

Supplementary Information for:

Synthesis of a Potassium Capped Terminal Cobalt-Oxido Complex

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General Methods

All chemicals were purchased from commercial suppliers and used without further purification. All manipulations were carried out under an atmosphere of N₂ using standard Schlenk and glovebox techniques. Glassware was dried at 180 °C for a minimum of two hours and cooled under vacuum prior to use. Solvents were dried on a solvent purification system from Pure Process Technologies and stored over 4 Å molecular sieves under N₂. Tetrahydrofuran (THF) was stirred over NaK alloy and run through an additional alumina column prior to use to ensure dryness. Solvents were tested for H₂O and O₂ using a standard solution of sodium-benzophenone ketyl radical anion. CD₃CN, C₆D₆, and *d*₈-toluene were dried over 4 Å molecular sieves under N₂. ¹H NMR spectra were recorded on Bruker DRX 400 or 500 spectrometers. Chemical shifts are reported in ppm units referenced to residual solvent resonances for ¹H NMR spectra. UV-visible spectra were recorded on a Bruker Evolution 300 spectrometer and analyzed using VisionPro software. A standard 1 cm quartz cuvette with an airtight screw cap with a puncturable Teflon seal was used for all measurements. A Unisoku CoolSpek cryostat was used for low temperature measurements. IR spectra were recorded on a Bruker Tensor II spectrometer with the OPUS software suite as DCM thin films between KBr plates. Single crystal X-ray diffraction data were collected in-house using Bruker D8 Venture diffractometer equipped with Mo microfocus X-ray tube ($\lambda = 0.71073 \text{ \AA}$). Electrochemical measurements were carried out using a BAS Epsilon potentiostat and using BAS Epsilon software version 1.40.67 NT. EPR spectra were recorded on an Elexsys E500 spectrometer with an Oxford ESR 900 X-band cryostat and a Bruker Cold-Edge Stinger and were simulated using the Easyspin suite in Matlab software.¹ Magnetic moments were determined using the Evans method.²

Synthesis of [^{*t*}Bu,^{*Tol*}DHP]CoOK (**1**)

In a 20 mL vial in the glovebox, 2 mL of toluene was added to [^{*t*}Bu,^{*Tol*}DHP]CoOH (0.002 g, 1 eq., 0.004 mmol).³ A suspension of potassium tert-butoxide (0.0022 g, 5 eq., 0.020 mmol) in toluene was added to the bright purple solution of [^{*t*}Bu,^{*Tol*}DHP]CoOH. After stirring for 1-2 h, or until the suspended white solids were no longer visible, the resulting green-purple solution was dried *in vacuo* and extracted into benzene. Complex **1** can then be isolated as a purple solid after crystallizations in petroleum ether. Yield: 0.0019 g, 88 %. Poor quality single crystals suitable for XRD of **1** were grown out of a cooled concentrated petroleum ether solution at -35°C. ¹H NMR (400 MHz, C₆D₆, RT): $\delta = 10.92$ (br s), 8.44 (s), 6.67 (s), 1.88(s), 1.50(s). Magnetic Susceptibility: Evans' Method for **1** (C₇D₈ RT, 500 MHz, μ_B): $\mu_{\text{eff}} = 3.62$, UV-vis, nm in toluene, (ϵ , M⁻¹cm⁻¹): 2213.32. HRMS (EI) *m/z*: [M]⁺ calculated for **1**: C₂₈H₃₄N₅OKCo 554.1732 found: 554.1775.

In practice, this compound can also be obtained from [^{*t*}Bu,^{*Tol*}DHP]CoCl or OTf via addition of wet KO^{*t*}Bu.⁴

Characterization of [^{*t*}Bu,^{*Tol*}DHP]Co(MeCN)

The [^{*t*}Bu,^{*Tol*}DHP]Co(MeCN) has been previously reported.⁵ In this work we report its crystal structure.

Preparation of UV-Vis Samples

An aliquot of complex **1** was dissolved in toluene in a quartz cuvette in the glove box. The 1 cm quartz cuvette was equipped with an airtight screw cap. The spectrum was collected under a blanketing flow of Nitrogen.

Preparation of IR Samples of (1)

Separate samples of complex **1** and [^tBu, Tol]DHP]CoOH were dissolved in dry dichloromethane to form a concentrated solution. This was dropcast onto a KBr plate, and a second plate was then placed on top. The sample was then transferred in an air-free temporary container to the spectrometer, and a spectrum was collected.

Electrochemical Experiments

Experiments were performed inside the glovebox with a 1:4 MeCN:THF 0.1 M KPF₆ electrolyte solution at room temperature. Cyclic voltammetry measurements were made with a [Co] = 2.4 mM using a glassy carbon working electrode, platinum wire counter electrode, and silver wire pseudo reference electrode and were referenced to internal Fc/Fc⁺ by adding ferrocene at the end of measurements. A one-compartment glass cell was filled with 4 mL of electrolyte solution. The working electrode was polished over a microcloth pad (Buehler) using alumina slurry (0.05mm EMS), followed by rinsing with deionized water and isopropyl alcohol. Reference and counter electrodes were rinsed with acetone. CVs were recorded at a scan rate of 200 mV/s scanning oxidatively.

Density Functional Theory (DFT) Geometry Optimizations

Geometry optimization calculations and single point energy calculations were performed with ORCA⁶ software suite using density functional theory (DFT). Geometries were fully optimized starting from coordinates generated from finalized cifs of the compound crystal structures when possible. The O3LYP functional was used for geometry optimizations, spin density plot calculations, and single point energy calculations. For the O3LYP calculations, def2-TZVPP was used on Co, N, S, O, and F, and def2-TZVP on C and H atoms. A CPCM solvation model for benzene was used throughout. Due to the challenge of simulating the dimeric OK complex, the calculation energies here do not include entropic contributions.

NMR Spectroscopy

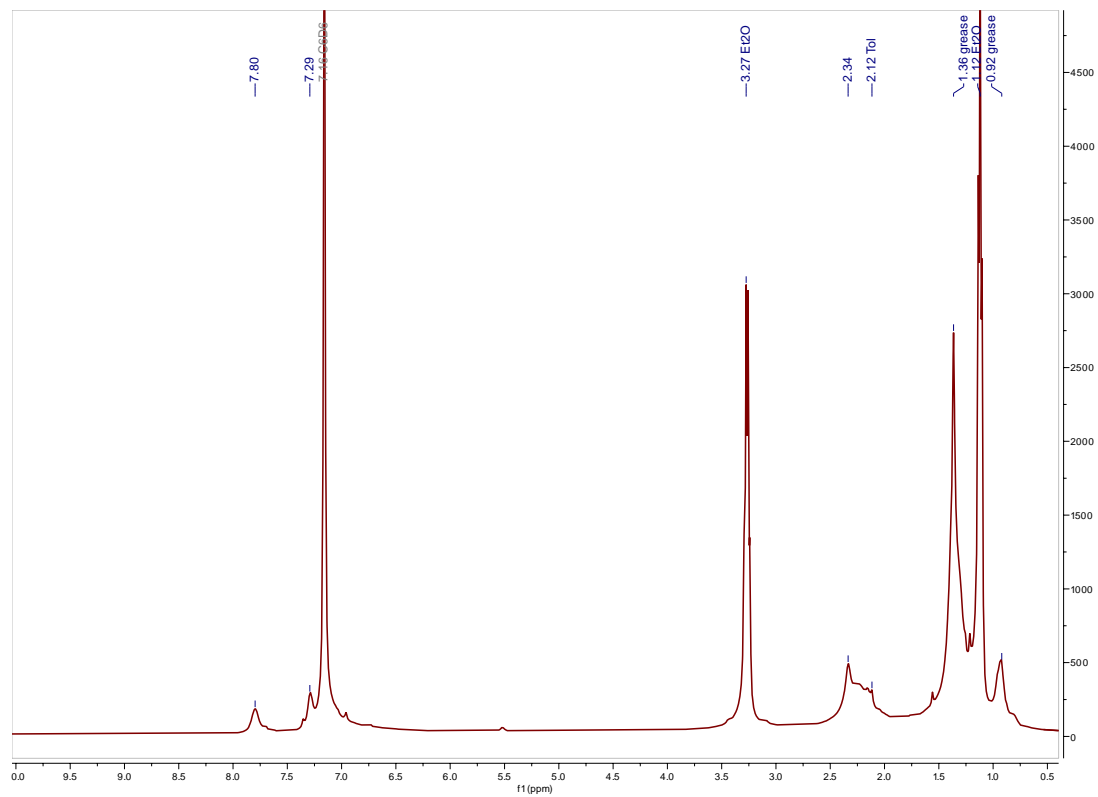


Figure S1. ^1H NMR of $[\text{tBu, Tol}]\text{DHP}]\text{CoOK}$ (1) in C_6D_6 .

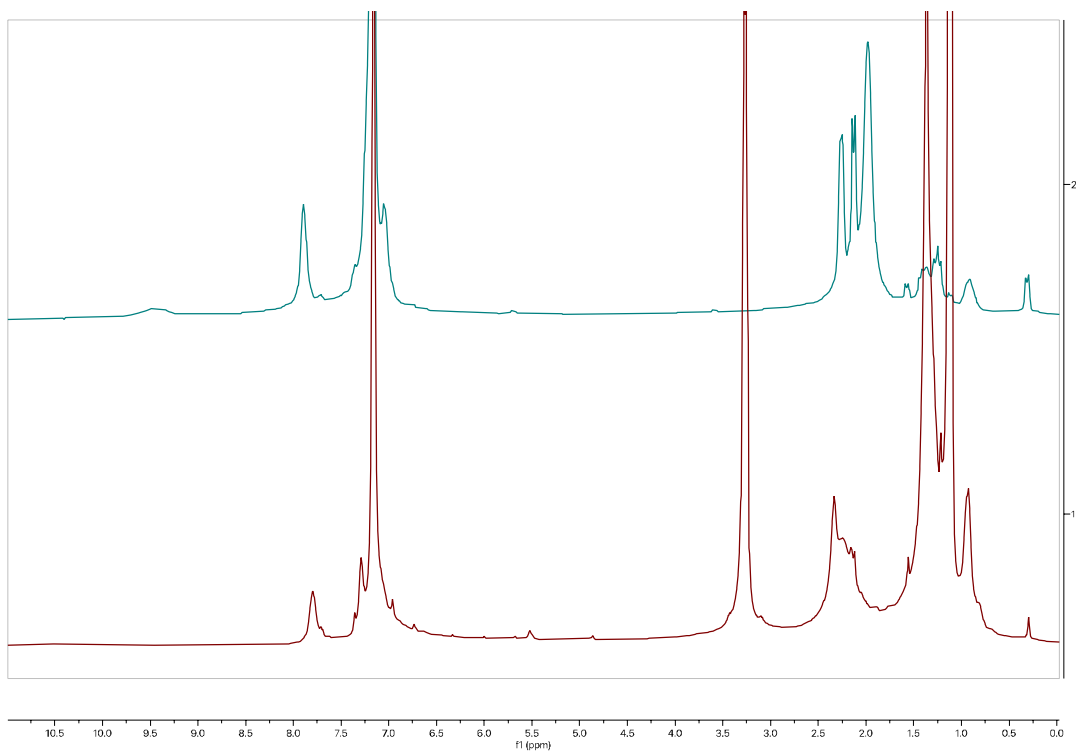


Figure S2. Comparison of ^1H NMR of $[\text{tBu, Tol}]\text{DHP}]\text{CoOH}$ in C_6D_6 (top) to ^1H NMR of $[\text{tBu, Tol}]\text{DHP}]\text{CoOK}$ (**1**) in C_6D_6 (bottom).

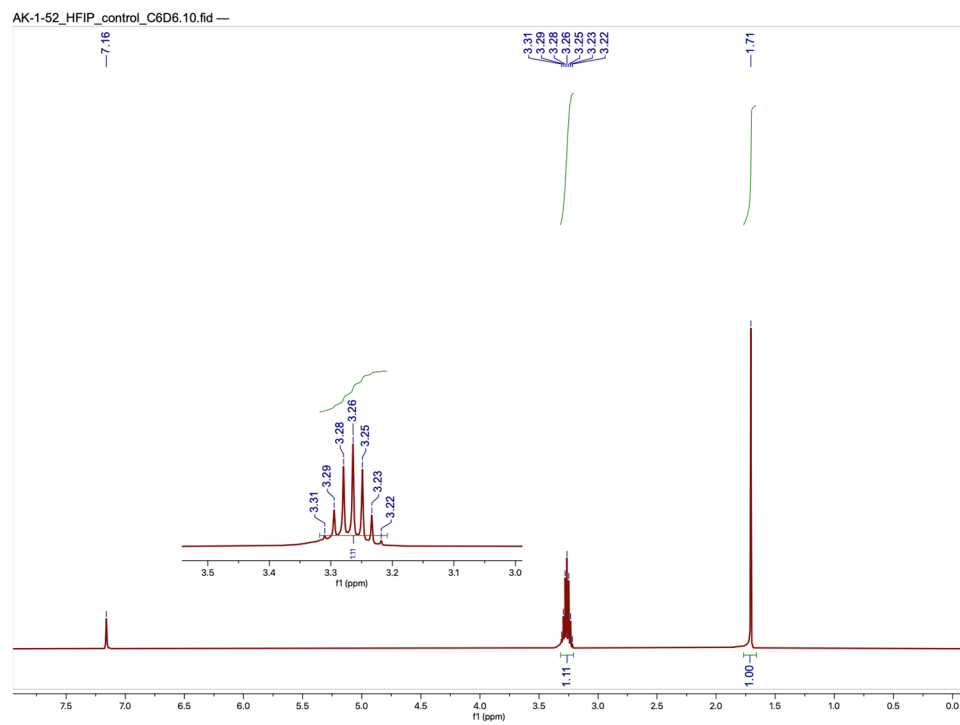


Figure S3. ^1H NMR of $(\text{CF}_3)_2\text{CHOH}$ (HFIP) in C_6D_6 .

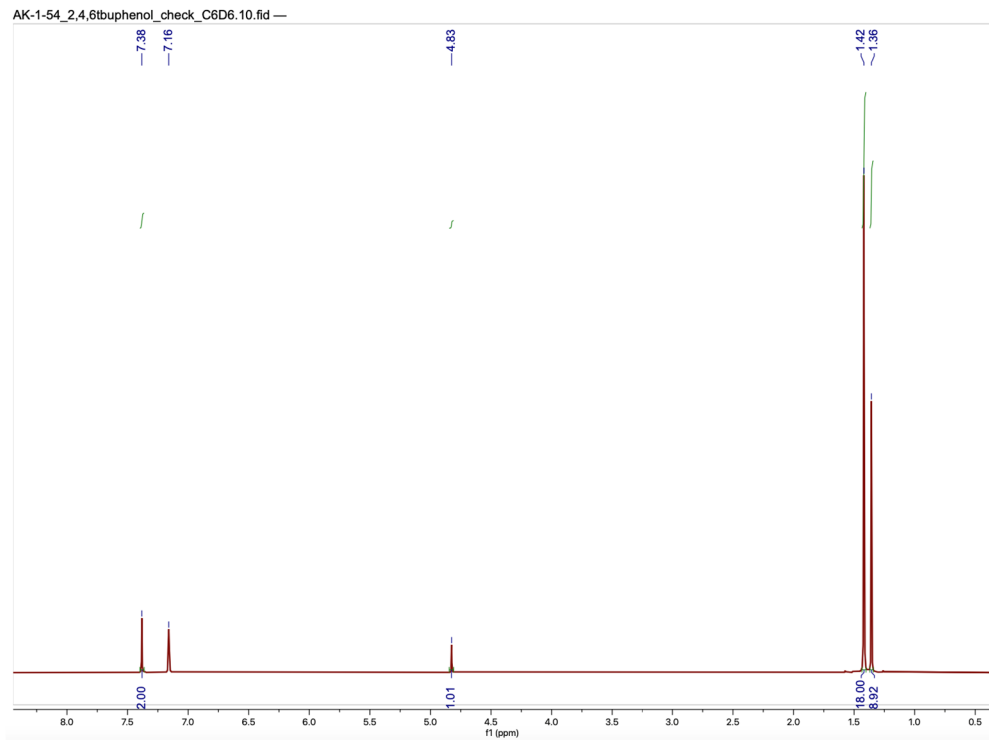


Figure S4. ^1H NMR of 2,4,6-tri-tert-butylphenol (2,4,6-TTBP) in C_6D_6 .

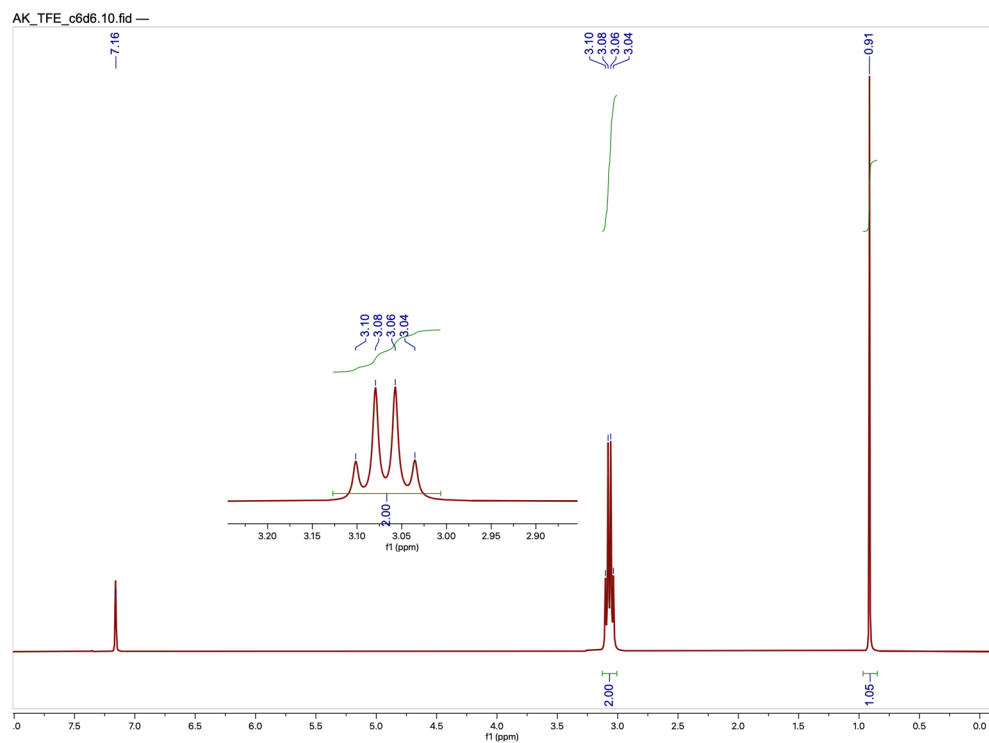


Figure S5. ^1H NMR of 2,2,2-Trifluoroethanol (TFE) in C_6D_6 .

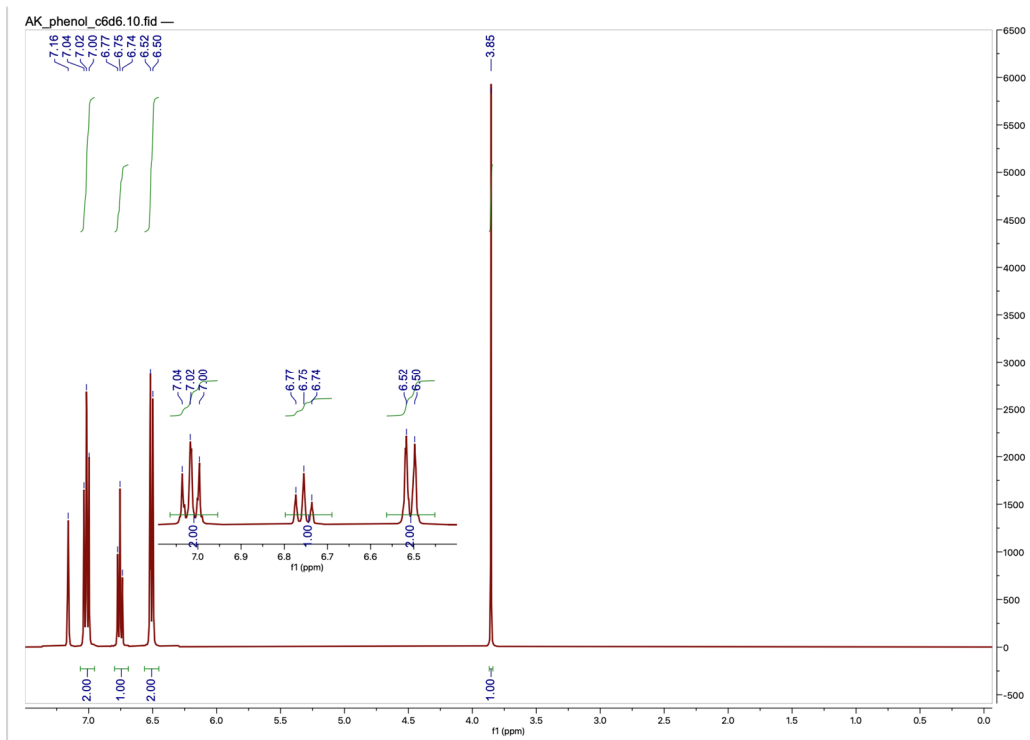


Figure S6. ^1H NMR of Phenol in C_6D_6 .

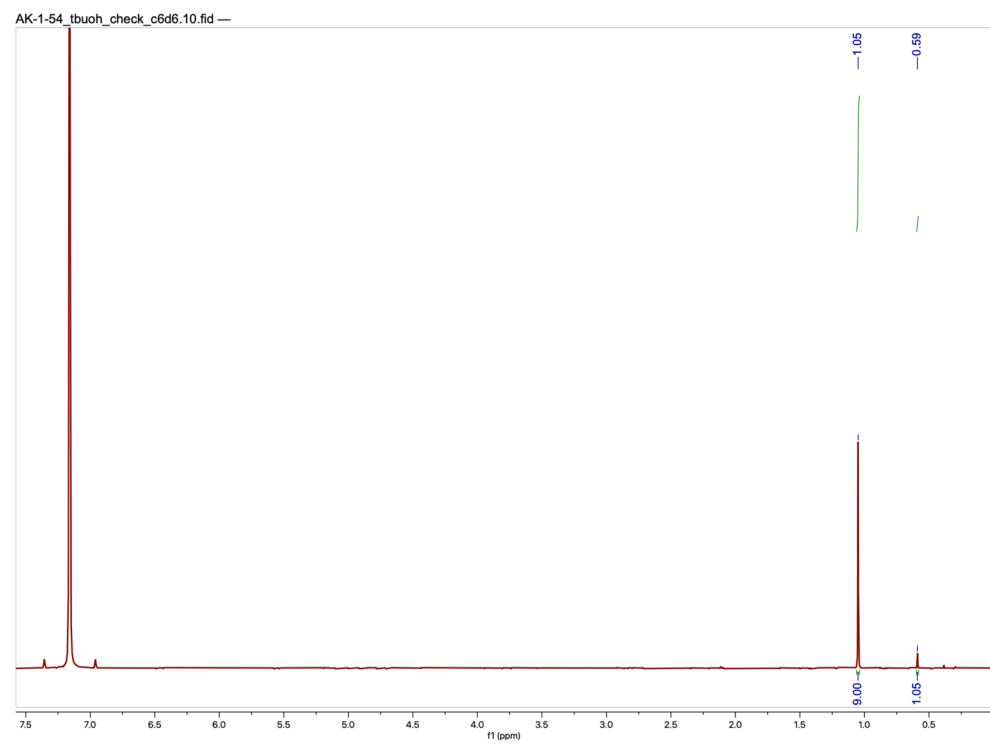


Figure S7. ^1H NMR of tert-butanol in C_6D_6 .

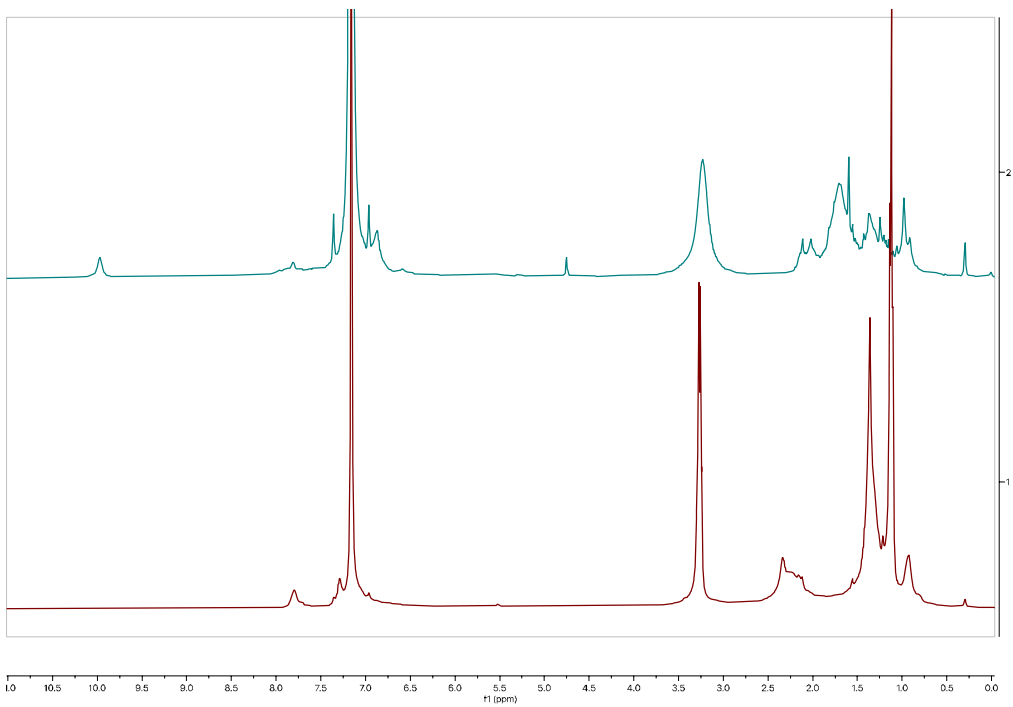


Figure S8. Comparison of ¹H NMR of **1** + HFIP in C₆D₆ (top) to **1** in C₆D₆ (bottom)

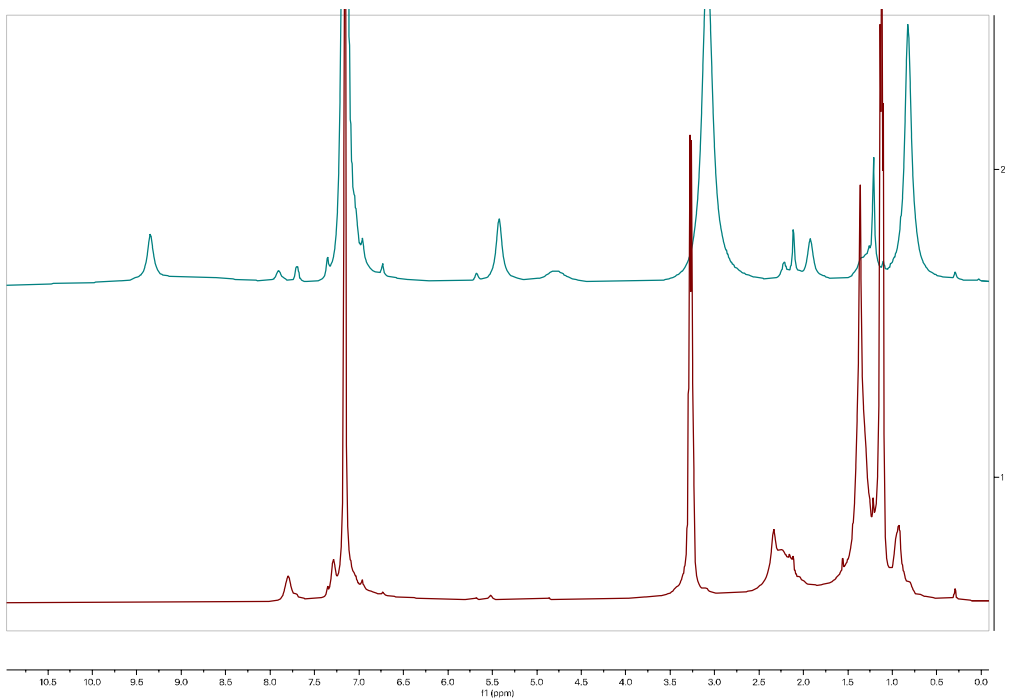


Figure S9. Comparison of ¹H NMR of **1** + TFE in C₆D₆ (top) to **1** in C₆D₆ (bottom)

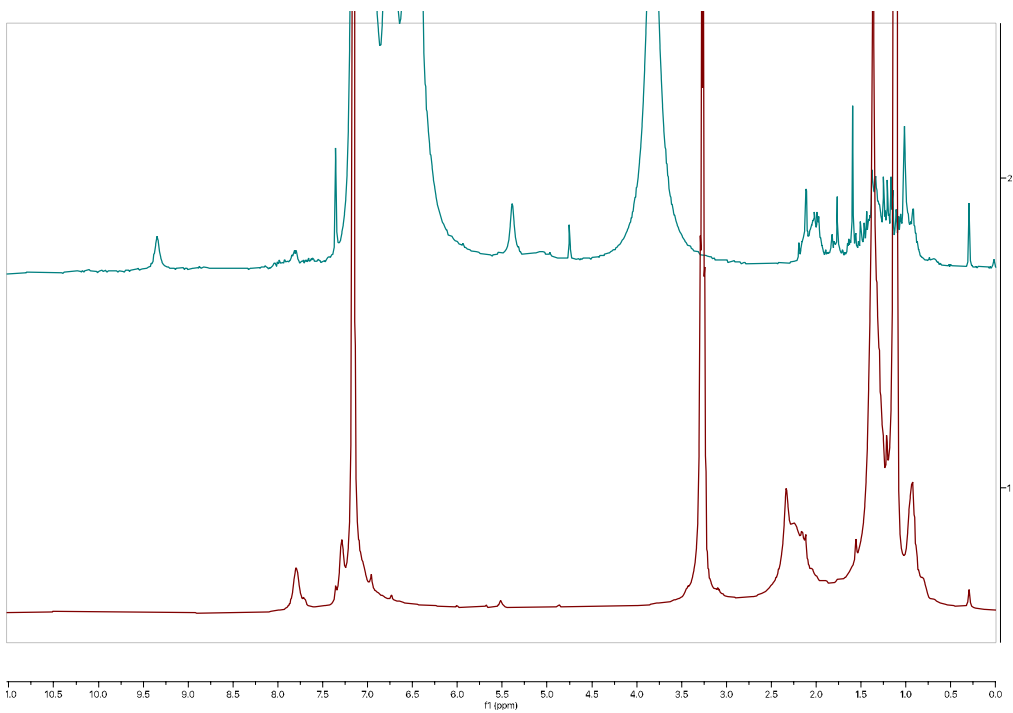


Figure S10. Comparison of ¹H NMR of **1** + Phenol in C₆D₆ (top) to **1** in C₆D₆ (bottom)

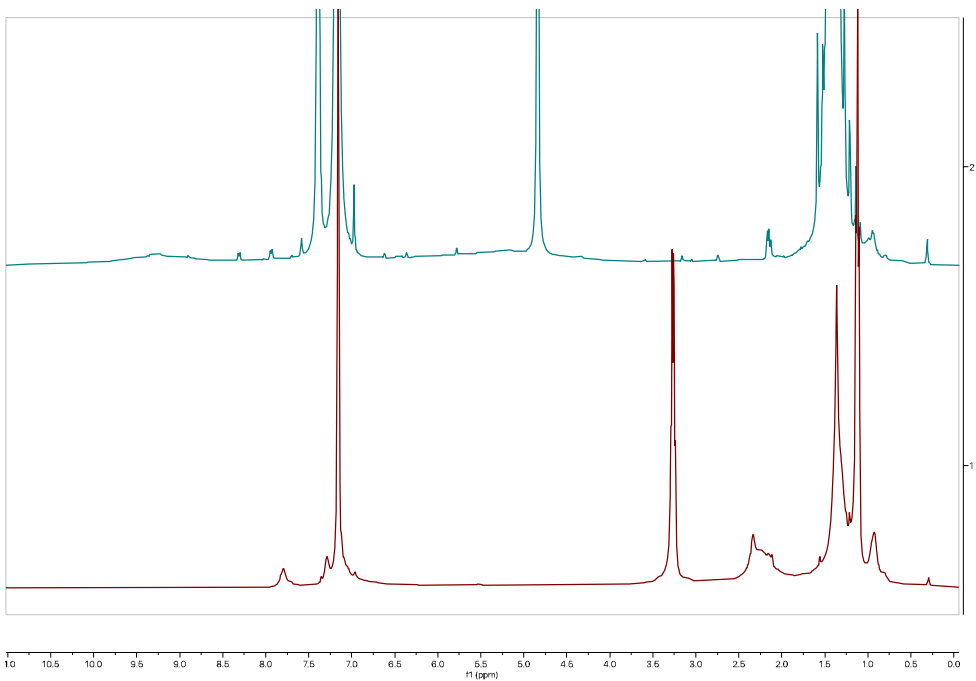


Figure S11. Comparison of ¹H NMR of **1** + 2,4,6-TTBP in C₆D₆ (top) to **1** in C₆D₆ (bottom)

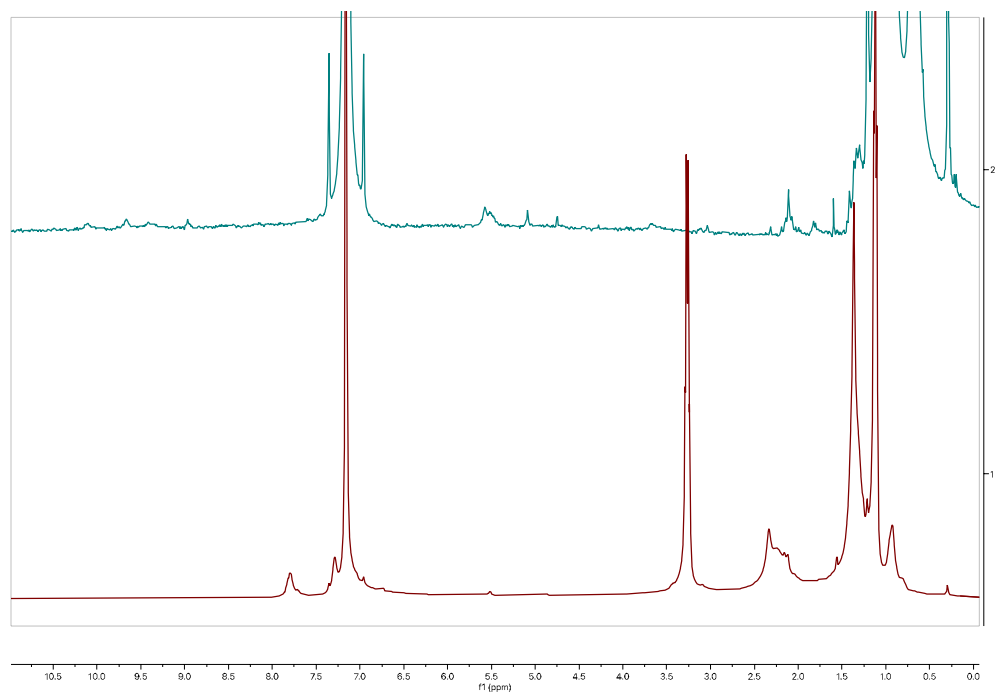


Figure S12. Comparison of ¹H NMR of **1** + tert-Butanol in C₆D₆ (top) to **1** in C₆D₆ (bottom)

UV-Vis Spectroscopy

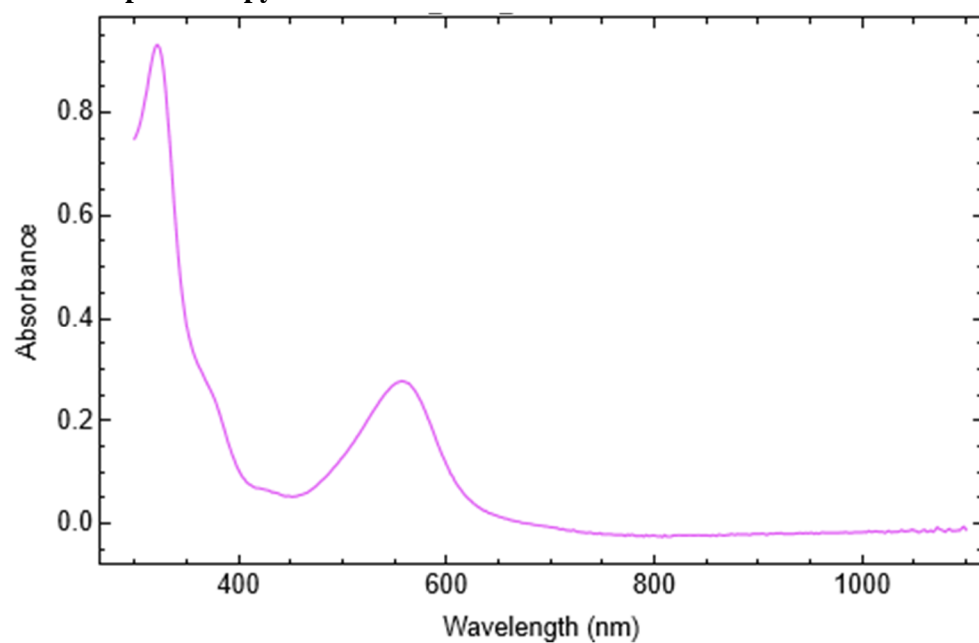


Figure S13. UV-vis of **1** from a 0.125 mM solution in toluene at room temperature.

IR Spectroscopy

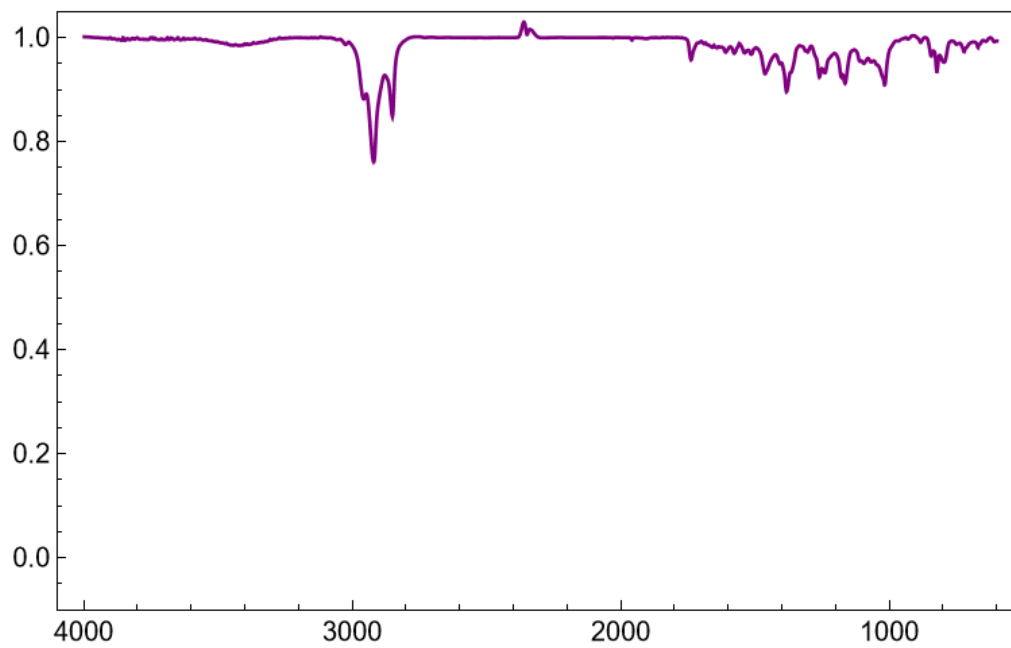


Figure S14. IR of **1** as a thin film.

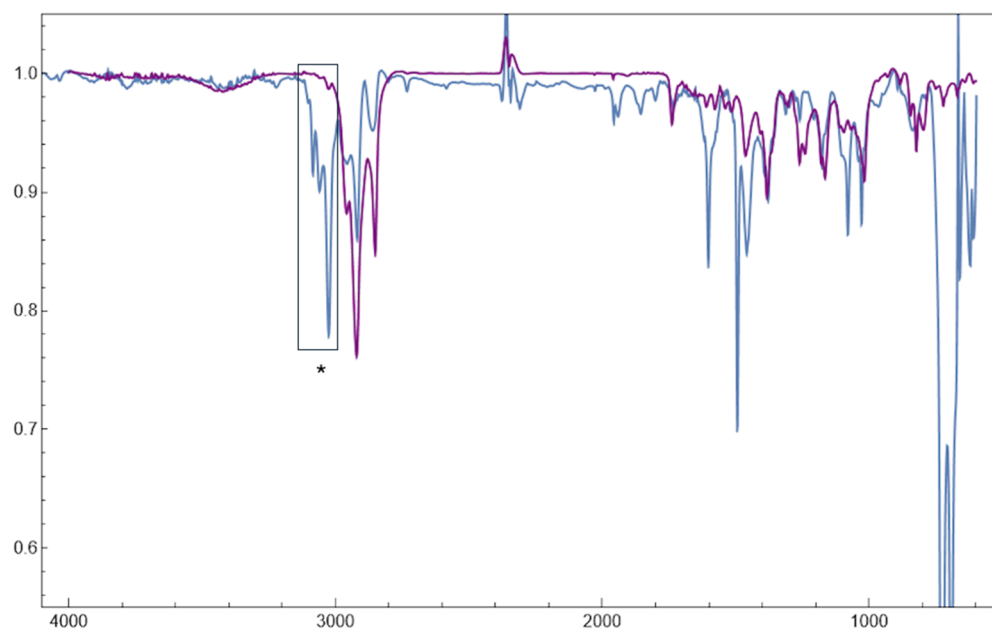


Figure S15. IR comparing IR of **1** (purple) as a thin film to IR of [^tBu, Tol]DHP]CoOH (blue) as a thin film. The OH peak of [tBu, Tol]DHP]CoOH is marked by an asterisk (*) and is generally consistent DFT calculated values.³ However, we note a few overlapping stretches, presumably from C–Hs. The low frequency of this OH made arise from hydrogen bonding interactions between molecules.

Cyclic Voltammetry

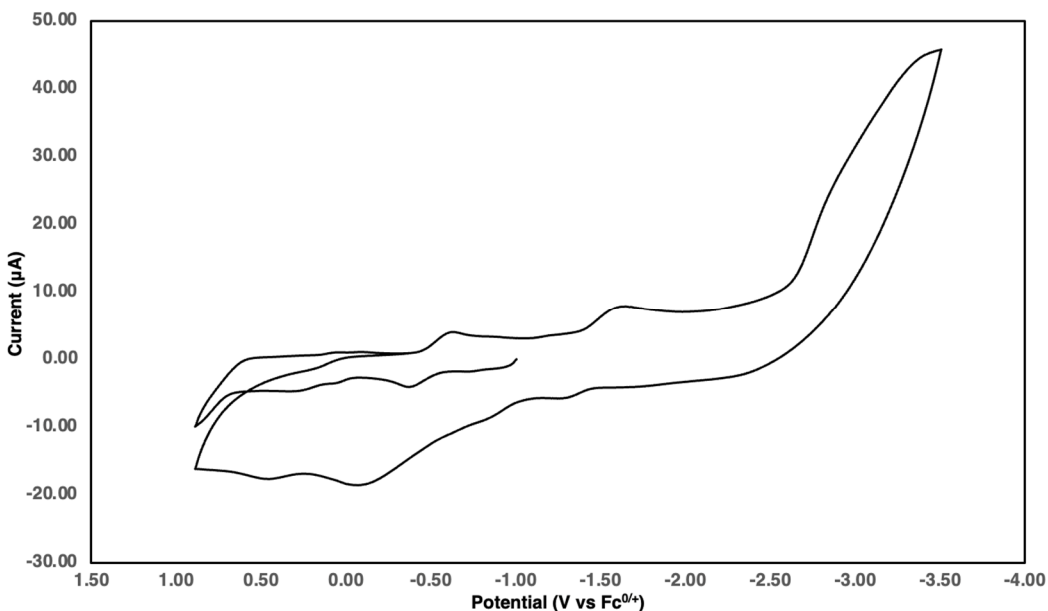


Figure S16. Cyclic Voltammogram of 2.4 mM of **1** in 0.1M KPF₆ electrolyte in a 1:4 MeCN:THF solution. Scan window: 1.5V to -3.5 V.

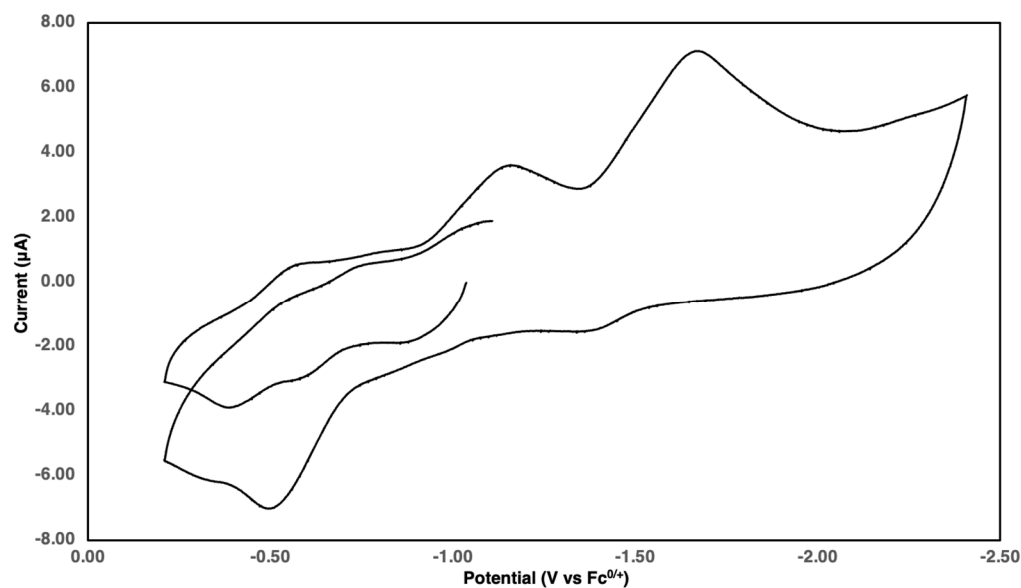


Figure S17. Cyclic Voltammogram of 2.4 mM of **1** in 0.1M KPF₆ electrolyte in a 1:4 MeCN:THF solution. Scan window: 0 V to -2.5 V

Single Crystal X-ray Diffraction

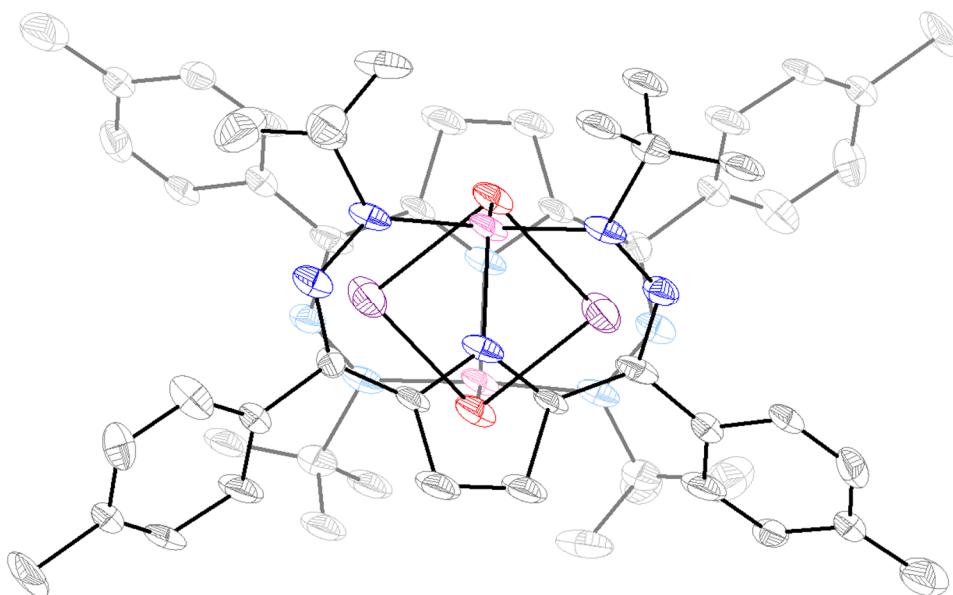


Figure S18. SXR D of **1**. Co (pink), N (blue), C (gray), O (red), K(violet). C-H H-atoms omitted.

Selected bond lengths (Å): Co-N1/N5: 1.94(1), 1.93(1); Co-N3: 1.94(1); N1-N2/N4-N5: 1.38(2), 1.32(2); Co-O: 1.96(1); N2-C5/N4-C10: 1.35(2), 1.33(2); C5-C6/C9-C10: 1.43(2), 1.41(2); C6-C7/C8-C9: 1.44(2), 1.42(2); C7-C8: 1.38(2). Selected bond angles (°): N1-M-N5: 149.4(6); N3-M-O: 107.4(5).

Table S1. SXRD of **1**.

Empirical formula	C ₂₈ H ₃₄ CoKN ₅ O
Formula weight	554.63
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.153(7)
b/Å	11.686(8)
c/Å	13.651(10)
α/°	89.533(19)
β/°	73.197(17)
γ/°	64.696(15)
Volume/Å ³	1389.1(17)
Z	2
ρ _{calc} /cm ³	1.326
μ/mm ⁻¹	0.797
F(000)	582.0
Crystal size/mm ³	0.242 × 0.072 × 0.052
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.566 to 46.918
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 13, -15 ≤ l ≤ 15
Reflections collected	14083
Independent reflections	4025 [R _{int} = 0.2607, R _{sigma} = 0.2678]
Data/restraints/parameters	4025/216/261
Goodness-of-fit on F ²	1.115
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.1435, wR ₂ = 0.3264
Final R indexes [all data]	R ₁ = 0.2880, wR ₂ = 0.4058
Largest diff. peak/hole / e Å ⁻³	1.76/-0.99

Table S2. Selected bond lengths (Å) and angles (°) of **1** and related Co complexes

	DHPCoOK	[DHP ²⁻]Co ^{II} (MeCN) ₂	[DHP ¹⁻]CoOTf	[DHP ²⁻]Co ^{III} OH
M—N1/M—N5	1.96(1) 1.92(1)	1.936(3) 1.938(3)	1.999(8) 2.000(8)	1.897(3) 1.889(3)
M—N3	1.94(1)	1.938(3)	1.918(7)	1.861(3)
N1—N2/ N4— N5	1.38(2) 1.32(2)	1.325(5) 1.320(5)	1.273(10) 1.249(10)	1.306(3) 1.302(3)
M—X(Cl/O/N)	1.96(1)	2.076(4)	2.166 2.128(6)	1.825(2)
N2—C5/ N4— C10	1.35(2) 1.33(2)	1.344(6) 1.339(6)	1.368(11) 1.383(11)	1.350(4) 1.342(4)
C5—C6/ C9— C10	1.44(2) 1.42(2)	1.402(6) 1.399(6)	1.387(13) 1.392(13)	1.390(4) 1.383(4)

C6—C7/ C8—C9	1.44(2)	1.441(6)	1.428(13)	1.439(4)
	1.41(2)	1.417(6)	1.445(13)	1.438(4)
C7—C8	1.39(2)	1.351(6)	1.315(13)	1.349(4)
N1—M—N5	149.1(5)	160.51(12)	178.1(3)	162.4(1)
N3—M—X	107.4(5)	114.32(13)	113.152	143.5(1)
			105.240	

L = PMe₃ as described in the text.

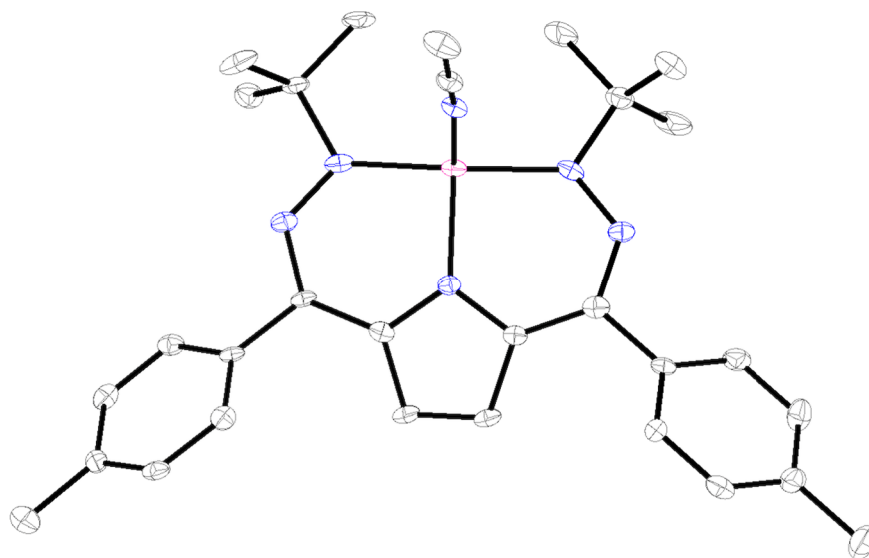


Figure S19. SXR of [^{tBu,Tol}DHP]Co(MeCN) . Co (pink), N (blue), C (gray), C–H H-atoms omitted for clarity.

Table S3. SXR of [^{tBu,Tol}DHP]Co(MeCN)

Empirical formula	C ₃₀ H ₃₇ CoN ₆
Formula weight	540.58
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	8.9652(6)
b/Å	11.2879(7)
c/Å	27.8086(17)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	2814.2(3)
Z	4
ρ _{calc} /cm ³	1.276
μ/mm ⁻¹	0.639

F(000)	1144.0
Crystal size/mm ³	0.297 × 0.122 × 0.059
Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection/ $^\circ$	4.648 to 50.264
Index ranges	-10 \leq h \leq 10, -13 \leq k \leq 13, -33 \leq l \leq 33
Reflections collected	54762
Independent reflections	5025 [$R_{\text{int}} = 0.1142$, $R_{\text{sigma}} = 0.0647$]
Data/restraints/parameters	5025/0/337
Goodness-of-fit on F^2	1.061
Final R indexes [$I > 2\sigma(I)$]	$R_1 = 0.0459$, $wR_2 = 0.0727$
Final R indexes [all data]	$R_1 = 0.0709$, $wR_2 = 0.0791$
Largest diff. peak/hole / e \AA^{-3}	0.38/-0.36

EPR Spectroscopy

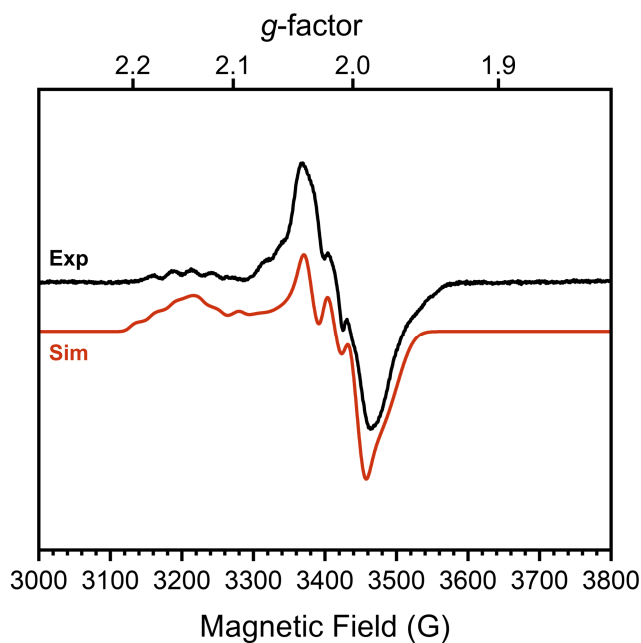


Figure S20. X-band EPR spectrum (black) and simulated spectrum (red) of a 15 mM solution of **1** (dimer) in toluene at 25 K. Conditions: MW frequency, 9.63 GHz; MW power, 2.0 mW.

Table S4. Simulated g -values for EPR of **1**

	$g(x,y,z)$	Co-A	N-A	H-strain
^t BuDHPCoOK	(2.14553 2.015 1.98313)	(37.85 7.0606 22.664)	(85.3902 87.9404 22.6612)	(41.7975 32.2248 100)

Code to generate simulations of EPR Spectra for 1.

```

Exp1.mwFreq=9.63;
Sys1.lw = 1
Exp1.Range = [300 380]
Exp1.nPoints = 2048
Sys1.g = [2.14553 2.015 1.98313]
Sys1.Nucs = 'Co,N';
Sys1.A = [37.85 7.0606 22.664;85.3902 87.9404 22.6612];
Sys1.HStrain = [41.7975 32.2248 100];
Vary1.g = [0.02 0.02 0.02];
Vary1.HStrain = [20 1.5 50];
Vary1.A = [10 10 10; 10 10 10];
plot(Bk,(((Ik)/max(Ik))*0.225)*2,Bk,pepper(Sys1,Exp1)/(max(pepper(Sys1,Exp1))))
)

```

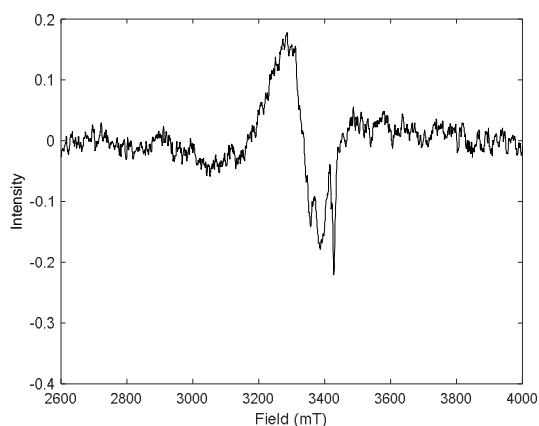
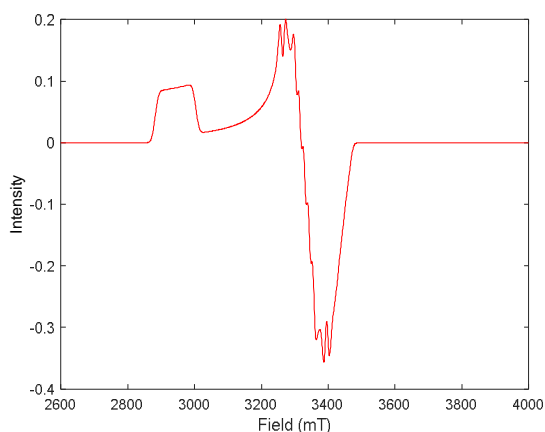


Figure S21. Small Window perpendicular-mode EPR spectrum (right) and simulated spectrum (left) of a 15 mM solution of [^tBu,^{Tol}DHP]CoOH in toluene at 25 K. Conditions: MW frequency, 9.63 GHz; MW power, 2.0 mW.

Code to generate simulations of EPR Spectra for [^tBu,^{Tol}DHP]CoOH.

```

Exp3.mwFreq=9.63913;
Sys3.lw = 1
Exp3.Range = [260 400]
Exp3.nPoints = 2048;
Sys3.g = [2.34 2.068 2.03];
Sys3.Nucs = 'Co, N';
Sys3.A = [50 40 40; 20 60 50];
Sys3.HStrain = [50 10 50];
Vary3.g = [0.02 0.02 0.02];
Vary3.HStrain = [50 10 50];
Vary3.A = [10 10 10; 10 10 10];
plot(BOH,((IOH)/max(IOH))-(-
0.000086*BOH+1.1044),BOH,0.2*pepper(Sys3,Exp3)/max(pepper(Sys3,Exp3)))

```

Density Functional Theory (DFT) Calculations

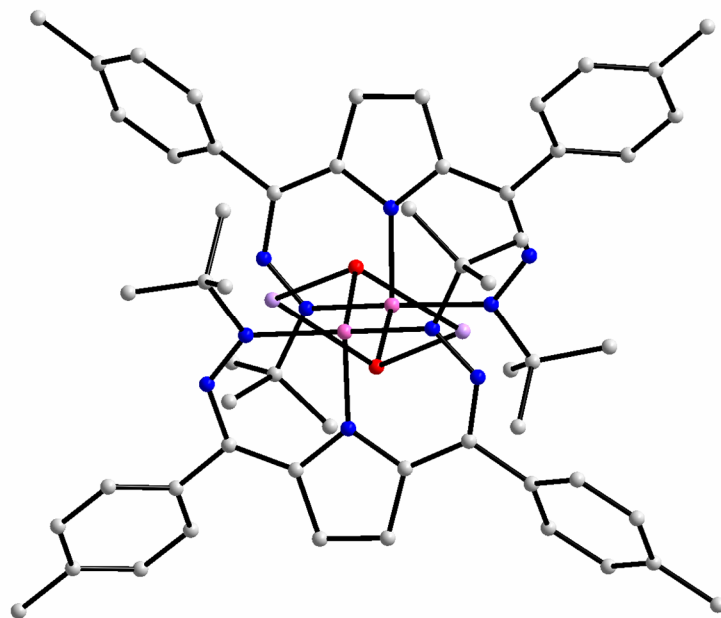


Figure S22. Calculated structure of **1**. All C–H hydrogen atoms have been removed for clarity

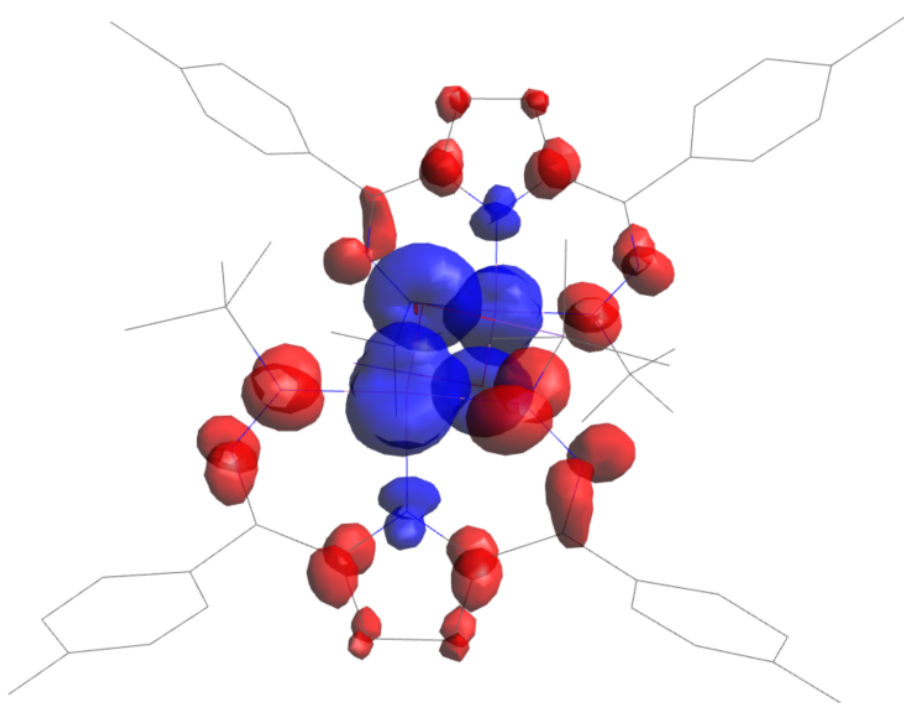


Figure S23. Spin density plot of **1** at an iso value of 0.005.

Table S5. Single Point Energy Calculations of **1** with the addition of different acids

Dimer		LCoOK+ tbuOH	LCoOK+ CyOH	LCoOK+ IPA	LCoOK+ acetamide	LCoOK+ TFE	LCoOK+ Phenol	LCoOK+ 2,4,6-TTBP	LCoOK+ PhenSL	LCoOK+ phthalamide	LCoOK+ HFIP	LCoOK+ BzCOOH	LCoOK dimer
Kcal/ mol	From LCoOH+ K[acid]	-18.01	-17.82	-17.19	-7.13	-6.05	-2.98	-2.63	-1.62	-0.80	1.77	12.48	-14.75
Monomer		LCoOK+ tbuOH	LCoOK+ CyOH	LCoOK+ IPA	LCoOK+ acetamide	LCoOK+ TFE	LCoOK+ Phenol	LCoOK+ 2,4,6-TTBP	LCoOK+ PhenSL	LCoOK+ phthalamide	LCoOK+ HFIP	LCoOK+ BzCOOH	All single point calculations (no entropy)
Kcal/ mol		-3.26	-3.07	-2.44	7.63	8.71	11.77	12.12	13.14	13.96	16.52	27.23	

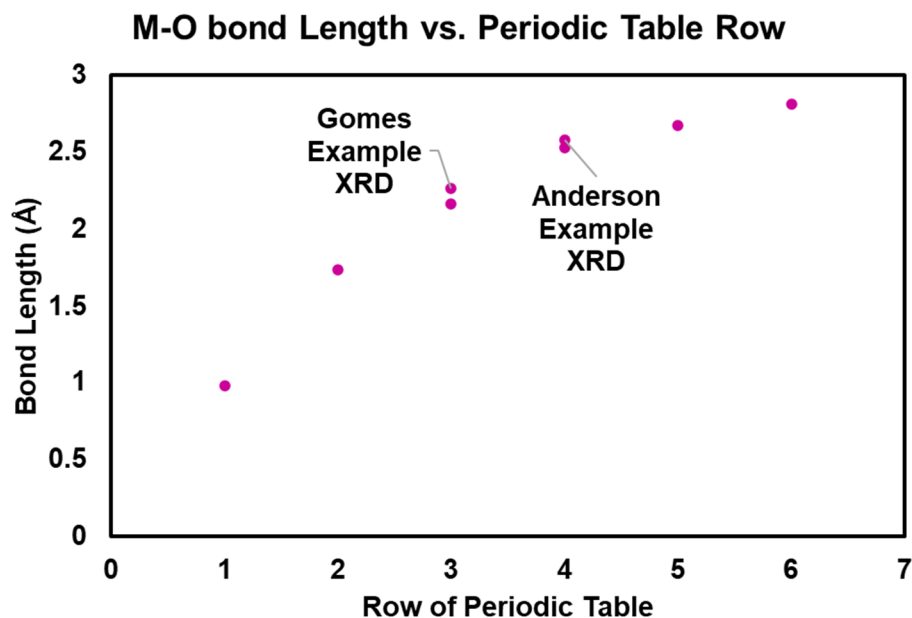


Figure S24. Calculated M–O bond lengths from monomeric (DHP)CoOM complexes ($S = \frac{1}{2}$) where M is each alkali metal (going down column 1 of the periodic table, rows 1-7).

Table S6. Single Point Energy Calculations of **1** with different alkali metal cations

Bond lengths in Å	LCoOH	LCoOLi	LCoONa	LCoOK	LCoORb	LCoOCs	LCoOK SXRD	Gomes SXRD	hydroxide
single O-M bond	0.976	1.738	2.164	2.53	2.675	2.808	2.58	2.263	--

pK_a Values of Weak Acids

Table S7. pK_a values for acids used in pK_a bracket study

pK _a	tbuOH	2,4,6-TTBP	TFE	Phenol	HFIP
Water	16.84 ⁷	12.19 ⁸	12.4 ⁹	10.0 ¹⁰	9.3 ¹¹
DMSO	29.4 ¹³	--	23.6 ⁹	18.0 ⁹	18.2 ¹⁵
MeCN	--	--	35.8 (calc.) ¹⁴	29.2 ¹²	--

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