	-C11X	1.41(3)
C9F	-H9FB	0.9700	N2X	-C7X	1.48(3)
C9F	-H9FA	0.9700	N2X	-C9X	1.43(3)
C12E	-H12E	0.9300	C3X	-H3XB	0.9700
C12F	-H12F	0.9300	C3X	-H3XA	0.9700
C13E	-H13E	0.9300	C4X	-H4XB	0.9600
C13F	-H13F	0.9300	C4X	-H4XC	0.9600
C14E	-H14E	0.9300	C4X	-H4XA	0.9600
C14F	-H14F	0.9300	C5X	-H5XB	0.9700
C15E	-H15E	0.9300	C5X	-H5XA	0.9700
C15F	-H15F	0.9300	C6X	-H6XC	0.9600
C17E	-H17E	0.9300	C6X	-H6XA	0.9600
C6X	-H6XB	0.9600	C13X	-H13D	0.9700
N2X	-H2X	0.9800	C14X	-H14C	0.9600
C7X	-C8X	1.21(4)	C14X	-H14D	0.9600
C9X	-C10X	1.40(3)	C14X	-H14G	0.9600
C11X	-C12X	1.30(4)	C15X	-H15C	0.9700
N3X	-C17X	1.39(3)	C15X	-H15D	0.9700
N3X	-C13X	1.46(3)	C16X	-H16C	0.9600
N3X	-C15X	1.40(3)	C16X	-H16B	0.9600
C7X	-H7XB	0.9700	C16X	-H16A	0.9600
C7X	-H7XA	0.9700	C17X	-H17D	0.9700
C9X	-H9XB	0.9700	C17X	-H17C	0.9800
C9X	-H9XA	0.9700	C18X	-H18B	0.9600
C10X	-H10A	0.9600	C18X	-H18C	0.9600
C10X	-H10C	0.9600	C18X	-H18A	0.9600
C10X	-H10B	0.9600	N4X	-H4X	0.9800
C11X	-H11B	0.9700	C19X	-C20X	1.40(3)
C11X	-H11A	0.9700	C21X	-C22X	1.33(3)
C12X	-H12C	0.9600	C23X	-C24X	1.36(4)
C12X	-H12D	0.9600	C19X	-H19M	0.9700
C12X	-H12G	0.9600	C19X	-H19N	0.9700
N3X	-H3X	0.9800	C21X	-H21A	0.9700
C13X	-C14X	1.35(3)	C21X	-H21B	0.9700
C15X	-C16X	1.33(3)	C22X	-H22B	0.9600
C17X	-C18X	1.28(3)	C22X	-H22C	0.9600
N4X	-C21X	1.54(2)	C22X	-H22A	0.9600
N4X	-C23X	1.35(4)	C23X	-H23A	0.9700
N4X	-C19X	1.53(3)	C23X	-H23B	0.9700
C13X	-H13C	0.9700	C24X	-H24B	0.9600

Angles

O1A	-Fe1	-O1B	91.4(3)	O2E	-Fe2	-O2F	90.0(3)
O1A	-Fe1	-O2A	165.7(3)	O2E	-Fe2	-N1E	75.7(3)
O1A	-Fe1	-O2B	91.0(3)	Fe1	-O1A	-C1A	125.1(6)
O1A	-Fe1	-N1A	89.1(3)	Fe1	-O1B	-C1B	122.1(6)
O1A	-Fe1	-N1B	104.8(3)	Fe1	-O2A	-C18A	117.5(6)
O1B	-Fe1	-O2A	91.0(3)	Fe1	-O2B	-C18B	116.5(6)
O1B	-Fe1	-O2B	165.3(3)	C2A	-O3A	-C19A	117.6(11)
O1B	-Fe1	-N1A	106.9(3)	C2B	-O3B	-C19B	117.5(10)
O1B	-Fe1	-N1B	89.2(3)	Fe1	-N1A	-C7A	111.4(6)
O2A	-Fe1	-O2B	90.2(3)	Fe1	-N1A	-C8A	108.7(6)
O2A	-Fe1	-N1A	76.7(3)	C7A	-N1A	-C8A	114.6(8)
O2A	-Fe1	-N1B	89.3(3)	Fe1	-N1B	-C8B	108.1(6)
O2B	-Fe1	-N1A	87.6(3)	Fe1	-N1B	-C7B	112.1(6)
O2B	-Fe1	-N1B	76.2(3)	C7B	-N1B	-C8B	115.0(8)
N1A	-Fe1	-N1B	158.6(3)	C16A	-N2A	-C17A	110.2(13)
O2E	-Fe2	-N1F	92.2(3)	C16B	-N2B	-C17B	108.8(12)
O2F	-Fe2	-N1E	89.1(3)	Fe1	-N1A	-H1A	107.00
O2F	-Fe2	-N1F	76.7(3)	O1A	-C1A	-C2A	120.3(10)
N1E	-Fe2	-N1F	161.4(3)	O1A	-C1A	-C6A	122.1(10)

O1E	-Fe2	-O1F	92.8(3)	C2A	-C1A	-C6A	117.4(10)
O1E	-Fe2	-O2E	165.6(3)	C8A	-N1A	-H1A	107.00
O1E	-Fe2	-O2F	91.1(3)	C7A	-N1A	-H1A	107.00
O1E	-Fe2	-N1E	90.0(3)	O1B	-C1B	-C6B	122.1(9)
O1E	-Fe2	-N1F	102.0(3)	O1B	-C1B	-C2B	120.7(9)
O1F	-Fe2	-O2E	89.6(3)	Fe1	-N1B	-H1B	107.00
O1F	-Fe2	-O2F	165.5(3)	C7B	-N1B	-H1B	107.00
O1F	-Fe2	-N1E	104.8(3)	C8B	-N1B	-H1B	107.00
O1F	-Fe2	-N1F	88.8(3)	C2B	-C1B	-C6B	117.3(10)
Fe2	-O1E	-C1E	121.3(6)	N1A	-C7A	-C6A	111.4(8)
Fe2	-O1F	-C1F	128.7(6)	N1B	-C7B	-C6B	109.9(8)
C16A	-N2A	-H2A	125.00	C9A	-C8A	-C18A	111.8(9)
C17A	-N2A	-H2A	125.00	N1A	-C8A	-C9A	114.3(9)
O3A	-C2A	-C3A	126.1(13)	N1A	-C8A	-C18A	108.9(9)
C1A	-C2A	-C3A	119.7(13)	N1B	-C8B	-C18B	107.9(8)
O3A	-C2A	-C1A	114.2(9)	N1B	-C8B	-C9B	114.0(9)
C16B	-N2B	-H2B	126.00	C9B	-C8B	-C18B	113.7(9)
O3B	-C2B	-C1B	114.9(9)	C8A	-C9A	-C10A	115.4(10)
O3B	-C2B	-C3B	124.2(11)	C8B	-C9B	-C10B	115.8(9)
C1B	-C2B	-C3B	120.9(11)	C9A	-C10A	-C11A	125.5(12)
C17B	-N2B	-H2B	126.00	C9A	-C10A	-C17A	129.1(13)
Fe2	-O2E	-C18E	115.9(7)	C11A	-C10A	-C17A	105.3(12)
Fe2	-O2F	-C18F	119.7(6)	C11B	-C10B	-C17B	106.4(11)
C2A	-C3A	-C4A	120.5(14)	C9B	-C10B	-C11B	128.4(11)
C2B	-C3B	-C4B	120.8(12)	C9B	-C10B	-C17B	125.1(11)
C2E	-O3E	-C19E	117.6(10)	C10A	-C11A	-C12A	135.6(12)
C2F	-O3F	-C19F	119.3(12)	C10A	-C11A	-C16A	107.9(14)
C3A	-C4A	-C5A	122.2(13)	C12A	-C11A	-C16A	116.5(14)
C3B	-C4B	-C5B	120.4(12)	C12B	-C11B	-C16B	116.8(11)
C4A	-C5A	-C6A	118.4(13)	C10B	-C11B	-C16B	106.7(11)
C4B	-C5B	-C6B	120.7(13)	C10B	-C11B	-C12B	136.5(13)
C1A	-C6A	-C7A	118.8(10)	C11A	-C12A	-C13A	122.9(13)
C5A	-C6A	-C7A	119.4(11)	C11B	-C12B	-C13B	121.6(14)
C1A	-C6A	-C5A	121.8(11)	C12A	-C13A	-C14A	119.3(16)
C5B	-C6B	-C7B	122.6(10)	C12B	-C13B	-C14B	119.2(16)
C1B	-C6B	-C5B	119.9(11)	C13A	-C14A	-C15A	119.2(17)
C1B	-C6B	-C7B	117.5(10)	C13B	-C14B	-C15B	123.9(16)
C14A	-C15A	-C16A	121.7(16)	C16E	-N2E	-C17E	110.0(13)
C14B	-C15B	-C16B	116.5(15)	C16F	-N2F	-C17F	109.3(11)
C11A	-C16A	-C15A	120.5(18)	C2A	-C3A	-H3A	120.00
N2A	-C16A	-C11A	106.1(15)	C4A	-C3A	-H3A	120.00
N2A	-C16A	-C15A	133.4(15)	C4B	-C3B	-H3B	120.00
C11B	-C16B	-C15B	122.0(13)	C2B	-C3B	-H3B	120.00
N2B	-C16B	-C11B	107.9(12)	C3A	-C4A	-H4A	119.00
N2B	-C16B	-C15B	130.1(14)	C5A	-C4A	-H4A	119.00
N2A	-C17A	-C10A	110.5(14)	C3B	-C4B	-H4B	120.00
N2B	-C17B	-C10B	110.3(12)	C5B	-C4B	-H4B	120.00
O2A	-C18A	-C8A	118.2(10)	C6A	-C5A	-H5A	121.00
O4A	-C18A	-C8A	118.3(11)	C4A	-C5A	-H5A	121.00
O2A	-C18A	-O4A	123.5(10)	C6B	-C5B	-H5B	120.00
O2B	-C18B	-C8B	118.0(9)	C4B	-C5B	-H5B	120.00
O4B	-C18B	-C8B	117.4(10)	N1A	-C7A	-H7AA	109.00
O2B	-C18B	-O4B	124.7(10)	N1A	-C7A	-H7AB	109.00
O3X	-Cl1	-O4X	112.2(11)	C6A	-C7A	-H7AA	109.00
O1X	-Cl1	-O3X	109.3(9)	C6A	-C7A	-H7AB	109.00
O1X	-Cl1	-O4X	109.5(9)	H7AA	-C7A	-H7AB	108.00
O1X	-Cl1	-O2X	107.8(10)	C6B	-C7B	-H7BA	110.00
O2X	-Cl1	-O4X	106.4(11)	N1B	-C7B	-H7BA	110.00
O2X	-Cl1	-O3X	111.5(10)	C6B	-C7B	-H7BB	110.00
Fe2	-N1E	-C8E	107.4(6)	H7BA	-C7B	-H7BB	108.00
C7E	-N1E	-C8E	113.8(8)	N1B	-C7B	-H7BB	110.00
Fe2	-N1E	-C7E	111.9(6)	C9A	-C8A	-H8A	107.00

Fe2	-N1F	-C8F	108.7(6)	C18A	-C8A	-H8A	107.00
C7F	-N1F	-C8F	114.9(7)	N1A	-C8A	-H8A	107.00
Fe2	-N1F	-C7F	111.8(6)	C9B	-C8B	-H8B	107.00
C18B	-C8B	-H8B	107.00	N2A	-C17A	-H17A	125.00
N1B	-C8B	-H8B	107.00	C10A	-C17A	-H17A	125.00
C10A	-C9A	-H9AA	108.00	C10B	-C17B	-H17B	125.00
C10A	-C9A	-H9AB	109.00	N2B	-C17B	-H17B	125.00
C8A	-C9A	-H9AB	108.00	O3A	-C19A	-H19D	110.00
C8A	-C9A	-H9AA	108.00	H19E	-C19A	-H19F	109.00
H9AA	-C9A	-H9AB	108.00	H19D	-C19A	-H19E	110.00
C10B	-C9B	-H9BA	108.00	H19D	-C19A	-H19F	109.00
H9BA	-C9B	-H9BB	107.00	O3A	-C19A	-H19F	109.00
C8B	-C9B	-H9BB	108.00	O3A	-C19A	-H19E	109.00
C10B	-C9B	-H9BB	108.00	H19B	-C19B	-H19C	109.00
C8B	-C9B	-H9BA	108.00	H19A	-C19B	-H19C	110.00
C13A	-C12A	-H12A	119.00	O3B	-C19B	-H19C	109.00
C11A	-C12A	-H12A	119.00	O3B	-C19B	-H19A	110.00
C11B	-C12B	-H12B	119.00	O3B	-C19B	-H19B	109.00
C13B	-C12B	-H12B	119.00	H19A	-C19B	-H19B	109.00
C14A	-C13A	-H13A	120.00	C2E	-C1E	-C6E	118.9(10)
C12A	-C13A	-H13A	120.00	O1E	-C1E	-C2E	119.9(9)
C12B	-C13B	-H13B	120.00	O1E	-C1E	-C6E	121.2(9)
C14B	-C13B	-H13B	120.00	C8E	-N1E	-H1E	108.00
C15A	-C14A	-H14A	121.00	Fe2	-N1E	-H1E	108.00
C13A	-C14A	-H14A	120.00	C7E	-N1E	-H1E	108.00
C13B	-C14B	-H14B	118.00	C7F	-N1F	-H1F	107.00
C15B	-C14B	-H14B	118.00	C8F	-N1F	-H1F	107.00
C16A	-C15A	-H15A	119.00	O1F	-C1F	-C2F	120.4(10)
C14A	-C15A	-H15A	119.00	O1F	-C1F	-C6F	120.7(9)
C16B	-C15B	-H15B	122.00	Fe2	-N1F	-H1F	107.00
C14B	-C15B	-H15B	122.00	C2F	-C1F	-C6F	118.7(10)
C16E	-N2E	-H2E	125.00	C9F	-C8F	-C18F	111.8(9)
C17E	-N2E	-H2E	125.00	N1F	-C8F	-C18F	109.5(8)
O3E	-C2E	-C3E	123.7(11)	C8E	-C9E	-C10E	115.9(9)
O3E	-C2E	-C1E	114.9(9)	C8F	-C9F	-C10F	114.1(8)
C1E	-C2E	-C3E	121.4(11)	C11E	-C10E	-C17E	106.0(12)
C16F	-N2F	-H2F	125.00	C9E	-C10E	-C11E	126.1(12)
C17F	-N2F	-H2F	125.00	C9E	-C10E	-C17E	127.9(11)
C1F	-C2F	-C3F	120.9(13)	C11F	-C10F	-C17F	105.6(10)
O3F	-C2F	-C1F	115.1(10)	C9F	-C10F	-C11F	126.1(10)
O3F	-C2F	-C3F	124.0(11)	C9F	-C10F	-C17F	128.2(11)
C2E	-C3E	-C4E	118.4(11)	C10E	-C11E	-C12E	133.1(14)
C2F	-C3F	-C4F	119.4(12)	C10E	-C11E	-C16E	108.5(13)
C3E	-C4E	-C5E	120.7(11)	C12E	-C11E	-C16E	118.4(13)
C3F	-C4F	-C5F	120.6(12)	C10F	-C11F	-C12F	135.7(10)
C4E	-C5E	-C6E	121.2(12)	C10F	-C11F	-C16F	106.7(10)
C4F	-C5F	-C6F	120.7(13)	C12F	-C11F	-C16F	117.5(10)
C5E	-C6E	-C7E	122.3(11)	C11E	-C12E	-C13E	118.1(15)
C1E	-C6E	-C7E	118.4(10)	C11F	-C12F	-C13F	119.5(11)
C1E	-C6E	-C5E	119.3(11)	C12E	-C13E	-C14E	120.8(17)
C1F	-C6F	-C7F	119.5(8)	C12F	-C13F	-C14F	120.8(13)
C5F	-C6F	-C7F	120.9(10)	C13E	-C14E	-C15E	124.3(16)
C1F	-C6F	-C5F	119.6(10)	C13F	-C14F	-C15F	120.7(14)
N1E	-C7E	-C6E	110.7(9)	C14E	-C15E	-C16E	115.0(18)
N1F	-C7F	-C6F	112.3(8)	C14F	-C15F	-C16F	119.8(13)
N1E	-C8E	-C9E	113.5(9)	N2E	-C16E	-C15E	130.2(17)
C9E	-C8E	-C18E	112.5(9)	N2E	-C16E	-C11E	106.5(14)
N1E	-C8E	-C18E	105.7(8)	C11E	-C16E	-C15E	123.4(16)
N1F	-C8F	-C9F	113.8(8)	C11F	-C16F	-C15F	121.7(12)
N2F	-C16F	-C11F	107.5(11)	C6E	-C5E	-H5E	119.00
N2F	-C16F	-C15F	130.7(12)	C6F	-C5F	-H5F	120.00
N2E	-C17E	-C10E	109.1(12)	C4F	-C5F	-H5F	120.00

N2F	-C17F	-C10F	111.0(12)	H7EA	-C7E	-H7EB	108.00
O4E	-C18E	-C8E	117.0(11)	C6E	-C7E	-H7EB	110.00
O2E	-C18E	-C8E	117.8(10)	N1E	-C7E	-H7EB	109.00
O2E	-C18E	-O4E	125.1(11)	C6E	-C7E	-H7EA	110.00
O2F	-C18F	-O4F	124.7(10)	N1E	-C7E	-H7EA	109.00
O2F	-C18F	-C8F	116.0(9)	N1F	-C7F	-H7FB	109.00
O4F	-C18F	-C8F	119.4(10)	C6F	-C7F	-H7FA	109.00
C3X	-N1X	-C5X	109.4(11)	C6F	-C7F	-H7FB	109.00
C1X	-N1X	-C5X	113.8(11)	N1F	-C7F	-H7FA	109.00
C1X	-N1X	-C3X	115.2(9)	H7FA	-C7F	-H7FB	108.00
O7X	-Cl2	-O8X	111.3(9)	N1E	-C8E	-H8E	108.00
O6X	-Cl2	-O8X	108.8(8)	C9E	-C8E	-H8E	108.00
O5X	-Cl2	-O6X	109.3(8)	C18E	-C8E	-H8E	108.00
O5X	-Cl2	-O7X	108.5(9)	C18F	-C8F	-H8F	107.00
O5X	-Cl2	-O8X	108.2(10)	N1F	-C8F	-H8F	107.00
O6X	-Cl2	-O7X	110.7(7)	C9F	-C8F	-H8F	107.00
C2E	-C3E	-H3E	121.00	H9EA	-C9E	-H9EB	107.00
C4E	-C3E	-H3E	121.00	C8E	-C9E	-H9EB	108.00
C4F	-C3F	-H3F	120.00	C10E	-C9E	-H9EA	108.00
C2F	-C3F	-H3F	120.00	C10E	-C9E	-H9EB	108.00
C3E	-C4E	-H4E	120.00	C8E	-C9E	-H9EA	108.00
C5E	-C4E	-H4E	120.00	C8F	-C9F	-H9FB	109.00
C5F	-C4F	-H4F	120.00	C10F	-C9F	-H9FA	109.00
C3F	-C4F	-H4F	120.00	C8F	-C9F	-H9FA	109.00
C4E	-C5E	-H5E	119.00	H9FA	-C9F	-H9FB	108.00
C10F	-C9F	-H9FB	109.00	O3F	-C19F	-H19L	109.00
C13E	-C12E	-H12E	121.00	H19J	-C19F	-H19K	109.00
C11E	-C12E	-H12E	121.00	H19K	-C19F	-H19L	110.00
C11F	-C12F	-H12F	120.00	O3F	-C19F	-H19J	109.00
C13F	-C12F	-H12F	120.00	H19J	-C19F	-H19L	110.00
C12E	-C13E	-H13E	120.00	N1X	-C1X	-C2X	114.6(13)
C14E	-C13E	-H13E	120.00	C1X	-N1X	-H1X	106.00
C14F	-C13F	-H13F	120.00	C5X	-N1X	-H1X	106.00
C12F	-C13F	-H13F	120.00	C3X	-N1X	-H1X	106.00
C13E	-C14E	-H14E	118.00	N1X	-C3X	-C4X	111.2(11)
C15E	-C14E	-H14E	118.00	N1X	-C5X	-C6X	112.2(12)
C15F	-C14F	-H14F	120.00	C2X	-C1X	-H1XA	109.00
C13F	-C14F	-H14F	120.00	C2X	-C1X	-H1XB	109.00
C16E	-C15E	-H15E	122.00	H1XA	-C1X	-H1XB	108.00
C14E	-C15E	-H15E	123.00	N1X	-C1X	-H1XB	109.00
C14F	-C15F	-H15F	120.00	N1X	-C1X	-H1XA	109.00
C16F	-C15F	-H15F	120.00	H2XA	-C2X	-H2XC	109.00
C10E	-C17E	-H17E	125.00	C7X	-N2X	-C9X	107(2)
N2E	-C17E	-H17E	125.00	C7X	-N2X	-C11X	109(2)
C10F	-C17F	-H17F	125.00	C1X	-C2X	-H2XA	110.00
N2F	-C17F	-H17F	125.00	C1X	-C2X	-H2XB	110.00
O3E	-C19E	-H19H	110.00	C1X	-C2X	-H2XC	109.00
O3E	-C19E	-H19G	110.00	H2XA	-C2X	-H2XB	109.00
O3E	-C19E	-H19I	110.00	H2XB	-C2X	-H2XC	109.00
H19G	-C19E	-H19H	109.00	C9X	-N2X	-C11X	111.3(19)
H19G	-C19E	-H19I	109.00	N1X	-C3X	-H3XB	109.00
H19H	-C19E	-H19I	109.00	N1X	-C3X	-H3XA	109.00
O3F	-C19F	-H19K	109.00	H3XA	-C3X	-H3XB	108.00
C4X	-C3X	-H3XB	109.00	C8X	-C7X	-H7XA	106.00
C4X	-C3X	-H3XA	109.00	N2X	-C7X	-H7XB	106.00
C3X	-C4X	-H4XB	109.00	H7XA	-C7X	-H7XB	106.00
C3X	-C4X	-H4XA	109.00	N2X	-C7X	-H7XA	106.00
C3X	-C4X	-H4XC	110.00	C8X	-C7X	-H7XB	106.00
H4XA	-C4X	-H4XB	109.00	H9XA	-C9X	-H9XB	107.00
H4XB	-C4X	-H4XC	110.00	C10X	-C9X	-H9XA	107.00
H4XA	-C4X	-H4XC	109.00	C10X	-C9X	-H9XB	107.00
C6X	-C5X	-H5XB	109.00	N2X	-C9X	-H9XA	106.00

H5XA	-C5X	-H5XB	108.00	N2X	-C9X	-H9XB	107.00
C6X	-C5X	-H5XA	109.00	C9X	-C10X	-H10A	110.00
N1X	-C5X	-H5XA	109.00	H10A	-C10X	-H10C	110.00
N1X	-C5X	-H5XB	109.00	H10B	-C10X	-H10C	109.00
H6XB	-C6X	-H6XC	109.00	C9X	-C10X	-H10B	109.00
C5X	-C6X	-H6XB	109.00	H10A	-C10X	-H10B	109.00
C5X	-C6X	-H6XC	109.00	C9X	-C10X	-H10C	109.00
C5X	-C6X	-H6XA	110.00	N2X	-C11X	-H11A	104.00
H6XA	-C6X	-H6XC	109.00	C12X	-C11X	-H11A	105.00
H6XA	-C6X	-H6XB	110.00	N2X	-C11X	-H11B	105.00
C11X	-N2X	-H2X	110.00	H11A	-C11X	-H11B	106.00
C9X	-N2X	-H2X	110.00	C12X	-C11X	-H11B	105.00
C7X	-N2X	-H2X	110.00	H12C	-C12X	-H12G	109.00
N2X	-C7X	-C8X	127(3)	H12C	-C12X	-H12D	109.00
N2X	-C9X	-C10X	123.0(17)	C11X	-C12X	-H12D	110.00
N2X	-C11X	-C12X	131(3)	H12D	-C12X	-H12G	110.00
C13X	-N3X	-C17X	115.0(19)	C11X	-C12X	-H12G	109.00
C15X	-N3X	-C17X	108(2)	C11X	-C12X	-H12C	109.00
C13X	-N3X	-C15X	105.1(19)	C15X	-N3X	-H3X	110.00
13X	-N3X	-H3X	110.00	C15X	-C16X	-H16A	109.00
C17X	-N3X	-H3X	109.00	C15X	-C16X	-H16B	110.00
N3X	-C13X	-C14X	124(2)	C18X	-C17X	-H17D	104.00
N3X	-C15X	-C16X	126.7(18)	N3X	-C17X	-H17C	104.00
N3X	-C17X	-C18X	132(3)	C18X	-C17X	-H17C	104.00
C19X	-N4X	-C23X	112(2)	N3X	-C17X	-H17D	104.00
C21X	-N4X	-C23X	118.4(19)	H17C	-C17X	-H17D	105.00
C19X	-N4X	-C21X	110.6(17)	C17X	-C18X	-H18C	109.00
H13C	-C13X	-H13D	106.00	H18A	-C18X	-H18C	110.00
N3X	-C13X	-H13C	106.00	H18B	-C18X	-H18C	109.00
N3X	-C13X	-H13D	106.00	C17X	-C18X	-H18B	109.00
C14X	-C13X	-H13C	106.00	C17X	-C18X	-H18A	109.00
C14X	-C13X	-H13D	106.00	H18A	-C18X	-H18B	109.00
C13X	-C14X	-H14C	109.00	C21X	-N4X	-H4X	105.00
C13X	-C14X	-H14G	109.00	C23X	-N4X	-H4X	105.00
H14C	-C14X	-H14D	110.00	C19X	-N4X	-H4X	105.00
C13X	-C14X	-H14D	109.00	N4X	-C19X	-C20X	122.5(19)
H14D	-C14X	-H14G	110.00	N4X	-C21X	-C22X	118.0(19)
H14C	-C14X	-H14G	109.00	N4X	-C23X	-C24X	130(2)
N3X	-C15X	-H15D	106.00	N4X	-C19X	-H19M	107.00
N3X	-C15X	-H15C	106.00	N4X	-C19X	-H19N	107.00
C16X	-C15X	-H15D	106.00	C20X	-C19X	-H19M	107.00
H15C	-C15X	-H15D	106.00	C20X	-C19X	-H19N	106.00
C16X	-C15X	-H15C	106.00	H19M	-C19X	-H19N	107.00
H16B	-C16X	-H16C	110.00	C22X	-C21X	-H21B	108.00
H16A	-C16X	-H16C	109.00	N4X	-C21X	-H21A	108.00
C15X	-C16X	-H16C	109.00	H21A	-C21X	-H21B	107.00
H16A	-C16X	-H16B	109.00	C22X	-C21X	-H21A	108.00
N4X	-C21X	-H21B	108.00	N4X	-C23X	-H23A	105.00
C21X	-C22X	-H22B	109.00	C24X	-C23X	-H23B	105.00
C21X	-C22X	-H22A	109.00	H23A	-C23X	-H23B	106.00
C21X	-C22X	-H22C	110.00	H24B	-C24X	-H24C	110.00
H22A	-C22X	-H22B	109.00	H24A	-C24X	-H24B	110.00
H22A	-C22X	-H22C	110.00	H24A	-C24X	-H24C	109.00
H22B	-C22X	-H22C	110.00	C23X	-C24X	-H24A	110.00
N4X	-C23X	-H23B	105.00	C23X	-C24X	-H24B	110.00
C24X	-C23X	-H23A	105.00	C23X	-C24X	-H24C	109.00

Table S11. Non-covalent interactions in Complex **5**.

Atoms	D-H (Å)	H…A (Å)	D…A(Å)	DHA(˚)
N1X-H1X…O4F	0.98	1.71	2.687(12)	172
N2A-H2A…O1B	0.86	2.26	3.113(15)	173
N2B-H2B…O6X	0.86	2.21	3.057(15)	167
N2E-H2E…O1X	0.86	2.19	2.989(19)	155
N2F-H2F…O1E	0.86	2.25	3.078(13)	161
N2X-H2X…O4E	0.98	1.69	2.672(14)	175
N3X-H3X…O4B	0.98	1.75	2.724(13)	171
N4X-H4X…O4A	0.98	1.63	2.602(14)	169

G. FTIR of the complexes.

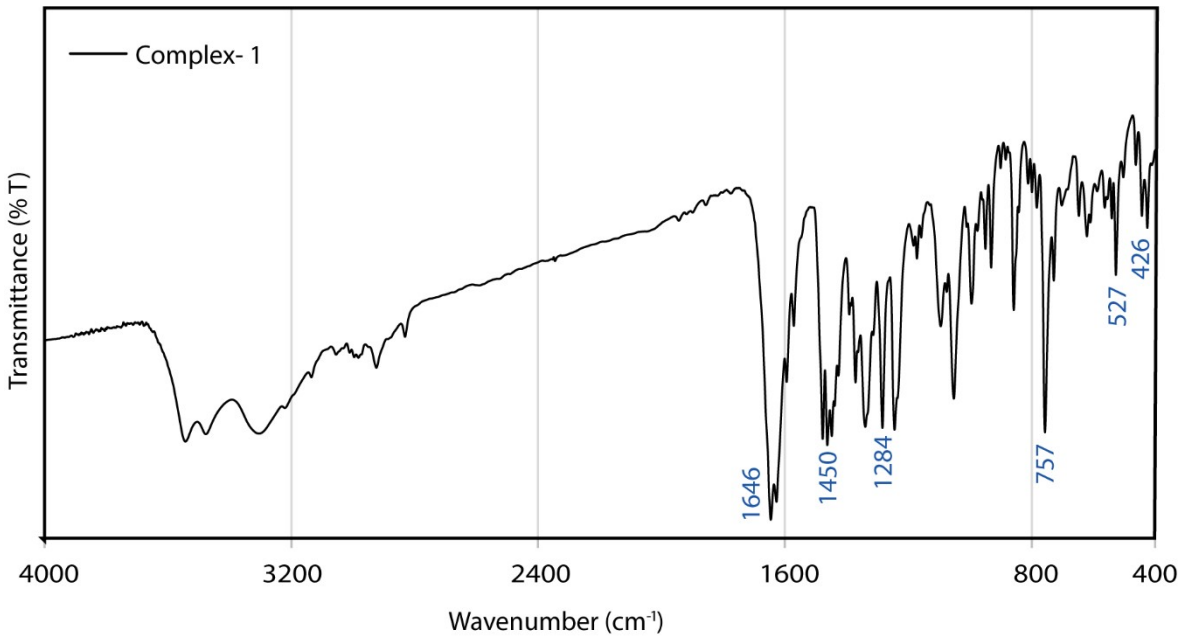


Figure S20. FTIR spectrum of **1**.

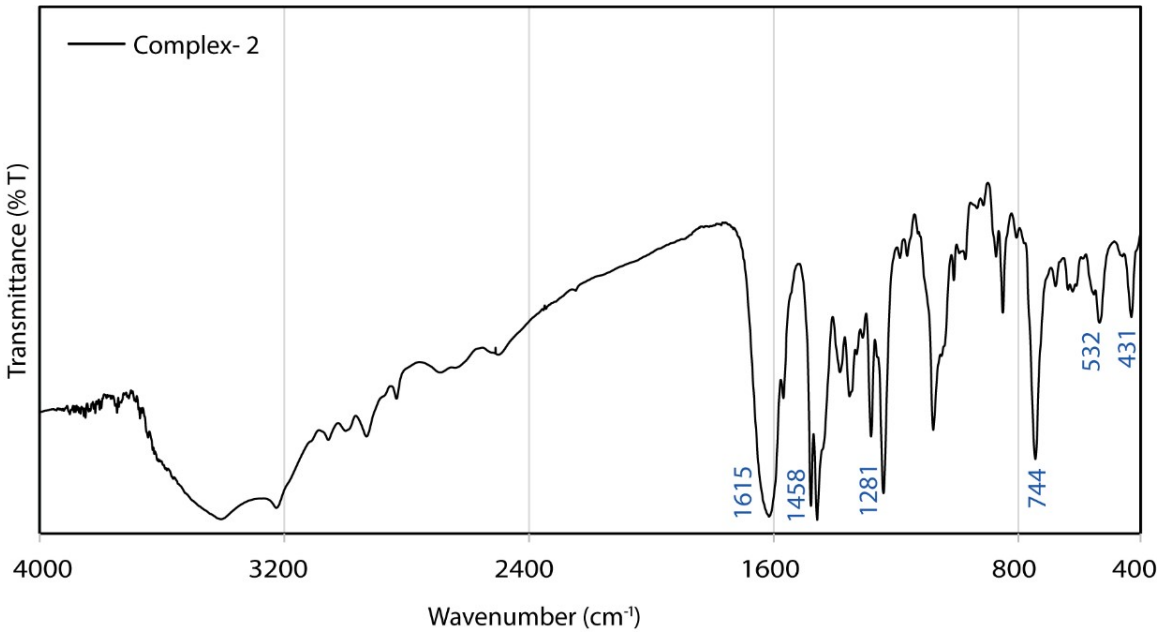


Figure S21. FTIR spectrum of **2**.

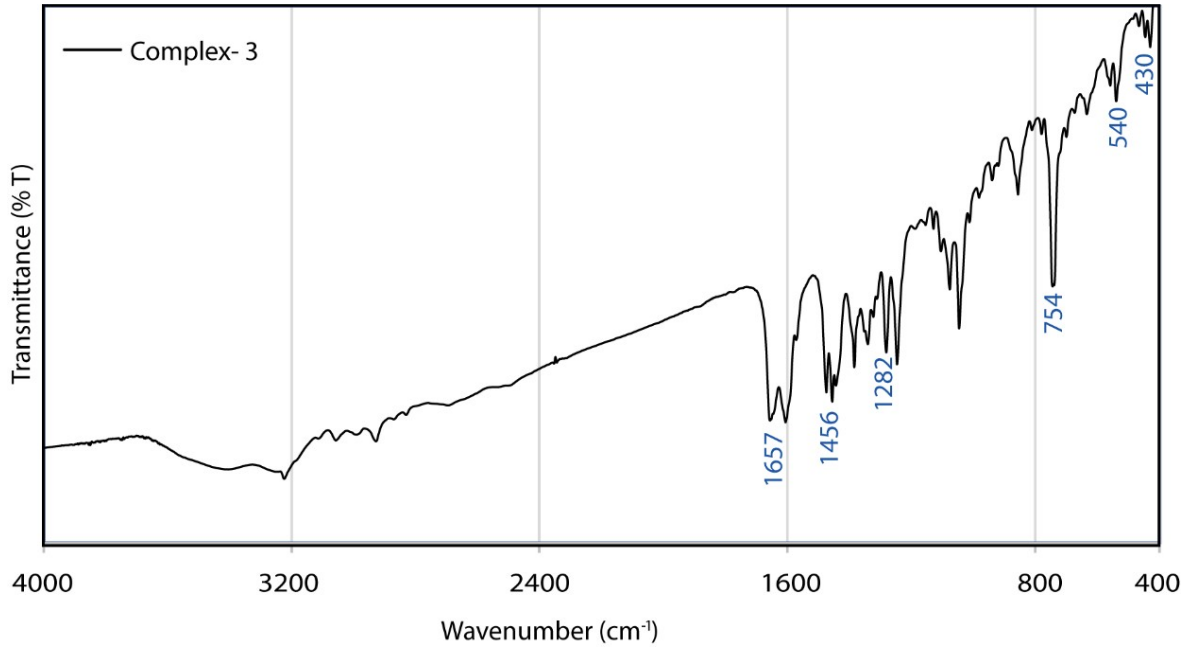


Figure S22. FTIR spectrum of **3**.

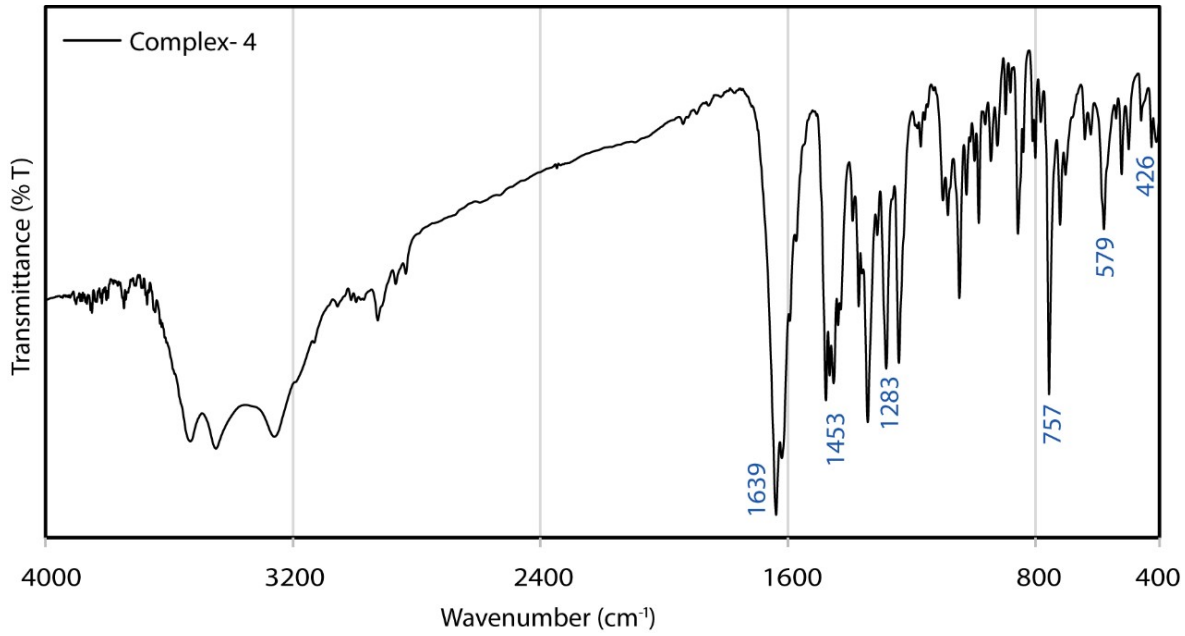


Figure S23. FTIR spectrum of **4**.

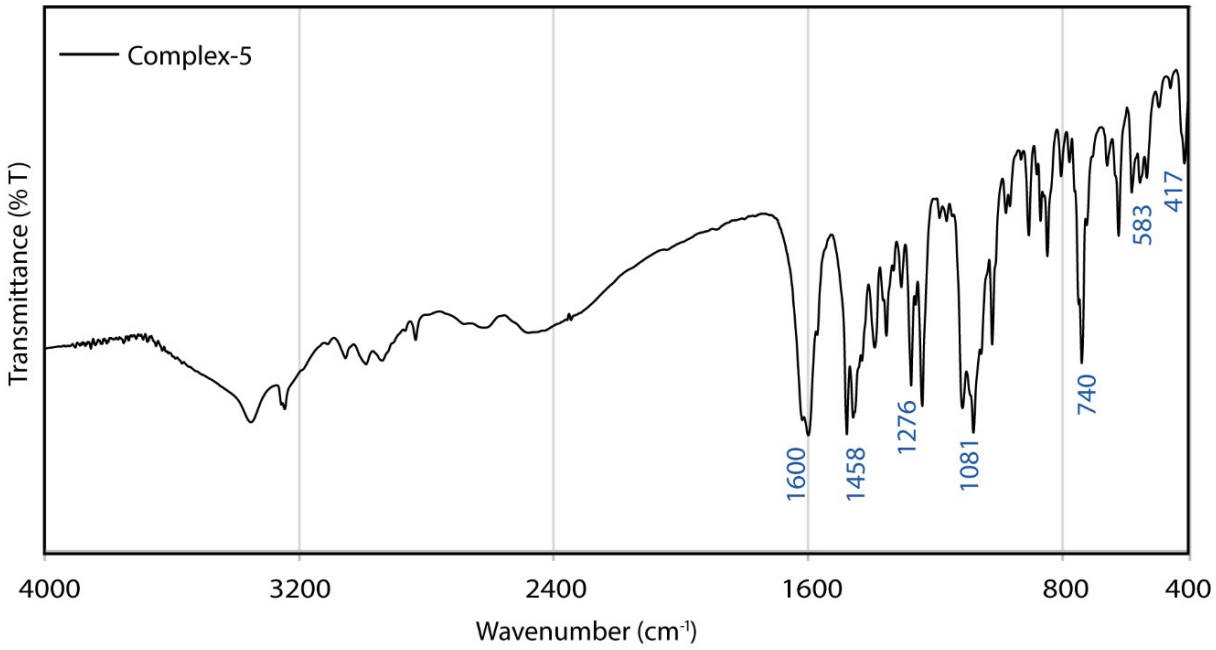


Figure S24. FTIR spectrum of **5**.