Supporting Information

Tunable Carbocation-based Redox Active Ambiphilic Ligands: Synthesis, Coordination and Characterization

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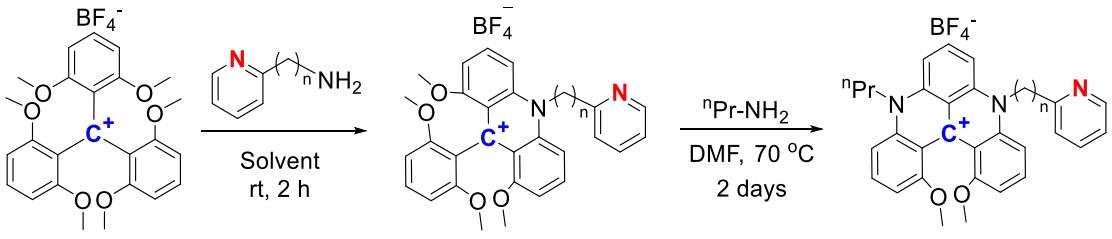
CONTENTS

1. General Remarks.

Unless otherwise specified, all reactions were carried out in oven-dried vials or reaction vessels with magnetic stirring in a glove box. Melting points are uncorrected and recorded using a MEL-TEMP® capillary melting point apparatus. ^{1}H NMR spectra and ^{13}C NMR spectra were recorded on Bruker Avance III-400 MHz or DRX-500 MHz spectrometers in appropriate solvents using TMS as internal standard or the solvent signals as secondary standards. The chemical shifts are shown in δ scales. Multiplicities of ^{1}H NMR signals are designated as s (singlet), d (doublet), dd (doublet of doublet), dt (doublet of triplet), t (triplet), quin (quintet), m (multiplet), etc.. HRMS (ESI) data were recorded on a Thermo LTQ Orbitrap Velos with nano ESI source by the Mass Spectrometry Facility of the University of Arizona. Elemental analyses were performed by the microanalytical laboratory of the ETH Zürich. Magnetic susceptibility data were recorded on a Sherwood scientific ltd Cambridge magnetic susceptibility balance mk1.[1] Absorption spectra were recorded on a ThermoScientific Evolution 220 UV-Visible spectrophotometer at 25 ˚C in analytical-grade solvents (con. 10^{-5} M). Compounds were named using ChemDraw and assignments of NMR spectra were done using MestReNova. All chemicals and solvents were purchased from Sigma Aldrich, Fisher Scientific, or VWR. Organic solvents used were dried by a standard solvent purification system. Commercially obtained reagents were used without further purification.

The $FeCl_2(THF)_{1.5}$[2] and $NiCl_2(DME)$[3] were synthesized by following procedures in previous literature.

2. Typical procedure for the preparation of the carbocation-based pyridine-containing ligands L1-L3



1

L1: n = 2, 90 % (Ethyl Acetate)
L2: n = 1, 76 % (MeCN)

L3: n = 2, 66 %

2-(2-Aminoethyl)pyridine (0.58 mL, 4.8 mmol, 1.2 equiv.) was added to a suspension of tris(2,6-dimethoxyphenyl)carbenium tetrafluoroborate **1** (2.04 g, 4.0 mmol, 1.0 equiv.) in EtOAc (100 mL).The solution was stirred at rt for 2 hr. Then 150 mL Et_2O was added and stirred at rt for 30 min. The red solid was filtered and further purified by recrystallization in DCM/hexanes to yield large dark red crystals (2.04 g, 90%).

L1: Yield: (2.04 g, 90%). A dark red solid. M.P.: 220-222 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (ddd, *J* = 4.8, 2.0, 0.8 Hz, 1H, Py), 8.26 (dd, *J* = 9.2, 8.0 Hz, 2H, ArH), 8.19 (d, *J* = 9.2 Hz, 2H, ArH), 7.70 (ddd, *J* = 7.6, 7.6, 2.0 Hz, 1H, Py), 7.57 (ddd, *J* = 7.6, 0.8, 0.8 Hz, 1H, Py), 7.37 (dd, *J* = 8.4, 8.4 Hz, 1H, ArH), 7.21 (ddd, *J* = 7.6, 4.8, 0.8 Hz, 1H, Py), 7.02 (d, *J* = 8.0 Hz, 2H, ArH), 6.66 (d, *J* = 8.4 Hz, 2H, ArH), 5.53 (t, *J* = 8.0 Hz, 2H, NC*H*$_2$CH$_2$Py), 3.69 (t, *J* = 8.0 Hz, 2H, NCH$_2$C*H*$_2$Py), 3.56 (s, 6H, OMe), 3.58 (s, 6H, OMe). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.90, 157.83, 156.23, 149.55, 141.67, 140.84, 137.53, 129.62, 124.60, 122.66, 119.91, 119.50, 109.15, 106.62, 103.54, 57.04, 56.08, 52.03, 35.66. ^{19}F NMR (376 MHz, $CDCl_3$) δ -153.42, -153.48. HRMS (ESI) Calcd. for $C30H29N2O4^{+1}$(M^++1) requires 481.2122, Found: 481.2119.

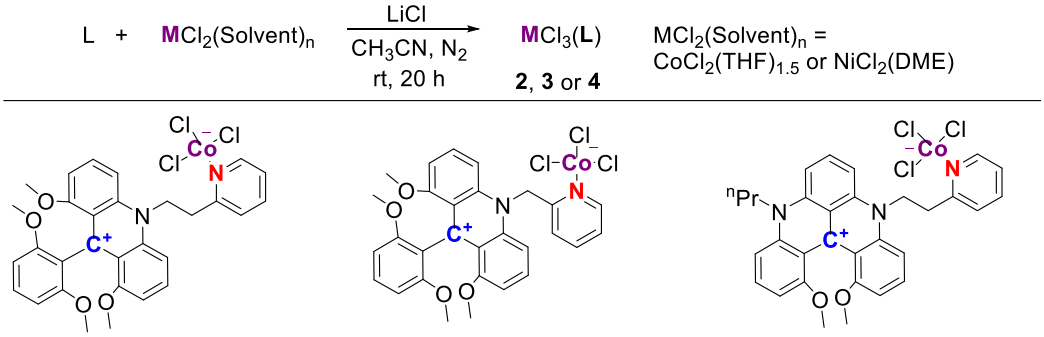
2-(2-Aminomethyl)pyridine (0.13 mL, 1.2 mmol, 1.2 equiv.) was added to a suspension of **1** (0.51 g, 1.0 mmol, 1.0 equiv.) in MeCN (15 mL). The solution was stirred at rt for 1 hr. MeCN was reduced to 5 mL under vacuum. Then 100 mL Et_2O was added and stirred at rt for 2 hr. The red solid was filtered and further purified by recrystallization in DCM/Et_2O to yield large dark red crystals (419 mg, 76%).

L2: Yield: (419 mg, 76%). A dark red solid. M.P.: 280-282 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.34 (ddd, *J* = 5.0, 2.0, 1.0 Hz, 1H, Py), 8.17 (dd, *J* = 9.0, 8.0 Hz, 2H, ArH), 7.99 (ddd, *J* = 8.0, 8.0 2.0 Hz, 1H, Py), 7.89 (d, *J* = 9.0 Hz, 2H, ArH), 7.81 (ddd, *J* = 8.0, 1.0, 1.0 Hz, 1H, Py), 7.46 (dd, *J* = 8.5 Hz, 1H, ArH), 7.38 (ddd, *J* = 8.0, 5.0, 1.0 Hz, 1H, Py), 7.20 (d, *J* = 8.0 Hz, 2H, ArH), 6.84 (d, *J* = 8.5 Hz, 2H, ArH), 6.70 (s, 2H, CH_2), 3.57 (s, 6H, OMe), 3.54 (s, 6H, OMe). ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.06, 157.06, 153.49, 149.53, 142.26, 140.22, 137.73, 129.53, 123.54, 122.43, 119.35, 119.13, 110.36, 106.97, 103.83, 57.21, 56.16, 55.89. ^{19}F NMR (376 MHz, DMSO-d_6) δ -148.25, -148.31. HRMS (ESI) Calcd. for $C29H27N2O4^{+1}$(M^++1) requires 467.1965, Found: 467.1965.

A solution of **L1** (1.14 g, 2.0 mmol, 1.0 equiv.) and n-propylamine (1.49 mL, 20.0 mmol, 10.0 equiv.) in 20 mL DMF was stirred in a pressure flask at 70 °C for 2 days. A dark green solution was formed. After cooling to rt, DMF was reduced to 4 mL under vacuum. 20 mL MeCN was added, followed by addition of a large excess of Et_2O (200 mL) and vigorous stirring at rt for 1 hr. Dark green solid crashed out and was filtered to yield crude product, which was further purified by recrystallization in DCM/Et_2O to yield dark green crystals (742 mg, 66%).

L3: Yield: (742 mg, 66%). A dark green solid. M.P.: 214-216 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.61-8.58 (m, 1H, Py), 8.24 (dd, *J* = 8.4, 8.4 Hz, 1H, ArH), 7.98-7.92 (m, 2H, ArH), 7.82 (d, *J* = 8.4 Hz, 1H, ArH), 7.77 (ddd, *J* = 7.6, 7.6, 2.0 Hz, 1H, Py), 7.71 (d, *J* = 8.4 Hz, 1H, ArH), 7.68 (d, *J* = 8.4 Hz, 1H, ArH), 7.62 (d, *J* = 8.4 Hz, 1H, ArH), 7.50-7.47 (m, 1H, Py), 7.33-7.29 (m, 1H, Py), 7.03-7.00 (m, 1H, ArH),5.17-5.08 (m, 1H, CH_2), 4.91-4.83 (m, 1H, CH_2),4.77-4.68 (m, 1H, CH_2),4.51-4.42 (m, 1H, CH_2), 3.73 (s, 6H, OMe), 3.44-3.39 (m, 2H, CH_2), 2.05-1.90 (m, 2H, CH_2), 1.17 (t, J = 7.2 Hz, 3H, CH_3). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.62, 157.85, 149.90, 142.31, 142.12, 142.02, 138.64, 137.71, 137.68, 137.37, 137.20, 124.44, 122.67, 118.98, 112.74, 108.11, 107.92, 105.61, 105.34, 103.54, 103.47, 56.02, 56.01, 50.91, 49.32, 33.93, 19.71, 11.07. ^{19}F NMR (376 MHz, DMSO-d_6) δ -148.25, -148.31. HRMS (ESI) Calcd. for $C31H30N3O2^{+1}$(M^++1) requires 476.2333, Found: 476.2331.

3. Typical procedure for the synthesis of Co(II) and Ni (II) complexes 2-4



2a [Co(**L1**)Cl_3], 84% yield
Ueff = 4.4 (0.1)[b]

3a [Co(**L2**)Cl_3], 69% yield[c]
Ueff = 4.3 (0.1)[b]

4a [Co(**L3**)Cl_3], 92% yield
Ueff = 4.3 (0.1)[b]

2b [Ni(**L1**)Cl_3], 90% yield
Ueff = 3.3 (0.1)[b]

3b [Ni(**L2**)Cl_3], 70% yield[c]
Ueff = 2.9 (0.1)[b]

4b [Ni(**L3**)Cl_3], 77% yield
Ueff = 3.3 (0.1)[b]

a) A solution of **L** (0.2 mmol, 1.0 equiv.), MCl_2(solvent)$_n$ (0.2 mmol, 1.0 equiv.) and LiCl (0.4 mmol, 2.0 equiv.) in MeCN (8 mL) was stirred in the glove box at rt for 20 hours.
b) Average value and the standard deviation of 3 different tests.
c) 4 mL MeCN was used as the solvent.

A solution of **L** (0.2 mmol, 1.0 equiv.), $CoCl_2(THF)_{1.5}$ or $NiCl_2(DME)$ (0.2 mmol, 1.0 equiv.) and LiCl (0.4 mmol, 2.0 equiv.) in MeCN (8 mL) was stirred in the glove box at rt for 20 hr. A cloudy solution was formed. The solid was filtered, washed with MeCN, THF and Et_2O, and dried under vacuum to give the final complexes **2**-**4**.

2a Co(**L1**)Cl_3: Yield: (108 mg, 84%). A dark red solid. M.P.: 262-264 ºC. Elemental Analysis (0.886 mg) requires: C, 55.70; H, 4.52; N, 4.33. Found: C, 55.62; H, 4.41; N, 4.56. μ_{eff} = 4.4 (0.1). X-ray crystals were obtained by layering the solution of ligand **L1** in MeCN on top of the solution of $CoCl_2(THF)_{1.5}$ and LiCl in MeCN without stirring at rt in the glove.

2b Ni(**L1**)Cl_3: Yield: (116 mg, 90%). A dark red solid. M.P.: 292-294 ºC (Decomposition). Elemental Analysis (0.974 mg) requires: C, 55.73; H, 4.52; N, 4.33. Found: C, 55.84; H, 4.52; N, 4.50. μ_{eff} = 3.3 (0.1). X-ray crystals were obtained by layering THF into a solution of **2b** in DMF.

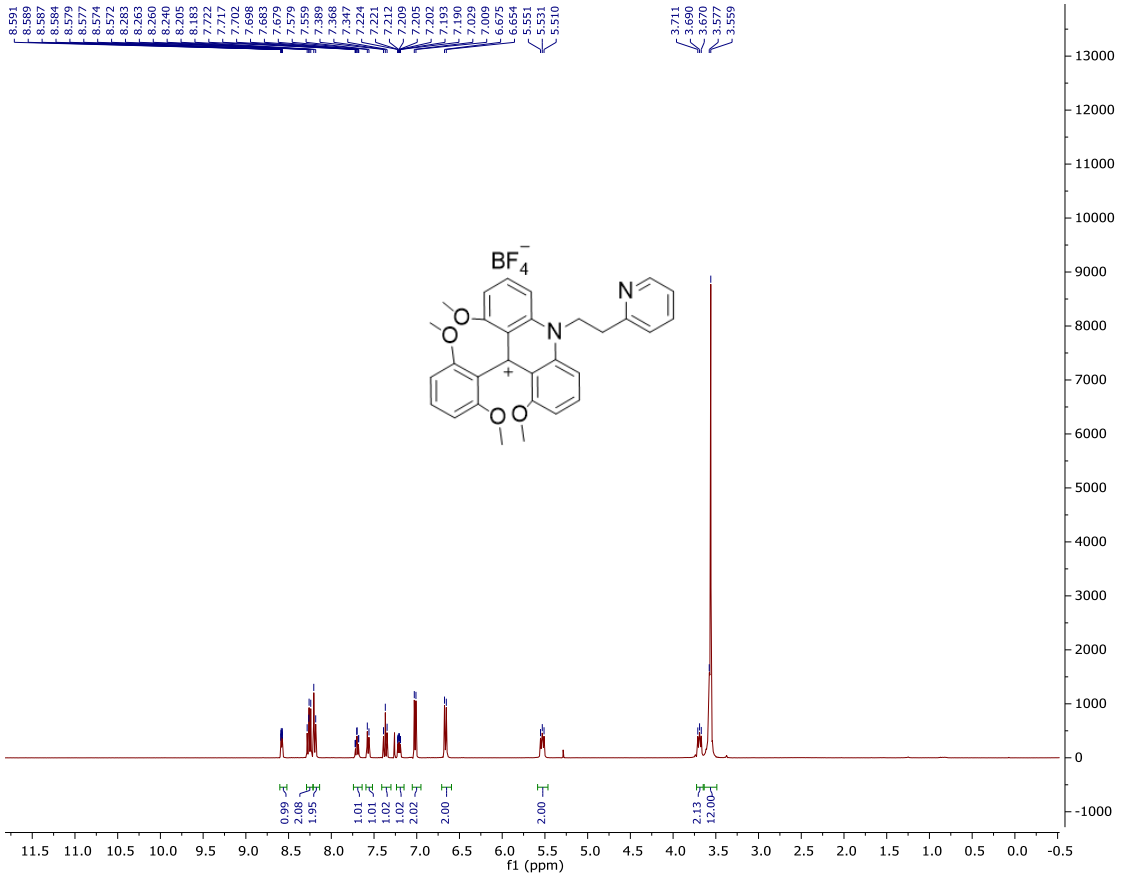
3a Co(**L2**)Cl_3: Yield: (87 mg, 69%). A dark red solid. M.P.: 298-300 ºC. Elemental Analysis (1.080 mg) requires: C, 55.04; H, 4.30; N, 4.43. Found: C, 55.24; H, 4.31; N, 4.59. μ_{eff} = 4.3 (0.1). 4 mL MeCN was used for the reaction, only washed with THF and Et_2O. X-ray crystals were obtained by layering the solution of ligand **L2** in MeCN on top of the solution of $CoCl_2(THF)_{1.5}$ and LiCl in MeCN without stirring at rt in the glove box.

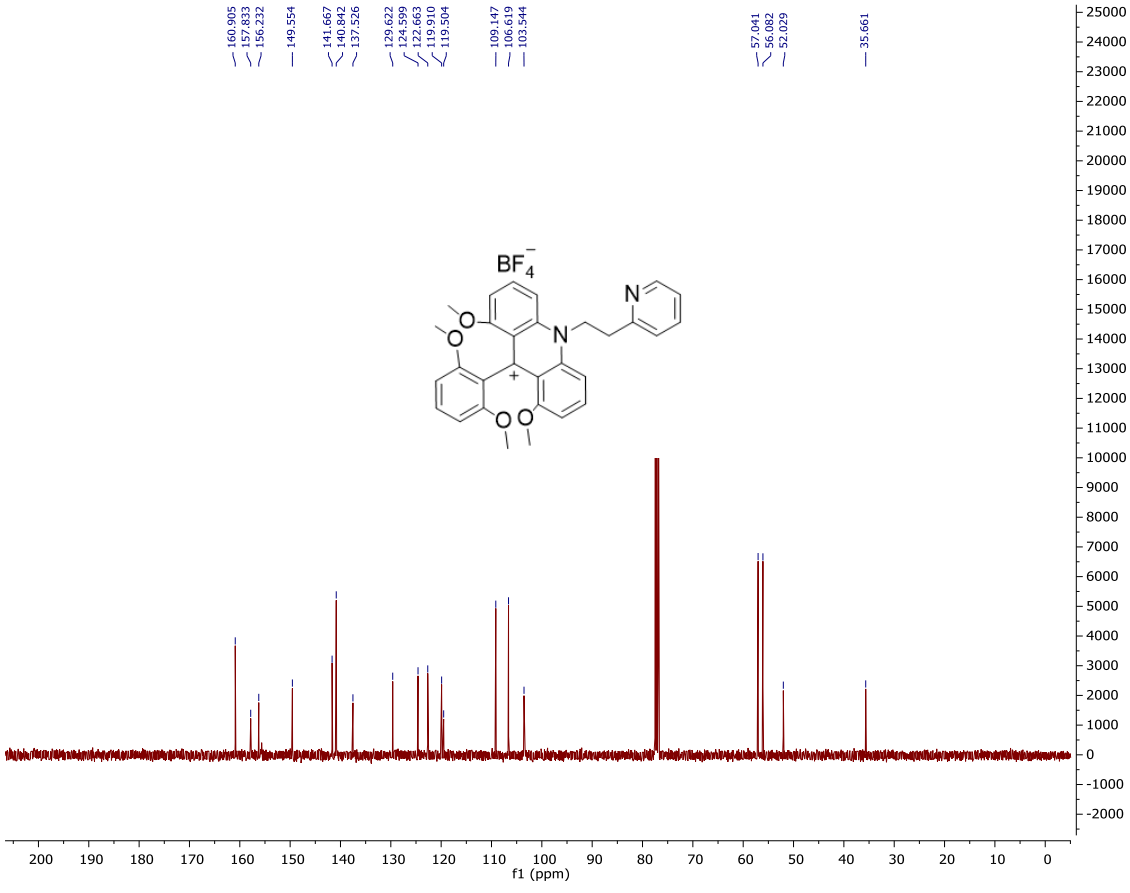
3b Ni(**L2**)Cl_3: Yield: (89 mg, 70%). A dark red solid. M.P.: 222-224 ºC. NMR: 1H NMR (500 MHz, Acetonitrile-d_3) δ 14.90 (br, 1H, Py), 10.26 (br, 1H, Py), 9.39 (br, 1H, Py), 8.93 (br, 1H, Py), 8.00 (dd, *J* = 8.5, 9.5 Hz, 2H, ArH), 7.67 (d, *J* = 9.5 Hz, 2H, ArH), 7.47 (dd, *J* = 8.5, 8.5 Hz, 1H, ArH), 7.07 (d, *J* = 8.5 Hz, 2H, ArH), 6.82 (d, *J* = 8.5 Hz, 2H, ArH), 5.05 (br, 2H, CH_2), 3.60 (s, 6H, OMe), 3.56 (s, 6H, OMe). Elemental Analysis (0.905 mg) requires: C, 55.06; H, 4.30; N, 4.43. Found: C, 55.23; H, 4.59; N, 4.32. μ_{eff} = 2.9 (0.1). 4 mL MeCN was used for the reaction so the product was only washed with THF and Et_2O. X-ray crystals were obtained by layering THF into solutions of **3b** in MeCN.

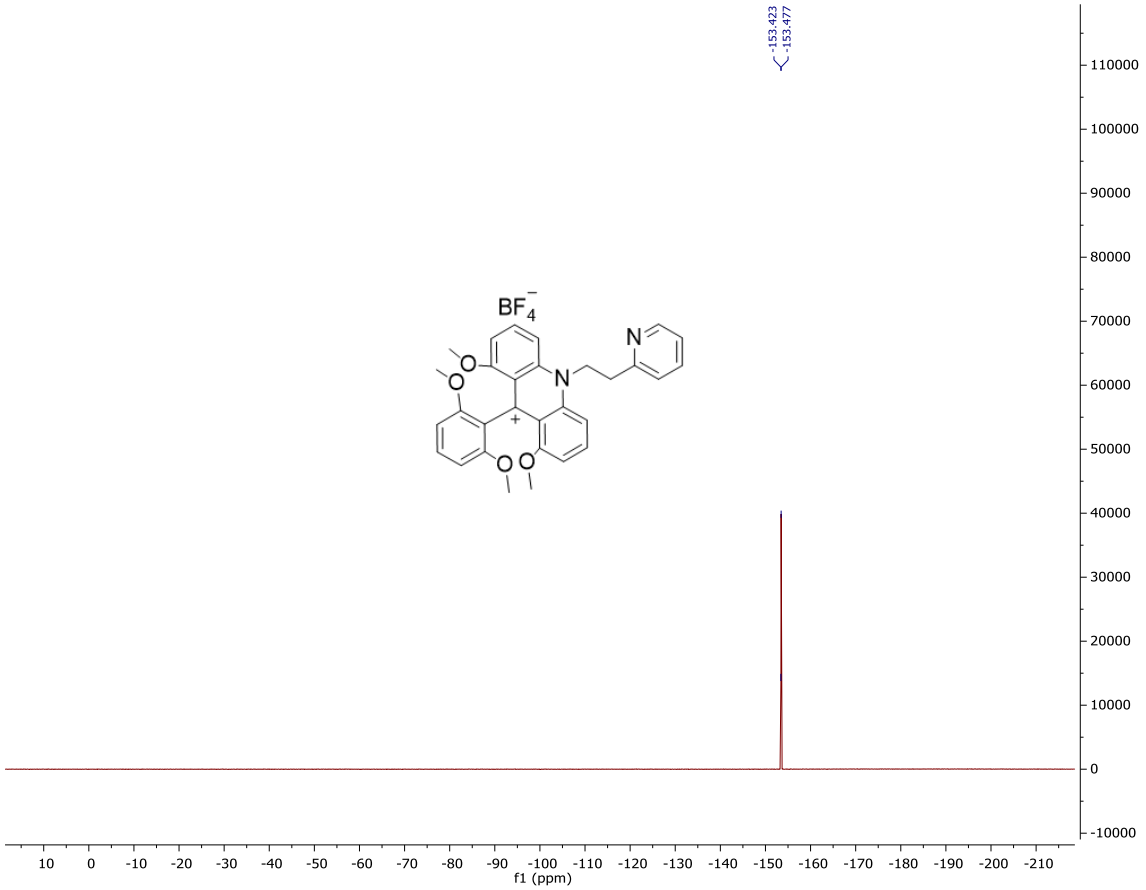
4a Co(**L3**)Cl_3: Yield: (118 mg, 92%). A dark green solid. M.P.: 218-220 ºC. Elemental Analysis (1.011 mg) requires: C, 58.01; H, 4.71; N, 6.55. Found: C, 57.98; H, 4.88; N, 8.18. μ_{eff} = 4.3 (0.1). X-ray crystals were obtained by layering the solution of ligand **L3** in MeCN into the solution of $CoCl_2(THF)_{1.5}$ and LiCl in MeCN without stirring at rt in the glove box.

4b Ni(**L3**)Cl_3: Yield: (99 mg, 77%). A dark green solid. M.P.: 216-218 ºC. Elemental Analysis (0.847 mg) requires: C, 58.03; H, 4.71; N, 6.55. Found: C, 58.13; H, 4.82; N, 8.18. μ_{eff} = 3.3 (0.1).

4. NMR spectra charts for ligands L1-L3, complexes 3b and the corresponding variable temperature-NMR.



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BF4−
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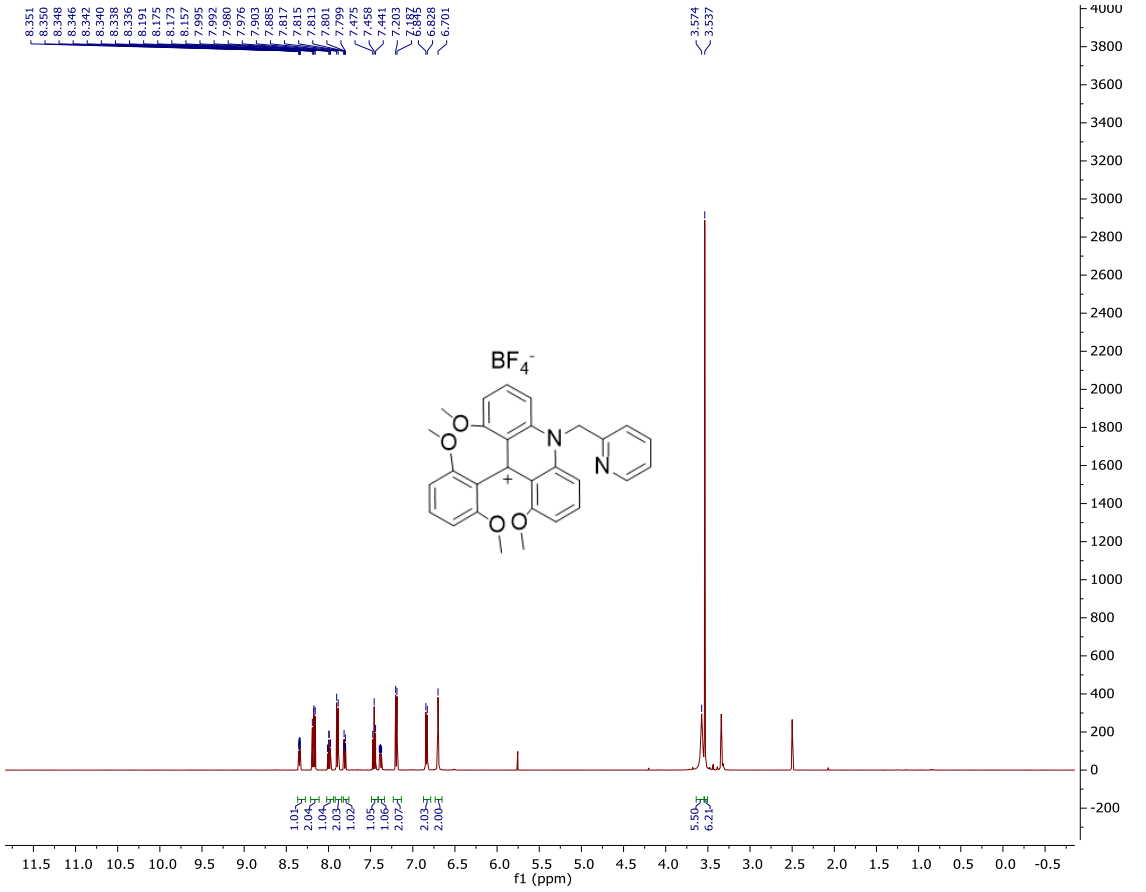
N
O
O
f1 (ppm)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8.350
8.348
8.346
8.342
8.340
8.338
8.336
8.191
8.175
8.173
8.157
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7.980
7.976
7.903
7.885
7.817
7.815
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7.801
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O
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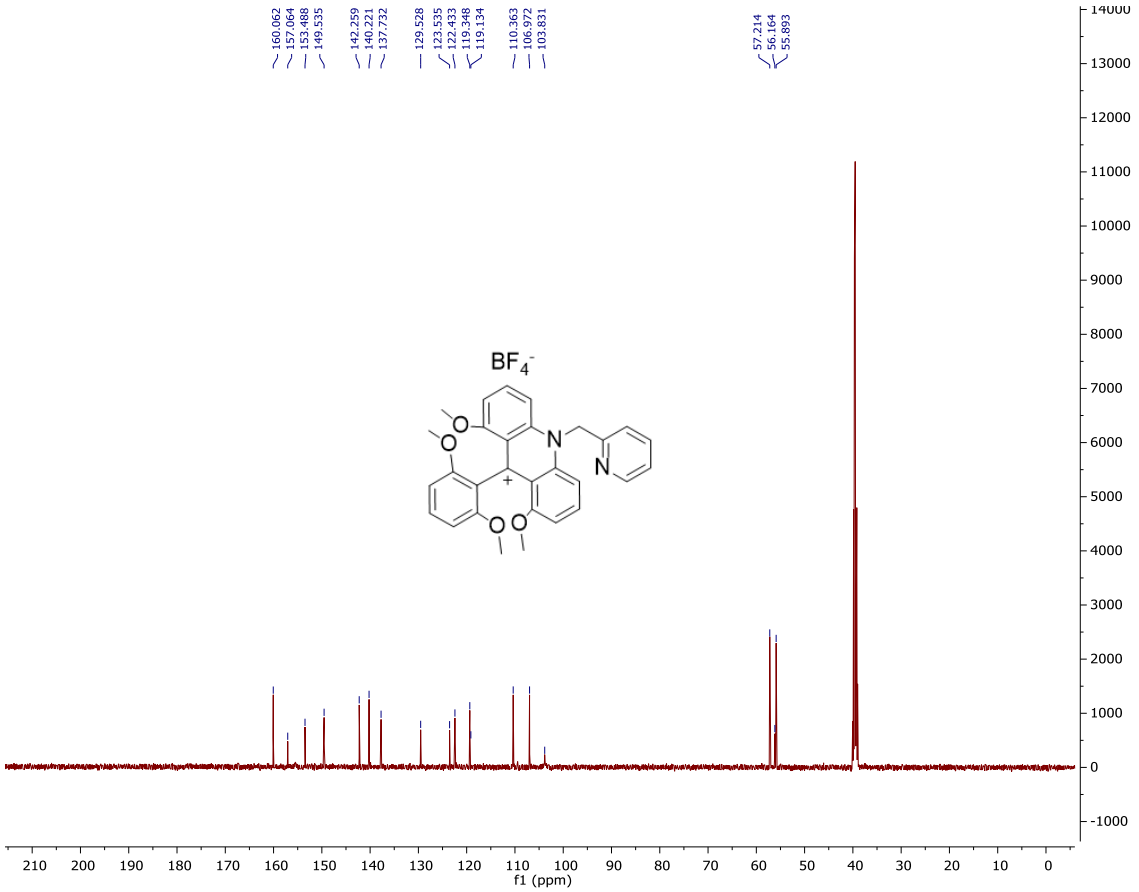
2.00
5.50
6.21
f1 (ppm)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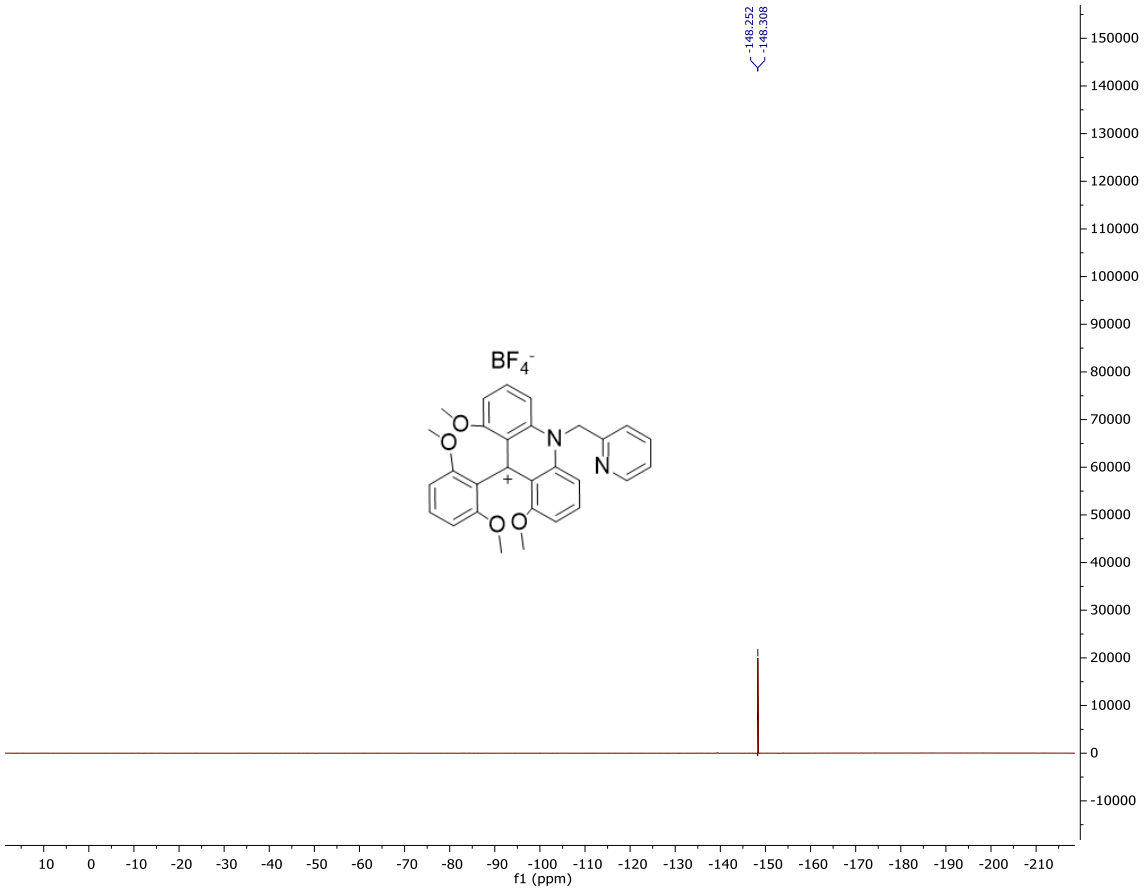
f1 (ppm)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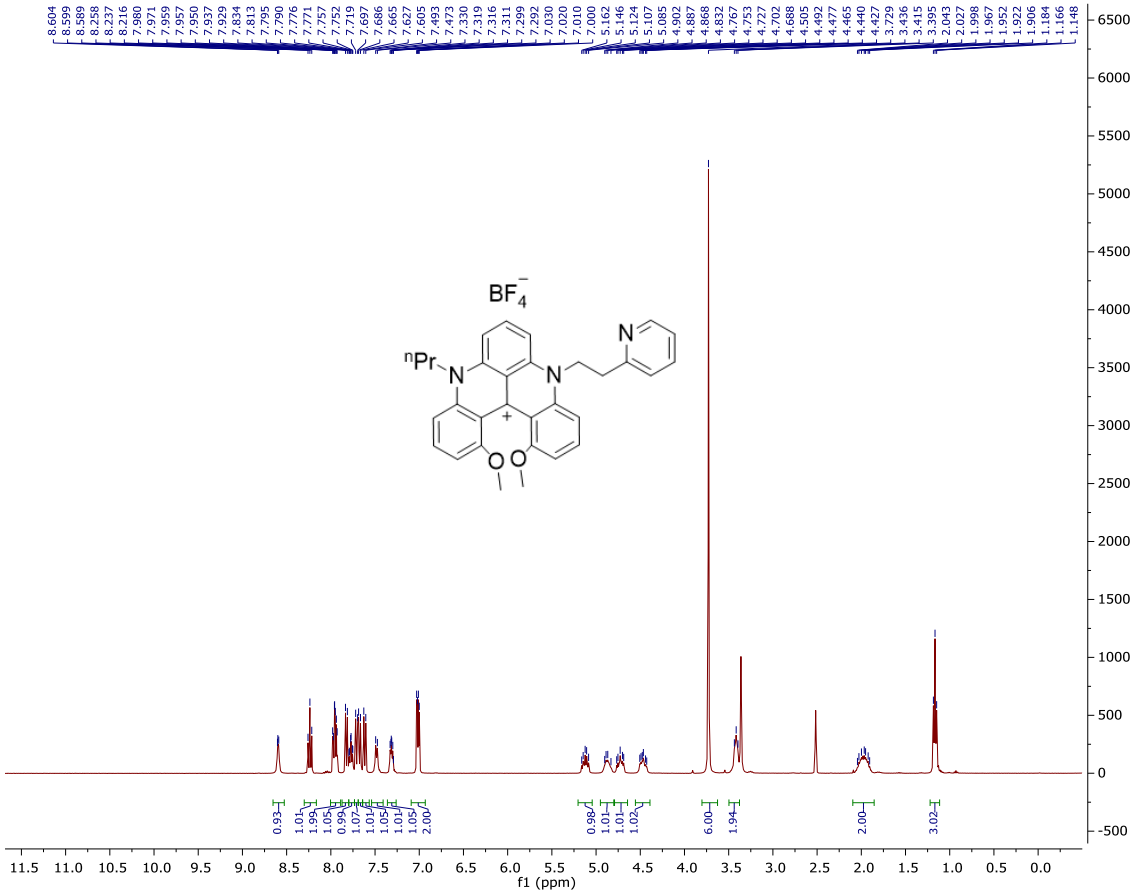
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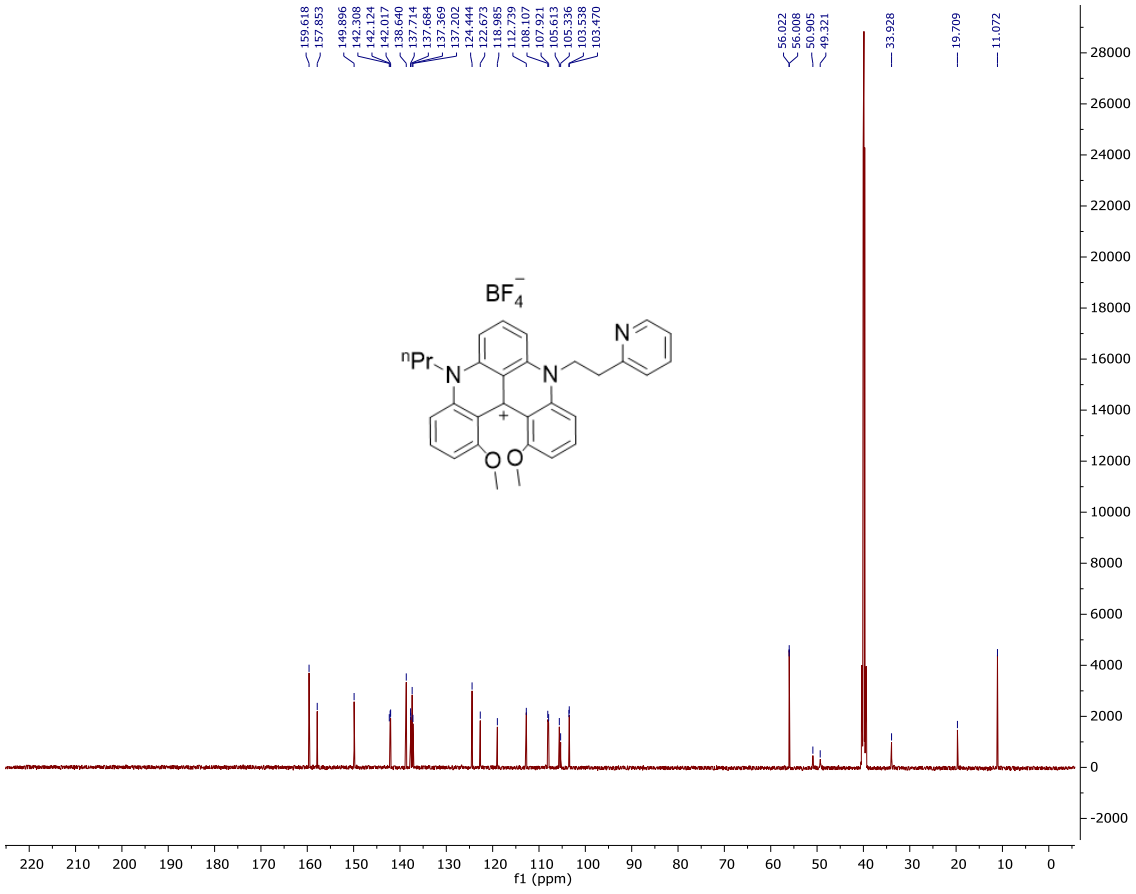
BF4−
nPr
N
N
N
O
O
0.93 1.01 1.99 1.05 0.99 1.07 1.01 1.05 1.01 1.05 2.00 0.98 1.01 1.01 1.02 6.00 1.94 2.00 3.02
f1 (ppm)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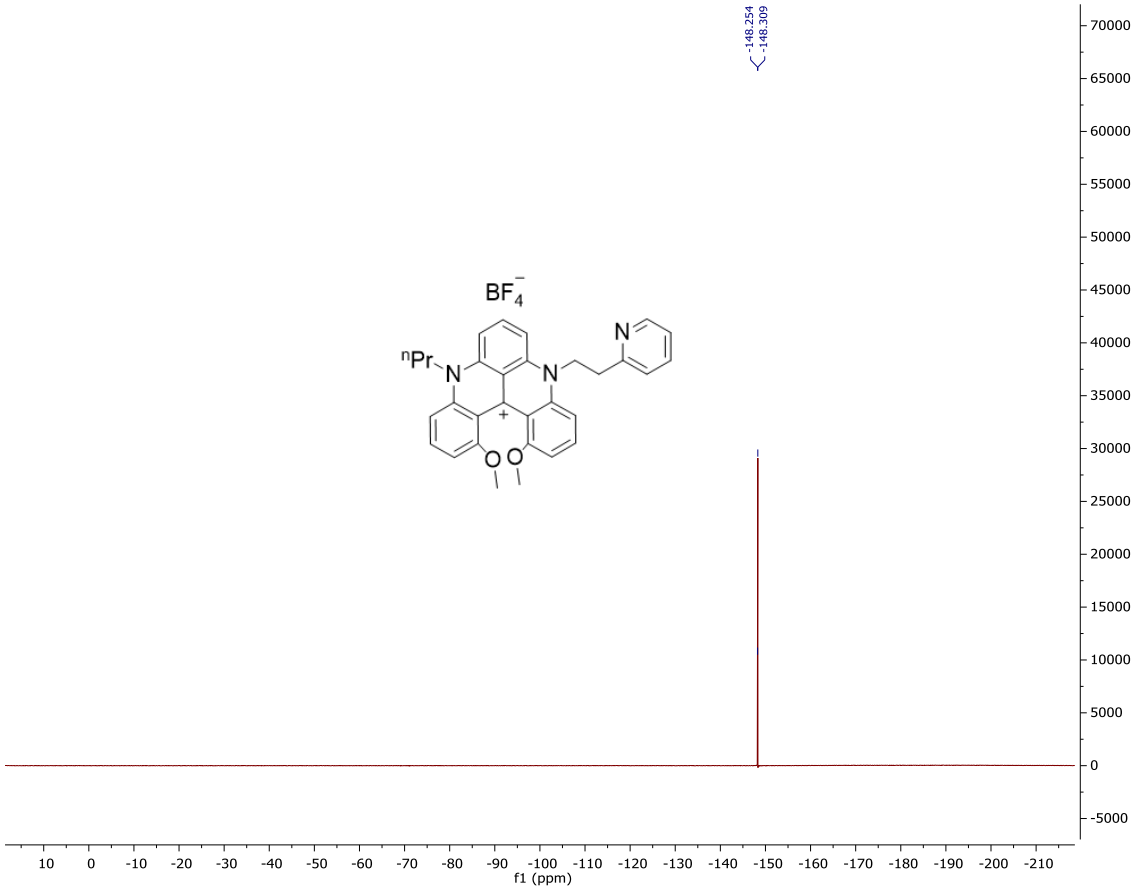
f1 (ppm)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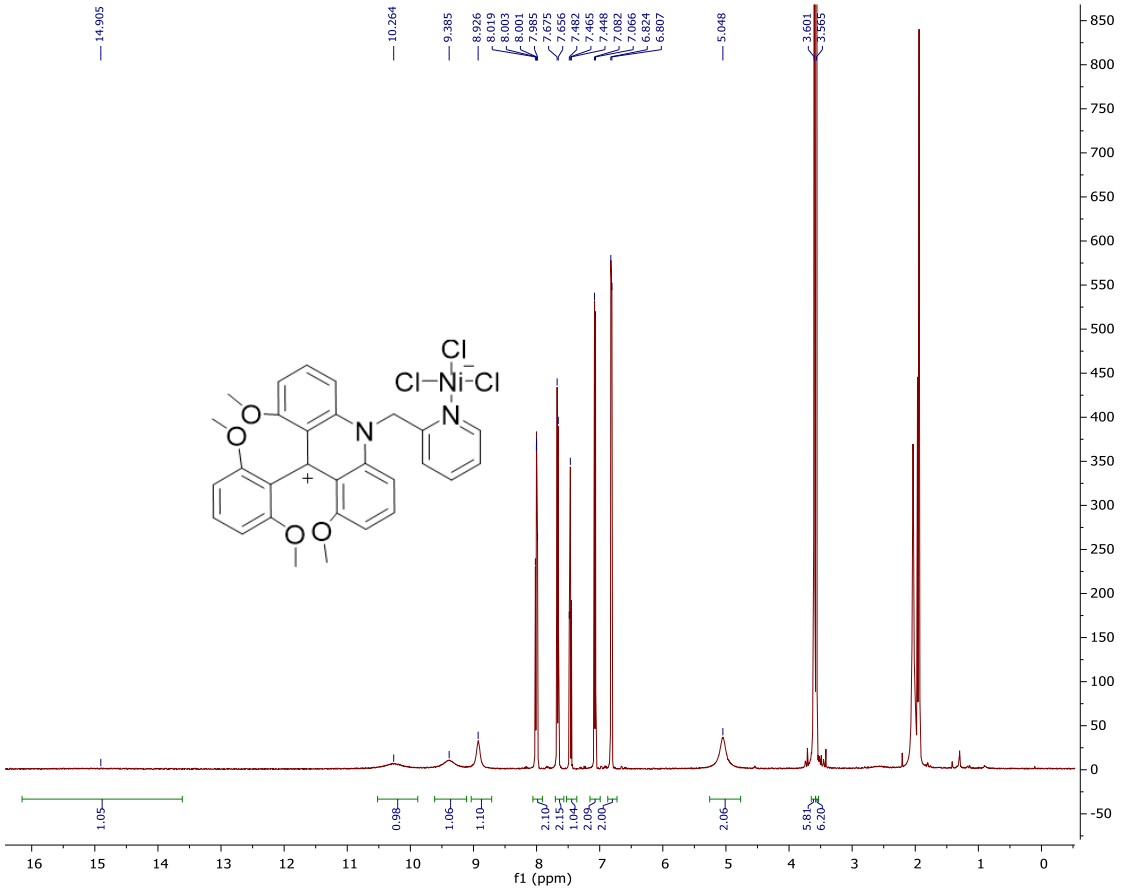
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8.001
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7.656
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7.082
7.066
6.824
6.807
5.048
3.601
3.565
Cl
Cl–Ni–Cl
N
N
O
O
O
O
1.05
0.98
1.06
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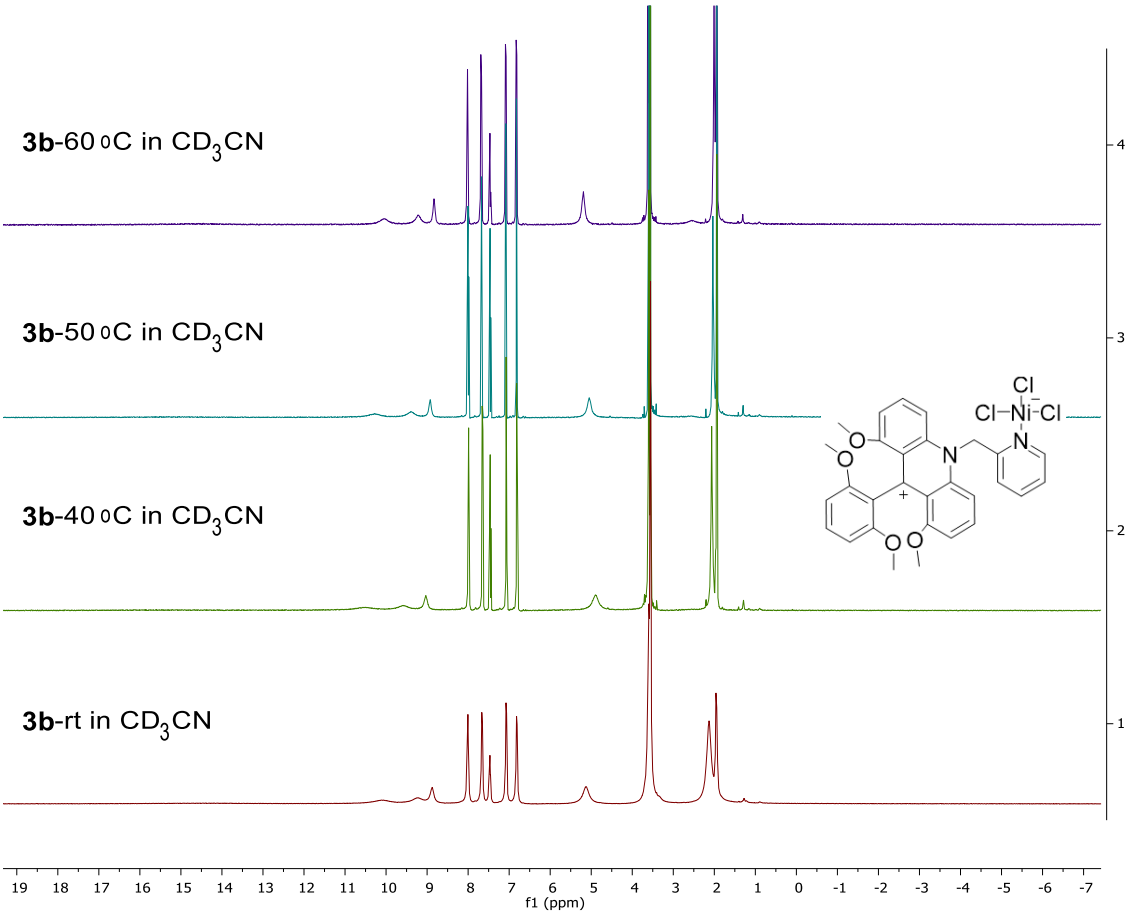
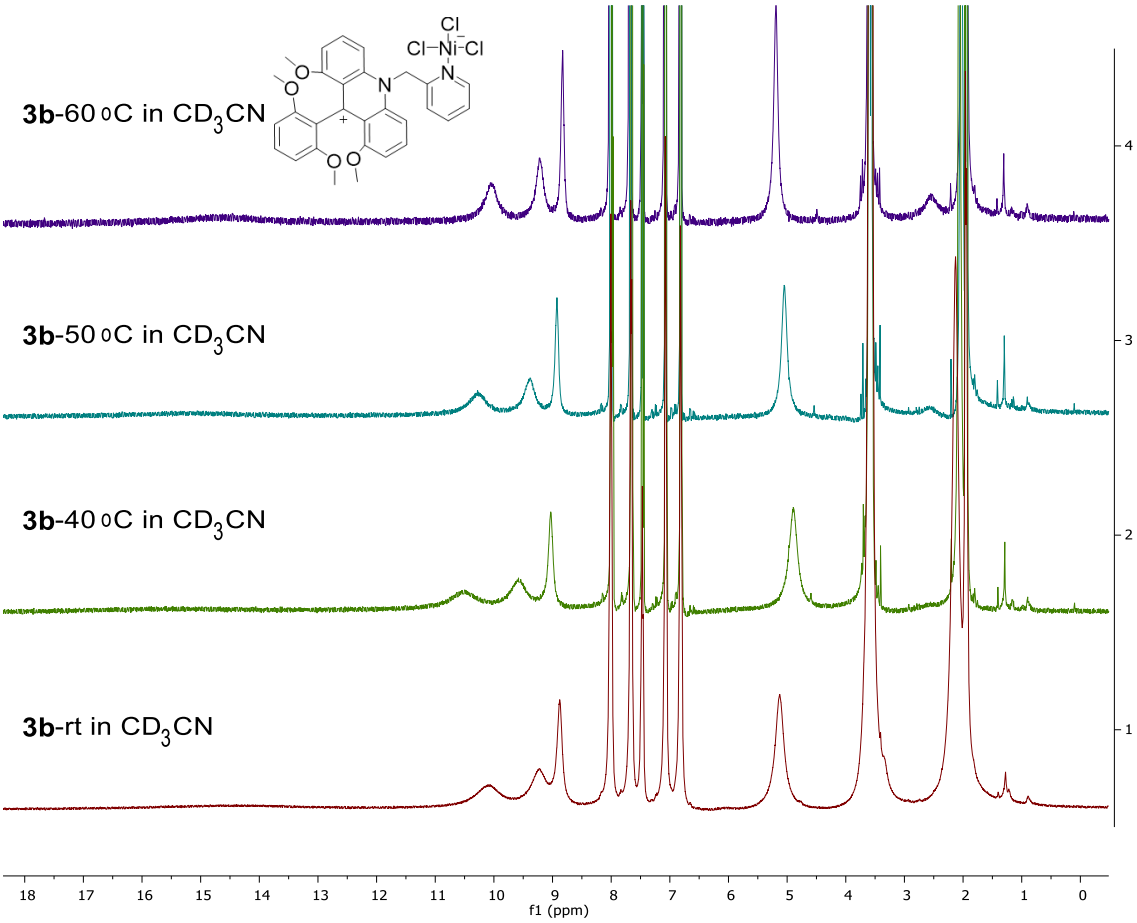
2.15
1.04
2.09
2.00
2.06
5.81
6.20
f1 (ppm)


3b-60 oC in CD3CN
3b-50 oC in CD3CN
3b-40 oC in CD3CN
3b-rt in CD3CN
Cl
Cl–Ni–Cl
N
O
O
O
O
+
4
3
2
1
19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)


3b-60 oC in CD3CN
3b-50 oC in CD3CN
3b-40 oC in CD3CN
3b-rt in CD3CN
Cl
Cl–Ni–Cl
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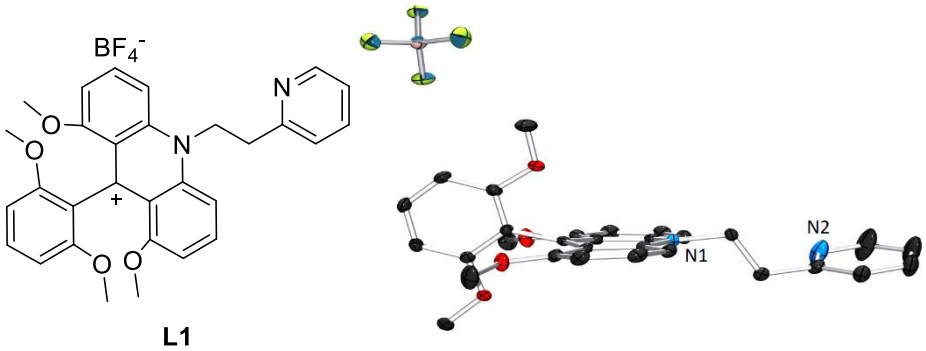
O
O
O
O
+
4
3
2
1
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

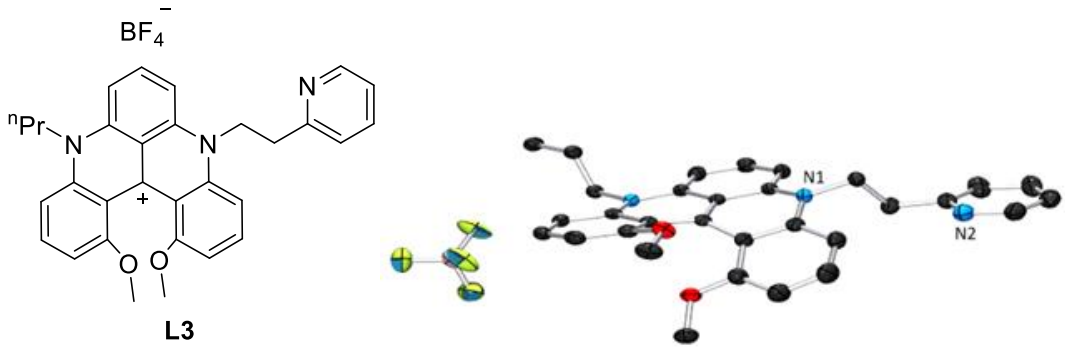
5. X-ray diffraction



L1

Crystal data and structure refinement for L1.

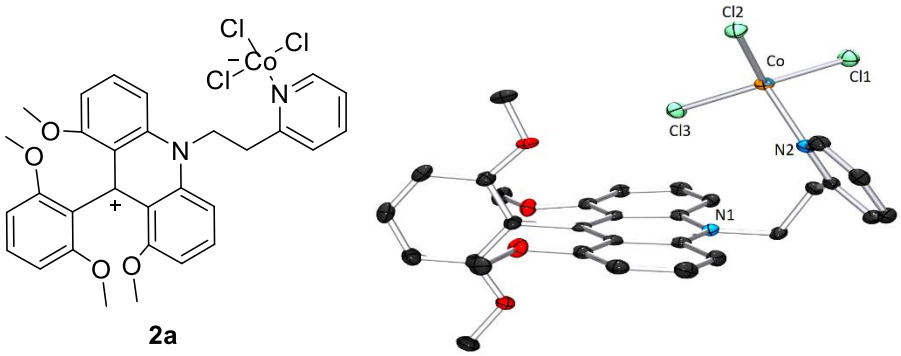
CCDC	1973583
Empirical formula	$C_{30.05}H_{29.1}BCl_{0.1}F_4N_2O_4$ ($C_{30}H_{29}N_2O_4BF_4$,0.05(C H_2 Cl_2))
Formula weight	572.61
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.8254(5)
b/Å	13.2164(4)
c/Å	15.3735(5)
α/°	90
β/°	98.088(3)
γ/°	90
Volume/$Å^3$	2781.15(16)
Z	4
$\rho_{calc}g/cm^3$	1.368
μ/mm^{-1}	0.117
F(000)	1192.0
Crystal size/mm^3	0.2 × 0.18 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.712 to 61.714
Index ranges	$-19 \leq h \leq 19$, $-17 \leq k \leq 18$, $-22 \leq l \leq 21$
Reflections collected	42410
Independent reflections	8104 [R_{int} = 0.0509, R_{sigma} = 0.0499]
Data/restraints/parameters	8104/24/402
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0513, wR_2 = 0.1024
Final R indexes [all data]	R_1 = 0.0850, wR_2 = 0.1179
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.25



L3

Crystal data and structure refinement for L3.

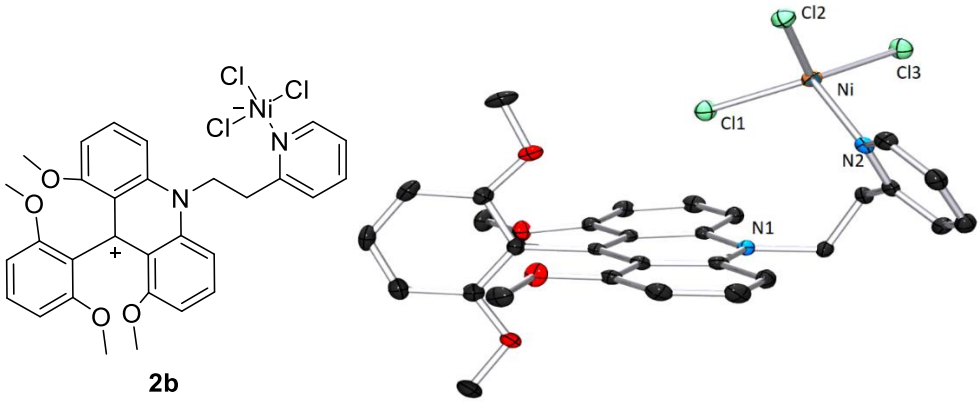
CCDC	1973584
Empirical formula	$C_{32}H_{31}BF_4N_2O_2$
Formula weight	562.40
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.823(3)
b/Å	21.139(5)
c/Å	12.359(3)
α/°	90
β/°	110.983(12)
γ/°	90
Volume/Å^3	2640.0(11)
Z	4
ρ_{calc}g/cm^3	1.415
μ/mm^{-1}	0.107
F(000)	1176.0
Crystal size/mm^3	0.27 × 0.12 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.854 to 51.484
Index ranges	$-13 \le h \le 12$, $-25 \le k \le 25$, $-14 \le l \le 14$
Reflections collected	23832
Independent reflections	4986 [R_{int} = 0.0430, R_{sigma} = 0.0341]
Data/restraints/parameters	4986/0/373
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0546, wR_2 = 0.1458
Final R indexes [all data]	R_1 = 0.0778, wR_2 = 0.1601
Largest diff. peak/hole / e Å^{-3}	0.58/-0.26



2a

Crystal data and structure refinement for 2a.

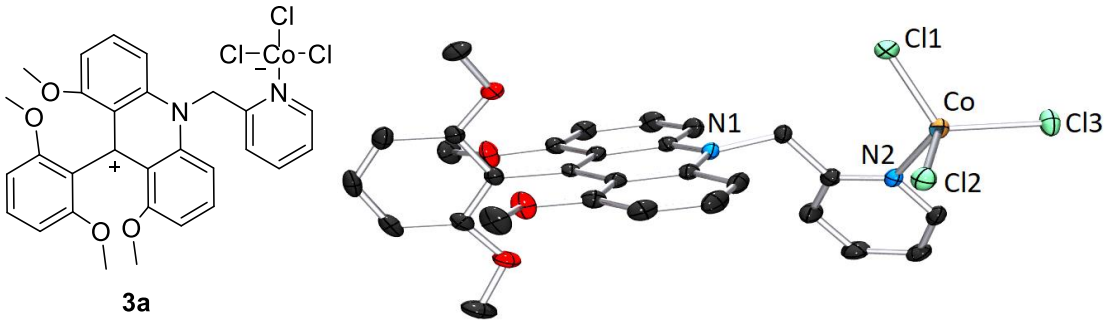
CCDC	1973585
Empirical formula	$C_{30}H_{29}Cl_3CoN_2O_4$
Formula weight	646.83
Temperature/K	100.00(16)
Crystal system	triclinic
Space group	P-1
a/Å	8.7176(3)
b/Å	12.5351(4)
c/Å	13.2082(5)
α/°	84.043(3)
β/°	74.577(3)
γ/°	85.088(3)
Volume/Å^3	1381.31(9)
Z	2
ρ_{calc}g/cm^3	1.555
μ/mm^{-1}	0.952
F(000)	666.0
Crystal size/mm^3	0.18 × 0.1 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.388 to 58.26
Index ranges	-11 ≤ h ≤ 11, -17 ≤ k ≤ 17, -18 ≤ l ≤ 18
Reflections collected	30805
Independent reflections	7414 [R_{int} = 0.0643, R_{sigma} = 0.0646]
Data/restraints/parameters	7414/0/365
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0430, wR_2 = 0.0869
Final R indexes [all data]	R_1 = 0.0673, wR_2 = 0.0990
Largest diff. peak/hole / e Å^{-3}	0.45/-0.47



2b

Crystal data and structure refinement for 2b.

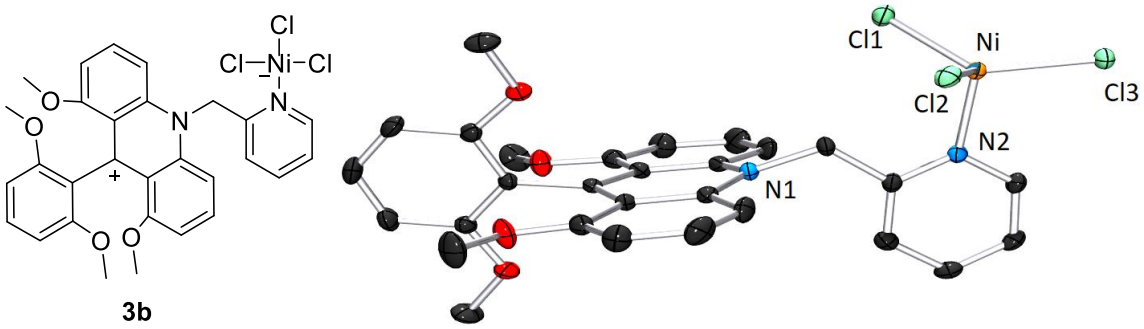
CCDC	1973588
Empirical formula	$C_{30}H_{29}Cl_3N_2NiO_4$
Formula weight	646.61
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.6529(3)
b/Å	12.5362(4)
c/Å	13.2372(5)
α/°	83.920(3)
β/°	74.506(3)
γ/°	84.865(3)
Volume/Å^3	1373.12(9)
Z	2
ρ_{calc}g/cm^3	1.564
μ/mm^{-1}	1.039
F(000)	668.0
Crystal size/mm^3	0.44 × 0.25 × 0.22
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.382 to 61.83
Index ranges	-11 ≤ h ≤ 12, -17 ≤ k ≤ 17, -18 ≤ l ≤ 18
Reflections collected	36350
Independent reflections	7966 [R_{int} = 0.0557, R_{sigma} = 0.0512]
Data/restraints/parameters	7966/0/365
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0414, wR_2 = 0.0956
Final R indexes [all data]	R_1 = 0.0568, wR_2 = 0.1067
Largest diff. peak/hole / e Å^{-3}	0.64/-0.40



3a

Crystal data and structure refinement for 3a.

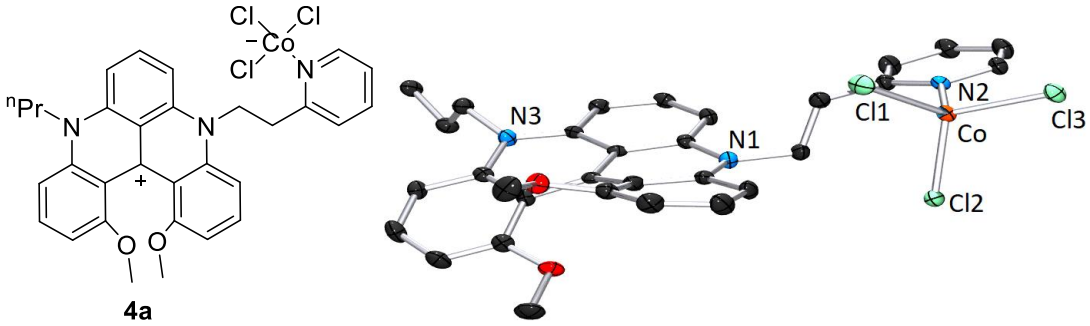
CCDC	1973587
Empirical formula	$C_{31}H_{30}Cl_3CoN_3O_4$
Formula weight	673.86
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.9579(3)
b/Å	12.8642(4)
c/Å	16.4462(5)
α/°	67.782(3)
β/°	76.185(3)
γ/°	78.925(3)
Volume/Å^3	1503.80(9)
Z	2
ρ_{calc}g/cm^3	1.488
μ/mm^{-1}	0.879
F(000)	694.0
Crystal size/mm^3	1 × 0.52 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.442 to 61.904
Index ranges	-10 ≤ h ≤ 11, -18 ≤ k ≤ 17, -23 ≤ l ≤ 23
Reflections collected	40695
Independent reflections	8835 [R_{int} = 0.0596, R_{sigma} = 0.0566]
Data/restraints/parameters	8835/0/384
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0431, wR_2 = 0.0894
Final R indexes [all data]	R_1 = 0.0664, wR_2 = 0.1025
Largest diff. peak/hole / e Å^{-3}	0.46/-0.56



3b

Crystal data and structure refinement for 3b.

CCDC	1973589
Empirical formula	$C_{31}H_{31}Cl_3N_2NiO_{4.5}$
Formula weight	668.64
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.5471(2)
b/Å	13.4245(4)
c/Å	16.5205(5)
α/°	110.441(3)
β/°	98.644(3)
γ/°	101.914(2)
Volume/Å^3	1488.78(8)
Z	2
ρ_{calc}g/cm^3	1.492
μ/mm^{-1}	0.963
F(000)	692.0
Crystal size/mm^3	0.6 × 0.4 × 0.08
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.092 to 61.726
Index ranges	-10 ≤ h ≤ 9, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23
Reflections collected	20068
Independent reflections	8217 [R_{int} = 0.0439, R_{sigma} = 0.0677]
Data/restraints/parameters	8217/36/401
Goodness-of-fit on F^2	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0455, wR_2 = 0.0961
Final R indexes [all data]	R_1 = 0.0623, wR_2 = 0.1071
Largest diff. peak/hole / e Å^{-3}	0.57/-0.49

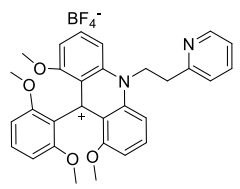


4a

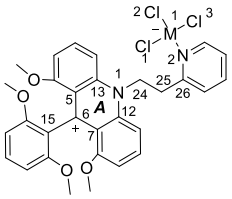
Crystal data and structure refinement for 4a.

CCDC	1973586
Empirical formula	$C_{33}H_{33}Cl_3CoN_4O_2$ ($C_{31}H_{30}Cl_3CoN_3O_2$-MeCN)
Formula weight	682.91
Temperature/K	100.0
Crystal system	monoclinic
Space group	C2/c
a/Å	25.405(6)
b/Å	10.880(2)
c/Å	25.515(8)
α/°	90
β/°	117.562(9)
γ/°	90
Volume/Å^3	6252(3)
Z	8
ρ_{calc}g/cm^3	1.451
μ/mm^{-1}	0.843
F(000)	2824.0
Crystal size/mm^3	0.23 × 0.11 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.602 to 54.312
Index ranges	-30 ≤ h ≤ 32, -13 ≤ k ≤ 13, -32 ≤ l ≤ 31
Reflections collected	31567
Independent reflections	6902 [R_{int} = 0.0695, R_{sigma} = 0.0549]
Data/restraints/parameters	6902/0/392
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0418, wR_2 = 0.0914
Final R indexes [all data]	R_1 = 0.0683, wR_2 = 0.1023
Largest diff. peak/hole / e Å^{-3}	0.52/-0.31

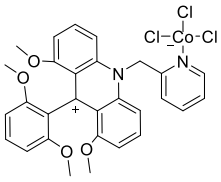
(a)



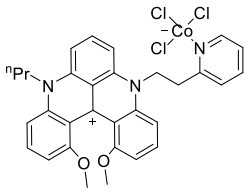
L1



2a: M = Co
2b: M = Ni



3a



4a

(b)

Compound	C6-C7	C6-C5	C6-C15	M1-Cl1	M1-Cl2	M1-Cl3	M1-N2	Cl1-C13	Cl1-N1	Cl1-centroid of ring A
L1	1.4139(19)	1.4122(19)	1.4982(19)	-	-	-	-	-	-	-
2a (Co)	1.411(3)	1.412(3)	1.499(3)	2.2462(7)	2.2656(7)	2.2710(6)	2.0842(18)	3.414	3.556	3.005
2b (Ni)	1.410(3)	1.414(3)	1.496(3)	2.2376(6)	2.2556(6)	2.2620(6)	2.0356(15)	3.439	3.521	3.481
3a (Co)	1.414(3)	1.412(3)	1.490(3)	2.2586(6)	2.2381(6)	2.2606(6)	2.1086(17)	-	-	-
4a (Co)	1.411(4)	1.430(4)	1.435(4)	2.2627(9)	2.2603(8)	2.2770(8)	2.082(2)	-	-	-

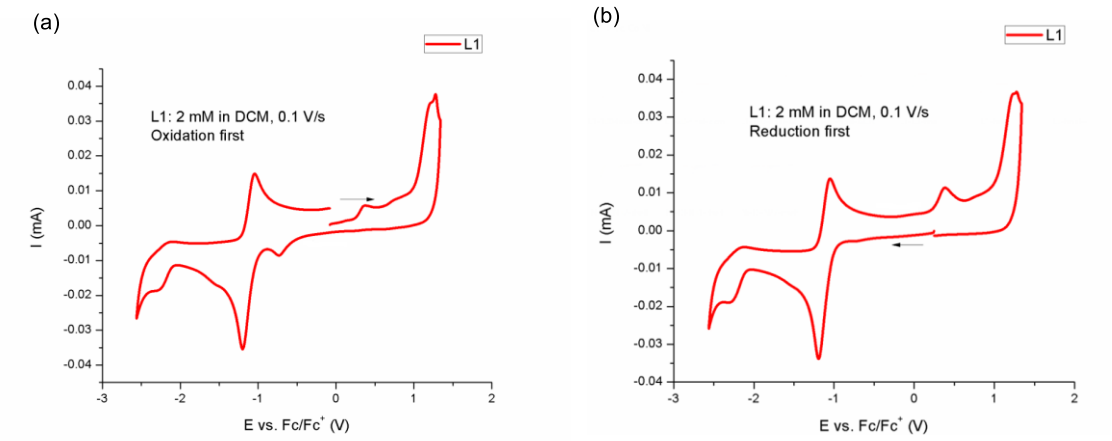
(c)

Compound	Cl3-M1-Cl2	Cl1-M1-Cl3	Cl1-M1-Cl2	N2-Co1-Cl3	N2-Co1-Cl1	N2-Co1-Cl2	N1-C24-C25-C26	N1-C24-C25-C26
L1	-	-	-	-	-	-	155.817	-64.951
2a (Co)	113.38(3)	116.79(3)	109.07(2)	101.52(5)	108.45(5)	106.83(6)	87.230	-116.393
2b (Ni)	113.73(2)	123.61(2)	106.06(2)	99.48(5)	106.18(5	106.05(5)	87.773	-117.503
2a (Co)	113.32(2)	115.39(2)	112.31(2	99.76(5)	112.80(5)	102.01(5)	-142.362 (N1-C24-C25-N2)	
4a (Co)	111.26(3)	112.96(3)	108.56(3)	104.28(6)	113.58(6)	105.98(6)	-162.739	-102.826

Figure S1. (a) Structures, (b) bond lengths (Å) and (c) bond/torsion angles (°) of ligand **L1** and complexes **2**, **3a** and **4a**.

6. CV curves of L1

I. Oxidation & Reduction -influence of scan direction



Initial anodic scan

Small signal at +0.42 V: product from C^- (Might be due to small amount in the analyte solution)

Large signal at -0.72 V: product from $C^{\bullet+}$

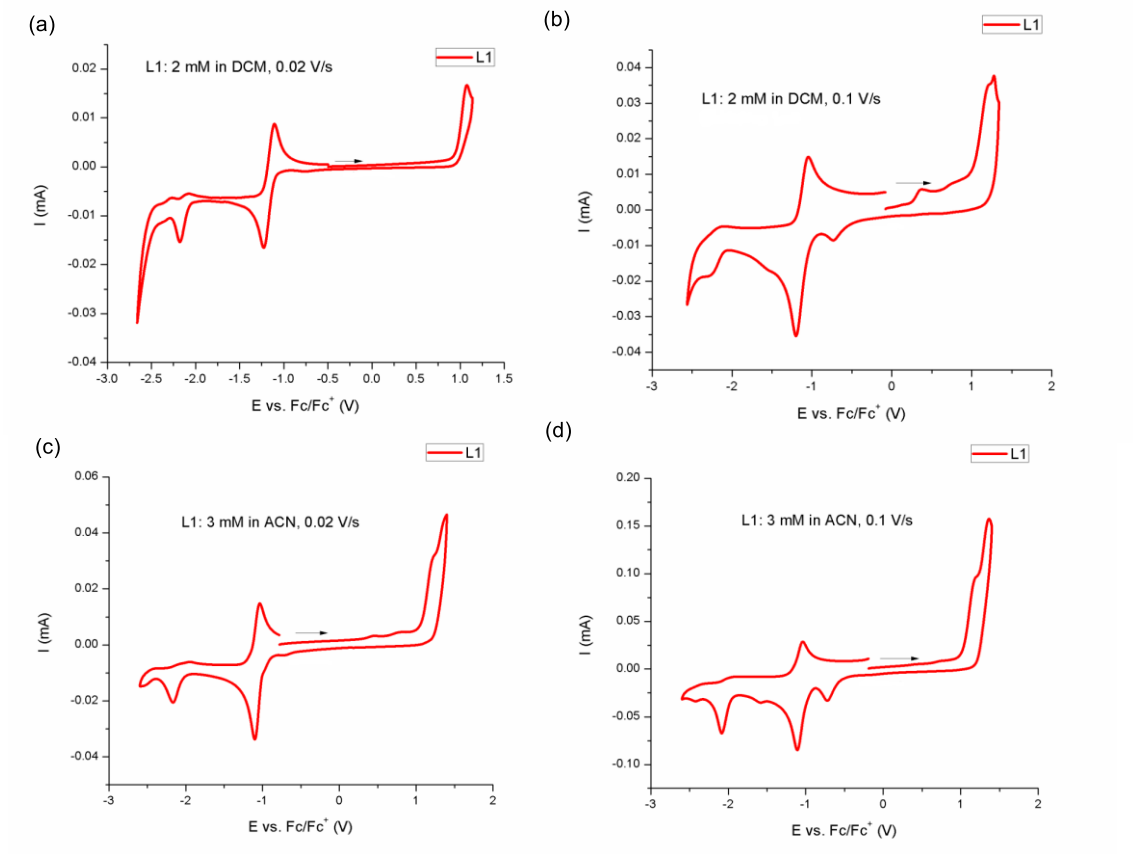
Initial cathodic scan

Large signal at +0.42 V: product from C^-

Trace signal at -0.72 V: product from $C^{\bullet+}$ (Might be due to trace amount from the analyte solution)

Figure S2 CV curves of **L1** (2 mM) in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode (ν = 0.1 V/s): (a) Oxidation first (initial anodic scan), (b) reduction first (initial cathodic scan).

II. DCM & MeCN -influence of scan rate and solvent



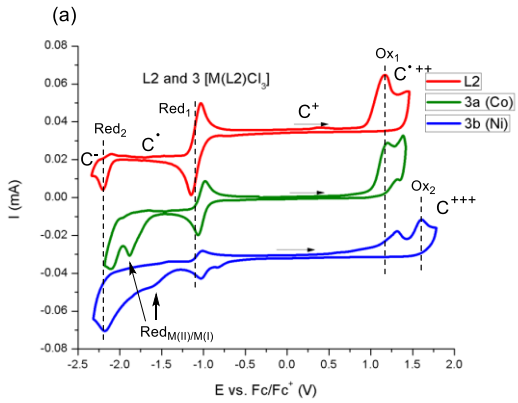
1. DCM and MeCN gave the same reduction and oxidation events for **L1**, though the potentials shifted a little bit.

2. Lower scan rate (0.02 V/s) gave cleaner CV curves in both solvents, presumably because the products generated from C^- and $C^{\cdot+}$ have enough time to diffuse away from the electrodes with lower scan rate.

Figure S3 CV curves of **L1** (2 mM) in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode with (a) ν = 0.02 V/s; (b) ν = 0.1 V/s; and CV curves of **L1** (3 mM) in MeCN ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode with (c) ν = 0.02 V/s; (d) ν = 0.1 V/s.

7. Selected CV curves of L2 and complex 3

(a)



(b)

Compound	Red_1	Reduction ΔE (Red **L2**)[a]	Red_2	$Red_{M(II)/M(I)}$	Ox_1	Ox_2
L2	-1.07	0	-2.19[b]	-	1.19[b]	-
3a	-1.02	0.05	-2.11[b]	-1.88[b]	1.20[b]	-
3b	-1.02	0.05	-2.18[b]	-1.62[b]	1.32[b]	1.61[b]

a Half-wave potential difference compared to the first reduction waves of ligand **L2**.
b The potential values for the irreversible processes are peak positions.

Figure S4 (a) Selected CV curves of **L2** (3 mM) and complexes **3a** (2 mM) and **3b** (1 mM) in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode (ν = 0.02 V/s). (b) Oxidation and reduction half-wave potential values [V] measured by CV for **L2** and **3**, E vs. the ferrocene/ferrocenium redox couple (Fc/Fc^+).

8. Individual CV curves of L and 2-4

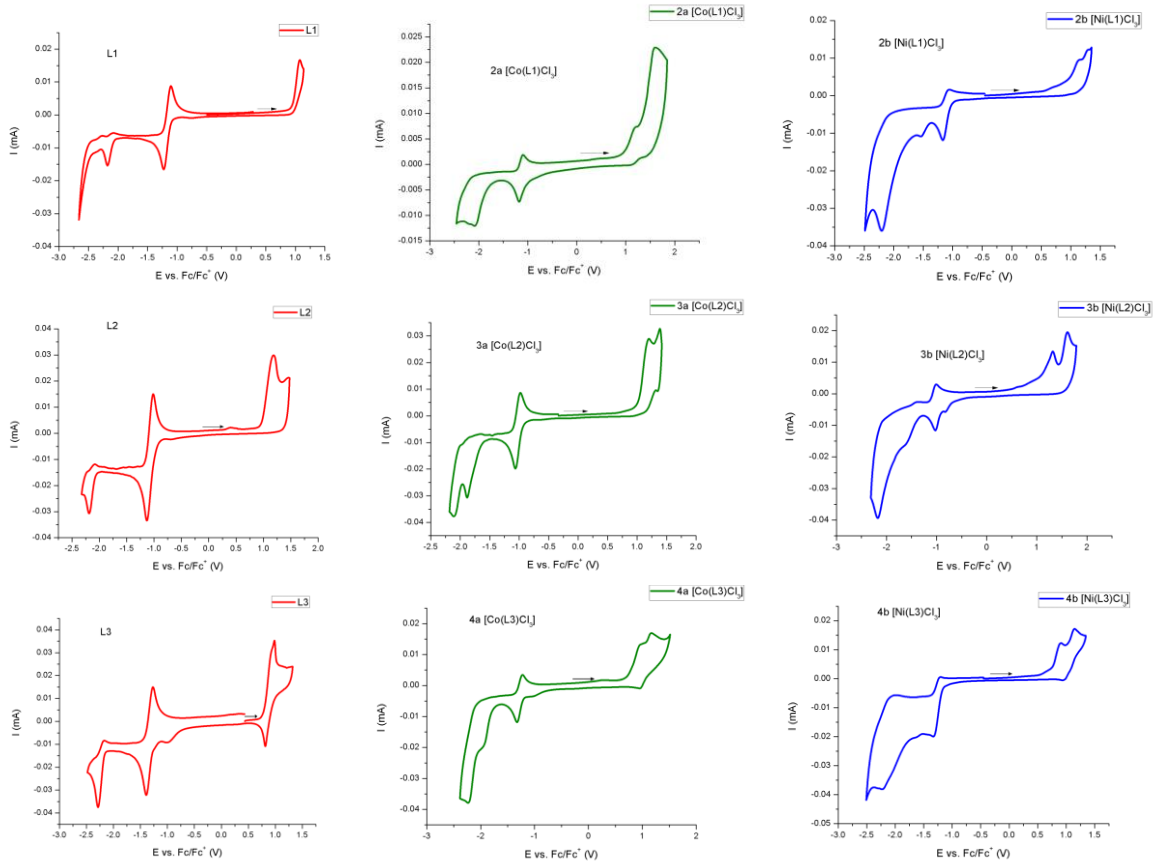


Figure S5 Individual CV curve of ligand **L1** (2 mM), **L2-L3** (3 mM) and complexes **2-4** (1 mM) [2 mM for **3a**] in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode (ν = 0.02 V/s).

9. Reversibility plots of the square root of the scan rate and current of L and 2-4.

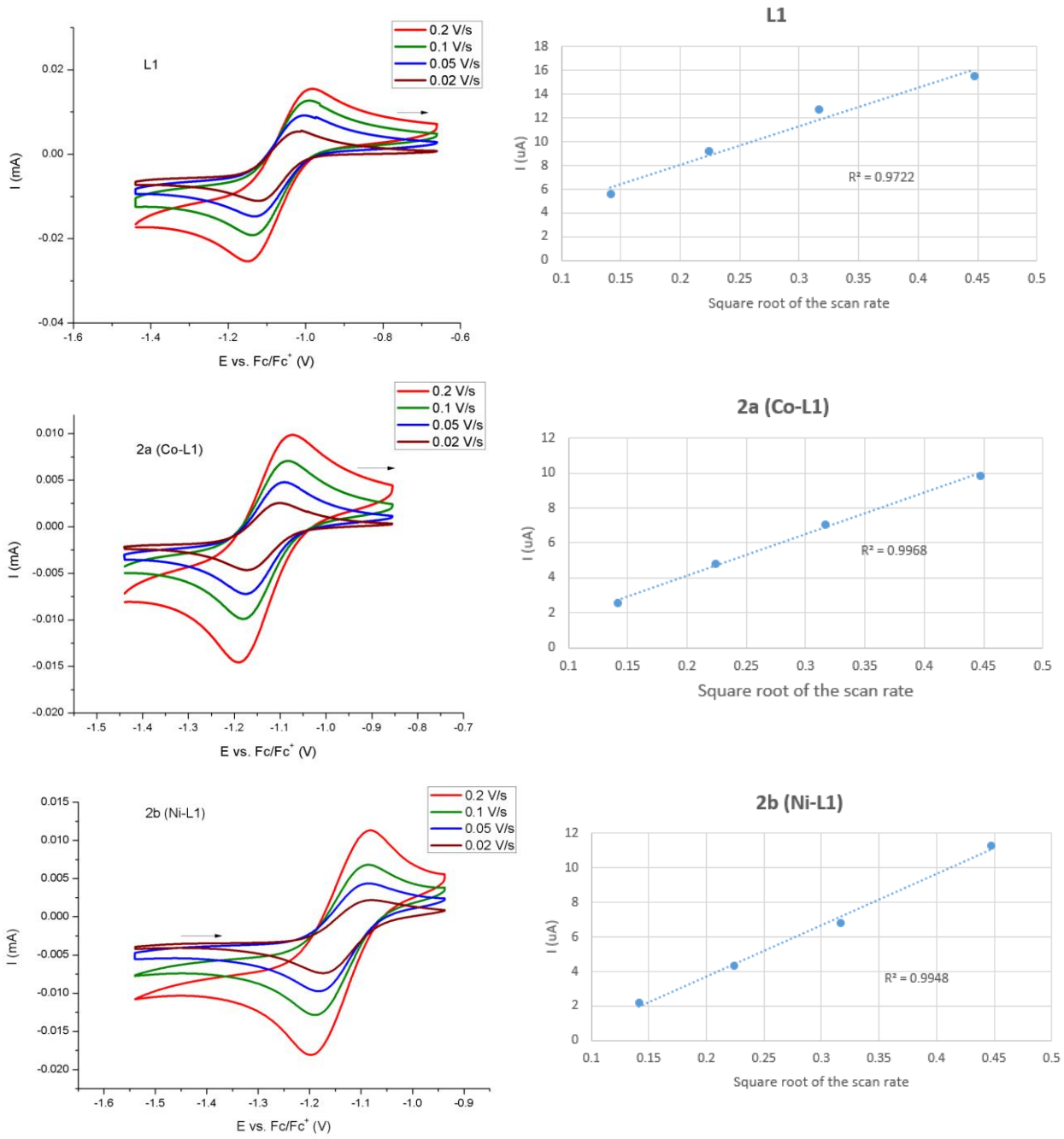


Figure S6 CV curves of ligand **L1** (2 mM) and complexes **2** (1 mM) in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode with different scan rate and the corresponding reversibility plots of square root of the scan rate and current. E vs the Fc/Fc^+ redox couple.

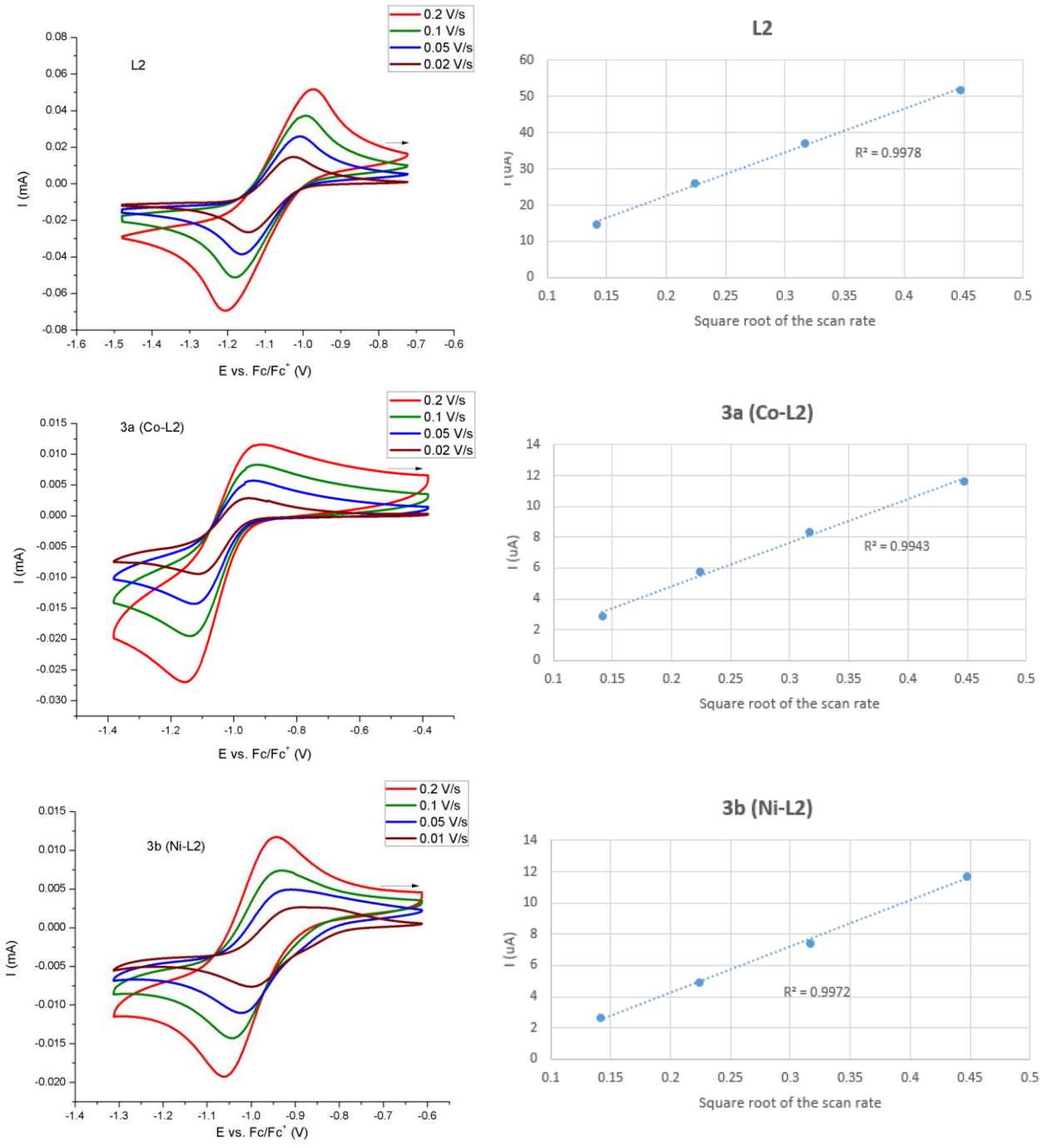


Figure S7 CV curves of ligand **L2** (3 mM), complex **3a** (2 mM) and **3b** (1 mM) in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode with different scan rate and the corresponding reversibility plots of square root of the scan rate and current. E vs the Fc/Fc^+ redox couple.

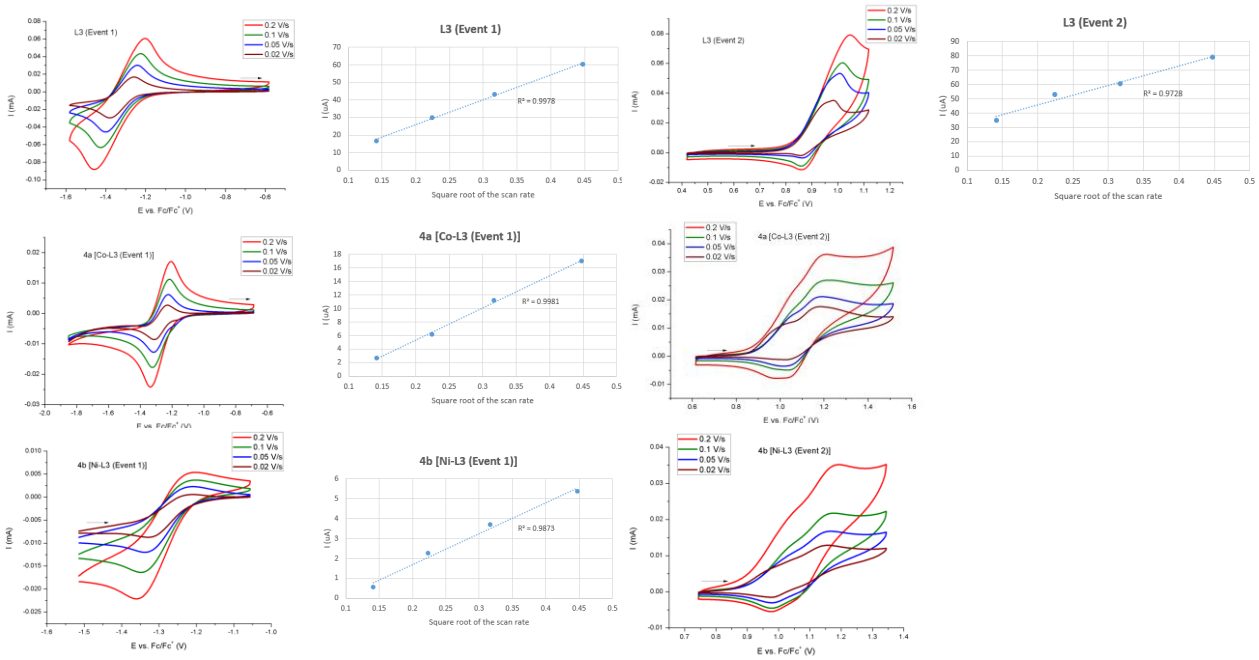
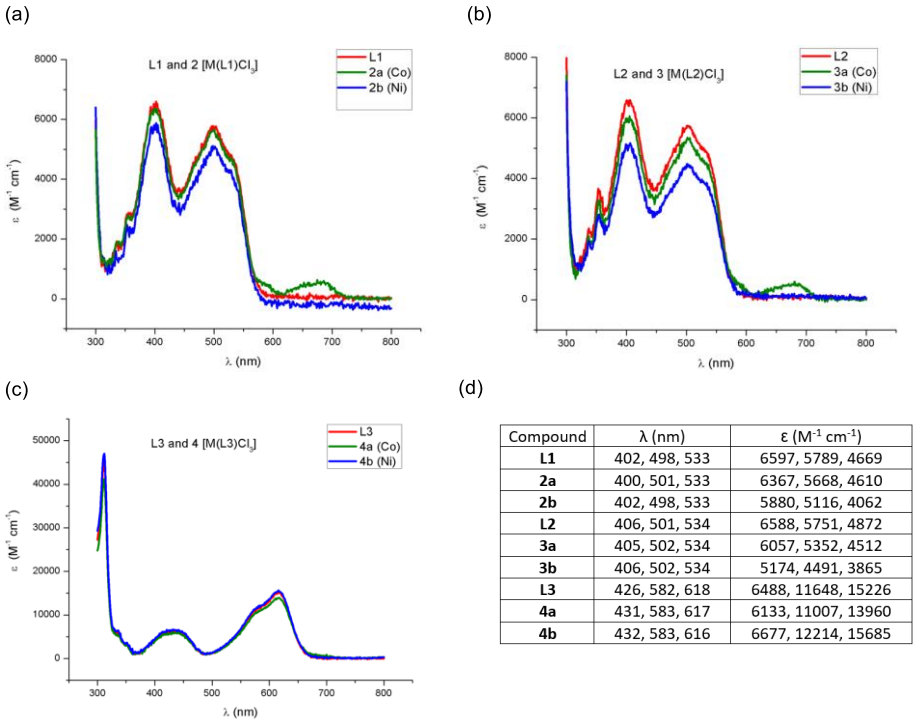


Figure S8 CV curves of ligand **L3** (3 mM) and complex **4** (1 mM) in DCM ([TBA][PF_6] 0.1 M) solutions recorded at a glassy carbon working electrode with different scan rates and the corresponding reversibility plots of square root of the scan rate and current. E vs the Fc/Fc^+ redox couple.

10. Absorption spectra and photophysical properties of L and 2-4



(d)

Compound	λ (nm)	ε (M^{-1} cm^{-1})
L1	402, 498, 533	6597, 5789, 4669
2a	400, 501, 533	6367, 5668, 4610
2b	402, 498, 533	5880, 5116, 4062
L2	406, 501, 534	6588, 5751, 4872
3a	405, 502, 534	6057, 5352, 4512
3b	406, 502, 534	5174, 4491, 3865
L3	426, 582, 618	6488, 11648, 15226
4a	431, 583, 617	6133, 11007, 13960
4b	432, 583, 616	6677, 12214, 15685

Figure S9. (a-c) Overlapped absorption spectra in MeCN (a) ligand **L1** and complex **2**, (b) **L2** and **3**, (c) **L3** and **4**, (d) photophysical properties of ligands **L1-L3** and complexes **2-4** in MeCN.

11. DFT calculations

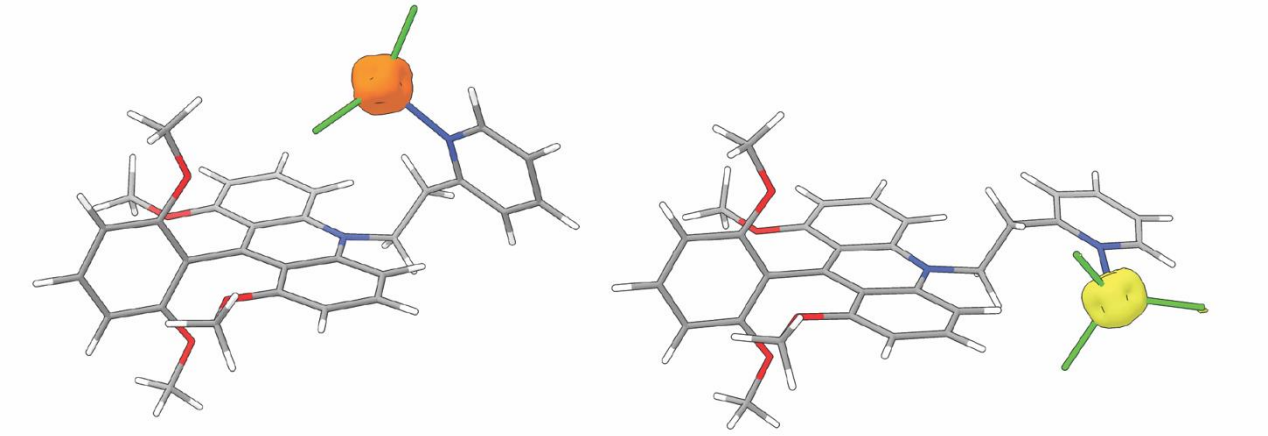
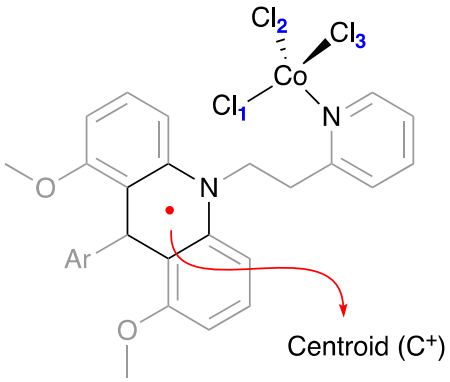


Figure S10. Spin density population plots of cobalt complexes **2a** in-plane (left) and out-of-plane (right). Self consistent field (SCF) surfaces were plotted at a 0.04 isovalue.

Table S1. Selected structural features from the DFT geometry optimized structure of complex **2a**. The presented bond lengths correspond to models from applied Grimme D3 empirical dispersion. A labeled illustration of the molecule is also presented.



	Bond Distances (Å)				
2a Complexes	Co–N	C^+–Cl**1**	Co–Cl**1**	Co–Cl**2**	Co–Cl**3**
Experimental (Crystal structure)	2.085(2)	3.506	2.2462(7)	2.2656(7)	2.2711(2)
In-plane complex (Gas)	2.178	3.726	2.297	2.277	2.322
In-plane complex (MeCN)	2.130	3.427	2.313	2.333	2.352
Out-of-plane complex (Gas)	2.182	5.522	2.313	2.279	2.322
Out-of-plane complex (MeCN)	2.122	5.730	2.333	2.334	2.338

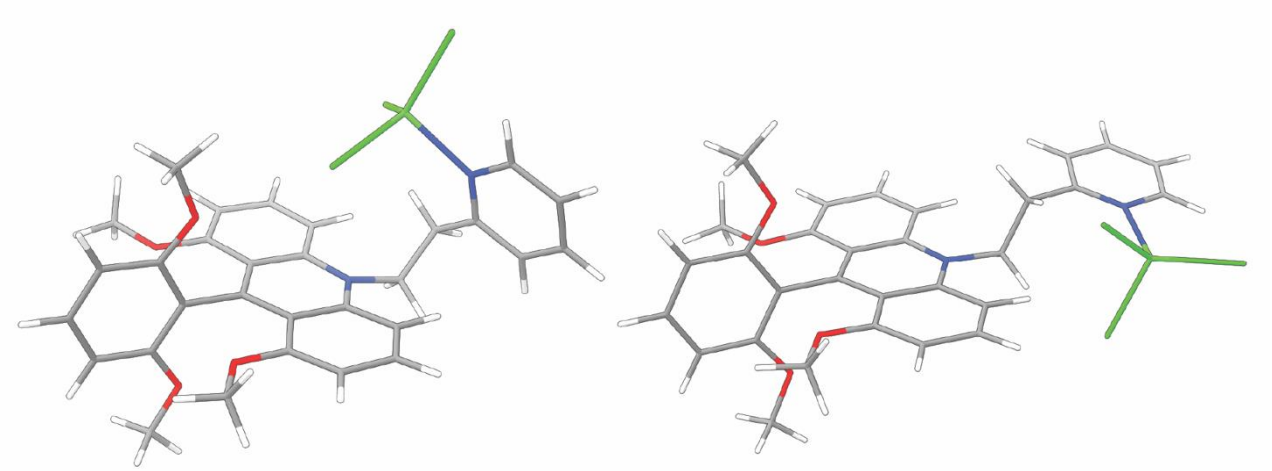


Figure S11. DFT geometry optimized structures for nickel complexes of **2b** in plane (left) and out of plane (right) of the carbocation moiety.

Table S2. Obtained energy values for the cobalt complexes of **2a**. [a]Overall energy difference was calculated by subtracting obtained energy values from our calculations using Grimme's D3 dispersion forces (GD3) and subtracting energy values from calculations where this keyword was omitted (ND).

Cobalt complexes		GD3		ND		ΔE^a
(**2a**)		Energy (Kcal mol^{-1})	$\Delta E_{(In-Out)}$	Energy (Kcal mol^{-1})	$\Delta E_{(In-Out)}$	(GD3–ND)
Gas	In	-1943327.60	-4.82	-1943255.96	4.71	-71.64
	Out	-1943322.79		-1943260.67		-62.12
Solution	In	-1943363.10	1.02	-1943294.56	8.58	-68.54
	Out	-1943364.12		-1943303.14		-60.98

Table S3. Obtained energy values for the nickel complexes of **2b**. [a]Overall energy difference was calculated by subtracting obtained energy values from our calculations using Grimme's D3 dispersion forces (GD3) and subtracting energy values from calculations where this keyword was omitted (ND).

Nickel complexes		GD3		ND		ΔE^a
(**2b**)		Energy (Kcal mol^{-1})	$\Delta E_{(In-Out)}$	Energy (Kcal mol^{-1})	$\Delta E_{(In-Out)}$	(GD3–ND)
Gas	In	-1958519.32	-5.58	-1958445.98	4.97	-73.35
	Out	-1958513.74		-1958450.95		-62.79
Solution	In	-1958553.32	2.31	-1958489.59	2.63	-63.73
	Out	-1958555.63		-1958492.22		-63.40

Table S4. Calculated energy for Cobalt complexes (**2a**) using different levels of theory. Energy difference was calculated by subtracting the energy from the *in*- from the *out*-of-plane models.

Functional	$Energy_{(solution)}$ (Kcal mol^{-1})			$Energy_{(gas)}$ (Kcal mol^{-1})		
	In	Out	$\Delta E_{(In-Out)}$	In	Out	$\Delta E_{(In-Out)}$
B97D	-1942845.36	-1942851.27	5.91	-1942814.38	-1942693.53	-120.85
PBE0	-1941874.81	-1941876.02	1.21	-1941837.07	-1941834.19	-2.88
B3LYP	-1943363.10	-1943364.12	1.02	-1943327.60	-1943322.79	-4.82

M06L	-1942845.36	-1943190.46	345.10	-1943180.30	-1943152.06	-28.24

Table S5. XYZ coordinates of the DFT geometry optimized models of cobalt **2a** in-plane of the carbocation moiety.

	Grimme Dispersion Forces						No Dispersion Forces					
	Solvated			Gas-Phase			Solvated			Gas-Phase		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
Co	-3.11023	-1.06146	0.98584	-2.21837	-0.58535	1.57338	-3.55914	-1.05487	0.93437	-3.24077	-1.12219	1.05317
Cl	-3.11788	-3.07924	-0.18549	-1.16262	-2.55030	1.02518	-3.74401	-2.99262	-0.38069	-3.20955	-2.95399	-0.36151
Cl	-1.04049	-0.52187	1.86607	-0.86975	1.23304	2.08840	-1.43970	-0.74522	1.86556	-1.15996	-0.31821	1.62679
Cl	-4.62623	-1.24078	2.77452	-3.96970	-0.80752	3.01183	-5.15576	-1.16908	2.66735	-4.75745	-1.19052	2.76467
O	3.45401	-2.19391	-0.79087	3.68872	-1.89682	-0.62089	3.34983	-2.40021	-0.46809	3.39037	-2.31089	-0.55316
O	2.29550	2.22144	1.49903	1.61065	2.69642	0.32656	2.88415	2.44875	1.18243	2.73490	2.53315	1.02974
O	3.76234	1.63963	-1.61252	3.71013	1.60634	-1.63740	4.31056	0.85371	-1.72882	4.32481	0.94578	-1.67522
O	2.58856	-1.19540	1.89483	1.79960	-0.93669	1.75254	2.41061	-0.67527	2.25033	2.16919	-0.66504	2.10979
N	-3.79933	0.64820	-0.08059	-3.36682	0.26838	-0.06909	-4.05894	0.71915	-0.16977	-4.01805	0.60104	-0.11211
N	-0.57077	0.23586	-1.79954	-0.67910	-0.70159	-2.18092	-0.35132	0.41897	-1.76699	-0.46965	0.30386	-1.80288
C	-1.67340	0.35517	-2.78943	-1.94430	-1.13195	-2.81664	-1.48406	0.60411	-2.71596	-1.61421	0.41490	-2.74877
H	-1.37438	-0.23444	-3.65686	-1.72104	-2.00049	-3.43395	-1.19261	0.09245	-3.63347	-1.33467	-0.19236	-3.61780
H	-1.70429	1.38905	-3.13347	-2.26506	-0.36262	-3.51831	-1.52745	1.65904	-2.97946	-1.63976	1.45088	-3.10349
C	-3.78831	0.85825	-1.41677	-3.75206	-0.23635	-1.25670	-3.71613	1.03165	-1.44169	-3.81433	0.90225	-1.41283
C	1.25743	2.36223	0.66341	0.64619	2.37475	-0.53779	1.72602	2.53376	0.51515	1.58100	2.57215	0.34164
C	3.24624	0.22158	0.17014	2.78081	0.40006	0.12574	3.42592	0.08486	0.29217	3.31628	0.13727	0.27016
C	-4.94892	2.74386	0.23543	-4.86761	2.12569	-0.37551	-5.28884	2.78827	0.00535	-5.34415	2.59907	0.13638
H	-5.38170	3.45862	0.92842	-5.27252	3.05436	0.01628	-5.89954	3.44477	0.61739	-5.94406	3.23193	0.79187
C	1.43043	-0.98351	-1.13006	1.47453	-1.27985	-1.22442	1.54724	-0.94338	-1.06055	1.47987	-0.96808	-1.07644
C	-4.36651	1.57828	0.71839	-3.91327	1.42424	0.35557	-4.82549	1.58759	0.52874	-4.76845	1.43351	0.63868
H	-4.36073	1.35435	1.78080	-3.55956	1.78259	1.31808	-5.07899	1.28215	1.53967	-4.91774	1.11222	1.67338
C	0.99062	1.25235	-0.23864	0.63019	1.01096	-1.04582	1.31464	1.36744	-0.26063	1.20217	1.36846	-0.38788
C	4.20104	1.01351	-0.48096	3.81661	1.22175	-0.32942	4.55880	0.44725	-0.44864	4.48968	0.52914	-0.38148
C	0.37274	-3.25450	-2.44499	0.92552	-3.99004	-1.77586	0.42209	-3.08852	-2.53693	0.30615	-3.24879	-2.28566
H	-0.04679	-4.14047	-2.91485	0.69327	-5.04013	-1.93603	-0.01372	-3.91593	-3.09115	-0.16956	-4.13878	-2.70038
C	5.50224	1.12204	0.03253	4.84290	1.61551	0.53597	5.83591	0.37735	0.12680	5.72177	0.48197	0.28964
H	6.25237	1.72582	-0.46570	5.65160	2.25332	0.19615	6.71950	0.65425	-0.43754	6.64367	0.78281	-0.20511
C	1.66783	-3.31431	-1.91100	2.18946	-3.63739	-1.27866	1.63542	-3.28257	-1.86528	1.57869	-3.35676	-1.70554
H	2.23787	-4.23116	-1.99774	2.93365	-4.40532	-1.10196	2.11996	-4.24954	-1.91489	2.08414	-4.31915	-1.70570
C	2.20920	-2.20362	-1.28310	2.47633	-2.30927	-1.02584	2.20011	-2.24712	-1.13704	2.16898	-2.25223	-1.11452
C	-0.21545	1.31635	-1.02270	-0.49758	0.63185	-1.85784	0.06523	1.47057	-0.97816	-0.05282	1.40830	-1.09653
C	1.86541	0.14752	-0.39330	1.62727	0.04776	-0.74988	2.07174	0.16776	-0.34482	1.98671	0.18443	-0.42096
C	-4.39780	1.99071	-1.97319	-4.73557	0.39667	-2.03028	-4.17702	2.21301	-2.03861	-4.38501	2.04788	-1.98927
H	-4.39500	2.11787	-3.05244	-5.04273	-0.05162	-2.97275	-3.91960	2.42207	-3.07371	-4.23568	2.24736	-3.05326
C	0.44277	3.48210	0.66923	-0.30694	3.29431	-0.94575	0.93728	3.67233	0.55872	0.77627	3.69950	0.32500
H	0.64443	4.31174	1.33545	-0.28411	4.30765	-0.56405	1.24332	4.53388	1.13874	1.06194	4.59096	0.87753

C	-0.37977	-2.09907	-2.40074	-0.02809	-3.04316	-2.07405	-0.24053	-1.87948	-2.50528	-0.37073	-2.05088	-2.32615
H	-1.37522	-2.11355	-2.81769	-0.99704	-3.38232	-2.40820	-1.18531	-1.80013	-3.02145	-1.37466	-2.03973	-2.73154
C	-3.06851	-0.11735	-2.31466	-3.05689	-1.46711	-1.79150	-2.86426	0.07159	-2.24702	-3.00410	-0.05332	-2.26212
H	-3.66268	-0.25396	-3.22668	-3.79331	-2.09455	-2.31074	-3.42042	-0.16795	-3.16340	-3.57988	-0.23467	-3.18682
H	-2.99535	-1.09432	-1.83138	-2.63067	-2.05258	-0.96901	-2.75022	-0.87164	-1.70981	-2.93857	-1.02330	-1.74583
C	0.13851	-0.94968	-1.76720	0.23888	-1.67374	-1.83852	0.30209	-0.79713	-1.77652	0.19836	-0.90210	-1.73426
C	3.59126	-0.45917	1.34753	2.78467	-0.06727	1.45100	3.57246	-0.34877	1.61918	3.36978	-0.30841	1.60225
C	-4.97847	2.94787	-1.14527	-5.29962	1.59128	-1.58987	-4.96378	3.10446	-1.31416	-5.15244	2.91113	-1.20920
H	-5.44408	3.83414	-1.56867	-6.06303	2.09298	-2.18106	-5.32016	4.02303	-1.77324	-5.60423	3.80336	-1.64927
C	5.82265	0.43767	1.20481	4.80328	1.18505	1.86637	5.95846	-0.05765	1.44673	5.75417	0.04080	1.61508
H	6.82911	0.52077	1.60928	5.58946	1.50278	2.54864	6.94697	-0.11396	1.89755	6.71193	0.00451	2.13956
C	-0.67326	3.53402	-0.17943	-1.31404	2.90713	-1.83419	-0.27722	3.71069	-0.13840	-0.43256	3.68738	-0.38667
H	-1.30836	4.41629	-0.16530	-2.05030	3.63941	-2.15765	-0.89412	4.60373	-0.07819	-1.06937	4.57405	-0.36830
C	-1.01059	2.48290	-1.00516	-1.42545	1.60763	-2.28300	-0.71471	2.64422	-0.89439	-0.84792	2.57828	-1.08697
H	-1.90975	2.56281	-1.59437	-2.26738	1.35790	-2.90903	-1.67435	2.72008	-1.38171	-1.81798	2.59954	-1.56832
C	4.88379	-0.35453	1.87270	3.78848	0.35262	2.33723	4.84213	-0.42266	2.20416	4.59368	-0.35610	2.28481
H	5.16265	-0.87448	2.78244	3.77838	0.02610	3.37160	4.96729	-0.75716	3.22812	4.64262	-0.69860	3.31745
C	2.63598	3.27446	2.40244	1.44392	3.82143	1.18881	3.32328	3.54558	1.98929	3.11972	3.64579	1.83067
H	3.51607	2.91234	2.93753	2.26007	3.74090	1.91009	4.26608	3.21438	2.42827	4.06123	3.34550	2.30604
H	1.82018	3.46476	3.11136	0.47830	3.75746	1.70384	2.59876	3.76278	2.78321	2.36407	3.86107	2.60436
H	2.88303	4.19539	1.85919	1.53456	4.76712	0.63573	3.49061	4.44096	1.37851	3.28688	4.54639	1.21545
C	2.86789	-1.97166	3.05524	1.45794	-1.17452	3.11801	2.47558	-1.12822	3.59992	2.05691	-1.09112	3.46169
H	3.65588	-2.71167	2.85802	2.26473	-1.71395	3.63683	3.06600	-2.05035	3.68303	2.62716	-2.02031	3.63847
H	1.93467	-2.48499	3.29857	0.55739	-1.78937	3.07712	1.44279	-1.32787	3.89448	0.98548	-1.27073	3.61381
H	3.16635	-1.33583	3.90012	1.23368	-0.22917	3.62491	2.90298	-0.36013	4.25816	2.40797	-0.31007	4.15888
C	4.66214	2.50241	-2.30186	4.61234	2.58619	-2.12050	5.41551	1.23664	-2.54261	5.47252	1.35365	-2.40239
H	5.53796	1.95349	-2.67442	5.64905	2.21778	-2.12368	6.11551	0.40234	-2.68421	6.20581	0.53379	-2.50246
H	4.99540	3.32850	-1.65861	4.55913	3.50922	-1.52419	5.95098	2.09340	-2.11230	5.96738	2.22242	-1.93283
H	4.09845	2.90388	-3.14772	4.30399	2.79798	-3.14827	4.98926	1.52146	-3.50764	5.11289	1.63935	-3.39974
C	4.21980	-3.39935	-0.74712	4.57191	-2.81634	0.01177	4.01553	-3.66692	-0.47802	4.07632	-3.55732	-0.48765
H	5.13617	-3.13088	-0.21756	5.35959	-2.19937	0.45083	4.90088	-3.52658	0.14449	5.01488	-3.34316	0.03755
H	4.46157	-3.75148	-1.75798	5.01042	-3.51656	-0.71322	4.31539	-3.94470	-1.49563	4.29730	-3.94848	-1.49550
H	3.68618	-4.18263	-0.19433	4.05079	-3.37257	0.80187	3.37790	-4.44863	-0.04802	3.49558	-4.30412	0.07891

Table S6. XYZ coordinates of the DFT geometry optimized models of cobalt **2a** out-of-plane of the carbocation moiety.

	Grimme Disperision Forces						**No Dispersion Forces**					
	Solvated			Gas-Phase			Solvated			Gas-Phase		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
Co	-4.80611	-0.99005	0.01853	-4.76091	-1.11453	0.01216	-4.95243	-0.97790	-0.03497	-3.55914	-1.05487	0.93437
Cl	-3.80305	-2.00390	-1.82864	-3.53913	-1.99125	-1.74493	-4.04464	-1.93513	-1.97728	-3.74401	-2.99262	-0.38069
Cl	-3.79830	-1.56411	2.04305	-3.68382	-1.35588	2.05481	-3.96935	-1.76558	1.94274	-1.43970	-0.74522	1.86556
Cl	-7.06001	-1.60398	0.12251	-6.98702	-1.60472	0.00830	-7.26432	-1.38995	0.01746	-5.15576	-1.16908	2.66735

O	4.36045	2.23886	-0.55144	4.38736	2.29336	0.17508	4.38381	2.29012	-0.44930	3.34983	-2.40021	-0.46809
O	3.31816	-2.69892	0.33107	3.27305	-2.66143	-0.31721	3.40916	-2.72642	0.27584	2.88415	2.44875	1.18243
O	4.07910	0.39837	2.30295	3.98019	-0.53072	2.32443	4.19988	0.15103	2.31921	4.31056	0.85371	-1.72882
O	3.92246	-0.84753	-2.18047	3.94914	0.09029	-2.28282	3.94756	-0.61831	-2.27639	2.41061	-0.67527	2.25033
N	-4.72699	1.12466	-0.13967	-4.74357	1.05801	-0.18666	-4.71888	1.14758	-0.05215	-4.05894	0.71915	-0.16977
N	-0.11639	0.66562	0.23940	-0.14219	0.68544	0.34663	-0.07055	0.60522	0.31211	-0.35132	0.41897	-1.76699
C	-1.54004	0.98718	0.50445	-1.57720	1.00044	0.58478	-1.49906	0.90459	0.59284	-1.48406	0.60411	-2.71596
H	-1.56267	1.86507	1.15116	-1.61449	1.88453	1.22226	-1.52292	1.76413	1.26321	-1.19261	0.09245	-3.63347
H	-1.97591	0.18018	1.09284	-2.03088	0.20143	1.17473	-1.91902	0.07684	1.16377	-1.52745	1.65904	-2.97946
C	-3.66667	1.88861	-0.49979	-3.69234	1.85209	-0.48473	-3.62482	1.87264	-0.39068	-3.71613	1.03165	-1.44169
C	2.01825	-2.39825	0.21558	1.96913	-2.36175	-0.16115	2.10427	-2.43067	0.20158	1.72602	2.53376	0.51515
C	4.08395	-0.24423	0.06222	4.05114	-0.24101	0.01720	4.14754	-0.24911	0.01912	3.42592	0.08486	0.29217
C	-6.06300	3.11080	0.14447	-6.13988	3.00606	0.05018	-5.97056	3.18641	0.26395	-5.28884	2.78827	0.00535
H	-7.02431	3.54184	0.40652	-7.12574	3.40765	0.26655	-6.91421	3.65174	0.53173	-5.89954	3.44477	0.61739
C	2.18092	1.40499	-0.07225	2.16484	1.43404	0.17577	2.21798	1.38621	0.00100	1.54724	-0.94338	-1.06055
C	-5.89257	1.73093	0.17299	-5.93639	1.62737	0.07128	-5.85746	1.80058	0.26820	-4.82549	1.58759	0.52874
H	-6.70830	1.06639	0.44243	-6.74176	0.92912	0.28699	-6.70461	1.16910	0.51975	-5.07899	1.28215	1.53967
C	1.67102	-0.98428	0.14477	1.63655	-0.95588	0.03109	1.74051	-1.01783	0.16065	1.31464	1.36744	-0.26063
C	4.80882	-0.06252	1.24586	4.73947	-0.55995	1.19201	4.90320	-0.18291	1.19806	4.55880	0.44725	-0.44864
C	1.22782	4.06853	-0.11500	1.20546	4.09855	0.20712	1.21744	4.03789	0.05260	0.42209	-3.08852	-2.53693
H	0.86430	5.09294	-0.12963	0.84082	5.12317	0.19105	0.83574	5.05550	0.07518	-0.01372	-3.91593	-3.09115
C	6.18091	-0.34771	1.28483	6.10348	-0.87906	1.14762	6.27905	-0.45033	1.17386	5.83591	0.37735	0.12680
H	6.75533	-0.21605	2.19504	6.65057	-1.12818	2.05027	6.87397	-0.40392	2.07946	6.71950	0.65425	-0.43754
C	2.59572	3.82889	-0.30875	2.59070	3.86723	0.18853	2.58588	3.82756	-0.16009	1.63542	-3.28257	-1.86528
H	3.26359	4.66463	-0.47635	3.27139	4.70977	0.17839	3.23811	4.67992	-0.30325	2.11996	-4.24954	-1.91489
C	3.07588	2.52904	-0.31065	3.07317	2.56987	0.18002	3.09067	2.53749	-0.20346	2.20011	-2.24712	-1.13704
C	0.26663	-0.65730	0.15611	0.23432	-0.63333	0.18282	0.33039	-0.71067	0.20452	0.06523	1.47057	-0.97816
C	2.62291	0.06028	0.04099	2.59375	0.08142	0.07776	2.67955	0.04235	0.05979	2.07174	0.16776	-0.34482
C	-3.77621	3.28219	-0.55914	-3.82830	3.24474	-0.53216	-3.67979	3.27094	-0.43433	-4.17702	2.21301	-2.03861
H	-2.91712	3.87098	-0.86861	-2.96827	3.85597	-0.79772	-2.79879	3.82873	-0.73900	-3.91960	2.42207	-3.07371
C	1.03180	-3.36964	0.16515	0.97610	-3.32198	-0.19885	1.12765	-3.41271	0.16758	0.93728	3.67233	0.55872
H	1.29080	-4.42091	0.19044	1.22360	-4.36493	-0.35723	1.39958	-4.46084	0.17505	1.24332	4.53388	1.13874
C	0.32545	3.04118	0.06578	0.29878	3.06467	0.24997	0.33702	2.98860	0.21032	-0.24053	-1.87948	-2.50528
H	-0.72016	3.28796	0.17130	-0.75623	3.29540	0.25243	-0.71052	3.21411	0.33637	-1.18531	-1.80013	-3.02145
C	-2.34237	1.22487	-0.79633	-2.34585	1.21556	-0.73793	-2.32044	1.16862	-0.69477	-2.86426	0.07159	-2.24702
H	-1.76201	1.86808	-1.46601	-1.75848	1.86930	-1.39507	-1.73389	1.80140	-1.36946	-3.42042	-0.16795	-3.16340
H	-2.50224	0.27269	-1.31227	-2.47836	0.25583	-1.25072	-2.50680	0.22521	-1.21825	-2.75022	-0.87164	-1.70981
C	0.77848	1.70182	0.07973	0.75662	1.72095	0.25786	0.81136	1.65740	0.17716	0.30209	-0.79713	-1.77652
C	4.73007	-0.70673	-1.09149	4.72341	-0.23991	-1.20995	4.77304	-0.58332	-1.19119	3.57246	-0.34877	1.61918
C	-4.98031	3.90424	-0.23383	-5.06268	3.83309	-0.26038	-4.85695	3.93934	-0.10417	-4.96378	3.10446	-1.31416
H	-5.07027	4.98657	-0.27925	-5.17967	4.91428	-0.29769	-4.90181	5.02490	-0.13871	-5.32016	4.02303	-1.77324
C	6.80613	-0.80765	0.12460	6.75642	-0.87470	-0.08598	6.88156	-0.77914	-0.04161	5.95846	-0.05765	1.44673
H	7.87093	-1.02895	0.14873	7.81478	-1.12367	-0.12678	7.94939	-0.98580	-0.06561	6.94697	-0.11396	1.89755

C	-0.31776	-2.99432	0.08395	-0.37163	-2.95055	-0.04925	-0.22734	-3.05542	0.12093	-0.27722	3.71069	-0.13840
H	-1.08094	-3.76596	0.02031	-1.15590	-3.70035	-0.10996	-0.97943	-3.83878	0.07007	-0.89412	4.60373	-0.07819
C	-0.70943	-1.67246	0.09760	-0.74519	-1.64130	0.15042	-0.63490	-1.73863	0.15267	-0.71471	2.64422	-0.89439
H	-1.76257	-1.45164	0.03643	-1.79793	-1.43533	0.24709	-1.69323	-1.52723	0.11921	-1.67435	2.72008	-1.38171
C	6.10009	-0.99165	-1.06774	6.08532	-0.55875	-1.27015	6.14749	-0.84906	-1.22834	4.84213	-0.42266	2.20416
H	6.61409	-1.35008	-1.95265	6.61958	-0.56529	-2.21401	6.64272	-1.10585	-2.15836	4.96729	-0.75716	3.22812
C	3.74481	-4.06269	0.29430	3.67159	-4.01179	-0.51636	3.82541	-4.09513	0.29780	3.32328	3.54558	1.98929
H	4.83430	-4.01773	0.34722	4.75972	-3.97414	-0.60661	4.91478	-4.05956	0.35410	4.26608	3.21438	2.42827
H	3.43637	-4.54511	-0.64171	3.23558	-4.42544	-1.43630	3.51612	-4.61463	-0.61716	2.59876	3.76278	2.78321
H	3.35140	-4.62252	1.15213	3.39083	-4.64113	0.33952	3.42324	-4.61318	1.17688	3.49061	4.44096	1.37851
C	4.48129	-1.40158	-3.36837	4.53929	0.07126	-3.57345	4.50804	-0.95482	-3.54253	2.47558	-1.12822	3.59992
H	5.27589	-0.76022	-3.77382	5.35753	0.80227	-3.65299	5.27351	-0.22813	-3.84568	3.06600	-2.05035	3.68303
H	3.65871	-1.45869	-4.08545	3.74190	0.34145	-4.27054	3.67750	-0.92622	-4.25200	1.44279	-1.32787	3.89448
H	4.88117	-2.40866	-3.18671	4.92096	-0.92862	-3.82600	4.94477	-1.96230	-3.53074	2.90298	-0.36013	4.25816
C	4.75338	0.64698	3.53322	4.58547	-0.89716	3.55528	4.90156	0.24676	3.55555	5.41551	1.23664	-2.54261
H	5.54090	1.40334	3.41079	5.40326	-0.21161	3.82199	5.68030	1.01995	3.51406	6.11551	0.40234	-2.68421
H	5.19160	-0.27371	3.94245	4.97100	-1.92655	3.52244	5.35478	-0.71423	3.83303	5.95098	2.09340	-2.11230
H	3.99034	1.02274	4.21935	3.79543	-0.82955	4.30757	4.15246	0.52426	4.30112	4.98926	1.52146	-3.50764
C	5.31102	3.28918	-0.74518	5.34380	3.34375	0.11539	5.28880	3.37755	-0.66311	4.01553	-3.66692	-0.47802
H	6.26619	2.78007	-0.88719	6.31251	2.83978	0.08683	6.25872	2.90784	-0.83570	4.90088	-3.52658	0.14449
H	5.36204	3.93976	0.13679	5.28567	3.98828	1.00348	5.34003	4.02553	0.22009	4.31539	-3.94470	-1.49563
H	5.06722	3.88188	-1.63588	5.21293	3.95017	-0.79157	4.99643	3.96394	-1.54266	3.37790	-4.44863	-0.04802

Table S7. XYZ coordinates of the DFT geometry optimized models of nickel **2b** in-plane of the carbocation moiety.

	Grimme Disperision Forces						**No Dispersion Forces**					
	Solvated			Gas-Phase			Solvated			Gas-Phase		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
Ni	-3.57025	-0.80973	1.28114	-1.97949	-0.51603	1.50231	-3.86304	-0.97490	1.06039	-3.43050	-1.16436	0.99092
Cl	-4.34843	-2.78798	0.28737	-1.24533	-2.64669	1.04838	-4.35971	-2.84444	-0.27120	-3.45651	-2.93050	-0.52206
Cl	-1.25223	-0.93919	1.34958	-0.83626	1.46341	1.94596	-1.55345	-0.92488	1.40780	-1.25760	-0.48004	1.37934
Cl	-4.14755	0.21559	3.30896	-3.59596	-0.61342	3.11877	-4.76372	-0.38280	3.15536	-4.62745	-0.95433	2.94477
O	3.19795	-2.33569	0.48410	3.63066	-1.91124	-0.53151	3.39491	-2.44822	-0.15366	3.30308	-2.38156	-0.40817
O	2.97035	2.77265	0.04809	1.64302	2.76519	0.05721	3.14911	2.63686	0.68737	2.96778	2.59476	0.82850
O	4.35371	-0.23565	-1.84028	3.74001	1.48830	-1.64210	4.54126	0.41838	-1.73451	4.47101	0.67832	-1.65063
O	2.27808	0.67004	2.23084	1.62307	-0.85466	1.77266	2.34931	-0.23009	2.33379	2.09061	-0.46863	2.16817
N	-3.97726	0.58540	-0.21025	-3.29879	0.24226	0.01273	-4.19327	0.65775	-0.20929	-4.06460	0.60255	-0.09661
N	-0.35252	-0.10874	-1.86500	-0.72281	-0.77601	-2.18428	-0.24235	0.27061	-1.78114	-0.39712	0.37918	-1.81555
C	-1.53884	-0.22037	-2.74746	-2.00436	-1.23234	-2.76768	-1.43879	0.35726	-2.65924	-1.56282	0.51170	-2.73042
H	-1.28009	-0.93077	-3.53220	-1.79892	-2.12144	-3.36104	-1.19247	-0.19582	-3.56537	-1.29820	-0.05751	-3.62470
H	-1.66805	0.73217	-3.25879	-2.34966	-0.49007	-3.48589	-1.53985	1.39217	-2.97873	-1.60741	1.55350	-3.04959
C	-3.71021	0.44479	-1.52927	-3.73942	-0.29288	-1.14397	-3.70553	0.81825	-1.46305	-3.75753	0.94758	-1.36624
C	1.71446	2.62057	-0.39026	0.64436	2.38644	-0.74270	1.91649	2.61749	0.16280	1.76388	2.62798	0.23261

C	3.38665	0.22184	0.23279	2.70044	0.39654	0.13173	3.51136	0.09237	0.33545	3.34799	0.09605	0.31144
C	-5.25380	2.57710	-0.67404	-4.86367	2.05541	-0.23639	-5.51232	2.66091	-0.45629	-5.32756	2.64180	0.14575
H	-5.84249	3.40209	-0.28508	-5.27240	2.97644	0.16910	-6.21714	3.35738	-0.01277	-5.94004	3.26998	0.78645
C	1.53926	-1.16949	-0.76669	1.42770	-1.31731	-1.19809	1.65409	-1.02568	-0.96795	1.49412	-0.95428	-1.05152
C	-4.72530	1.63388	0.19860	-3.85673	1.38792	0.45433	-5.07135	1.56419	0.27409	-4.82919	1.43713	0.63646
H	-4.89575	1.69363	1.26868	-3.47036	1.76115	1.39638	-5.41903	1.38201	1.28656	-5.04007	1.09553	1.64725
C	1.29504	1.26753	-0.72836	0.60490	0.99019	-1.15270	1.46205	1.36354	-0.43015	1.31713	1.41149	-0.43239
C	4.55431	0.03645	-0.51799	3.77919	1.16700	-0.31416	4.70162	0.23464	-0.39127	4.56630	0.34343	-0.32742
C	0.54224	-3.66431	-1.64547	0.89913	-4.04391	-1.68796	0.55093	-3.27827	-2.28931	0.27861	-3.19383	-2.29321
H	0.16388	-4.62493	-1.98605	0.67495	-5.09855	-1.82824	0.12847	-4.14429	-2.79265	-0.20895	-4.06136	-2.73037
C	5.81204	0.13083	0.09386	4.78028	1.57066	0.57449	5.94091	0.18492	0.26109	5.77120	0.24059	0.38219
H	6.72433	-0.00641	-0.47579	5.61945	2.17160	0.24147	6.86849	0.29525	-0.28984	6.72395	0.42879	-0.10106
C	1.67896	-3.63394	-0.82399	2.15182	-3.67356	-1.17647	1.73590	-3.42698	-1.55667	1.51230	-3.35289	-1.64668
H	2.15173	-4.56468	-0.53608	2.89518	-4.43405	-0.96791	2.20843	-4.39979	-1.50455	1.97072	-4.33357	-1.61292
C	2.16457	-2.42112	-0.36412	2.42794	-2.33847	-0.94944	2.28339	-2.34031	-0.89369	2.12004	-2.27018	-1.03645
C	0.01227	1.12204	-1.36653	-0.53557	0.57184	-1.92843	0.17873	1.38511	-1.08984	0.04588	1.47116	-1.10658
C	2.05491	0.10772	-0.43076	1.57925	0.02949	-0.77877	2.19134	0.14564	-0.36917	2.04424	0.19040	-0.42037
C	-4.24680	1.34133	-2.46347	-4.77284	0.31160	-1.87407	-4.13084	1.89144	-2.25776	-4.24818	2.13516	-1.92877
H	-4.04469	1.18848	-3.52037	-5.11841	-0.15903	-2.79188	-3.75743	1.98487	-3.27411	-4.01964	2.36627	-2.96771
C	0.84180	3.68722	-0.53087	-0.31626	3.28397	-1.18068	1.09742	3.73511	0.17121	0.97610	3.76591	0.24225
H	1.14202	4.68795	-0.24565	-0.27592	4.31954	-0.86590	1.42943	4.65868	0.62871	1.30878	4.66266	0.75055
C	-0.13150	-2.51560	-2.00296	-0.05481	-3.10972	-2.02175	-0.10574	-2.06881	-2.37196	-0.34687	-1.97043	-2.36721
H	-1.03502	-2.61298	-2.58637	-1.01549	-3.46397	-2.36305	-1.03755	-2.02808	-2.91583	-1.32390	-1.92633	-2.82205
C	-2.82286	-0.68083	-2.01143	-3.07821	-1.53489	-1.69542	-2.74044	-0.20535	-2.02733	-2.92954	0.00309	-2.21255
H	-3.40390	-1.28855	-2.71611	-3.84501	-2.15563	-2.17714	-3.27388	-0.75348	-2.81534	-3.51602	-0.21952	-3.11651
H	-2.55098	-1.33434	-1.18272	-2.63103	-2.12030	-0.88479	-2.48732	-0.93760	-1.25999	-2.81972	-0.94887	-1.68686
C	0.33817	-1.25910	-1.55677	0.20111	-1.73343	-1.81626	0.42272	-0.93456	-1.71433	0.23525	-0.84356	-1.74663
C	3.47514	0.49914	1.60439	2.63972	-0.01977	1.47263	3.56211	-0.10331	1.72361	3.32919	-0.25725	1.67077
C	-5.02070	2.41853	-2.04063	-5.34026	1.50010	-1.42332	-5.03594	2.82357	-1.75675	-5.03667	2.99680	-1.16961
H	-5.43235	3.11844	-2.76326	-6.14216	1.97746	-1.98295	-5.36532	3.65625	-2.37309	-5.42318	3.91797	-1.60150
C	5.87735	0.40380	1.46127	4.67543	1.19644	1.91867	5.96868	-0.01223	1.64313	5.73230	-0.11305	1.73325
H	6.85082	0.47503	1.94160	5.44164	1.52173	2.61980	6.92837	-0.05352	2.15395	6.66636	-0.19451	2.28594
C	-0.43916	3.47551	-1.06255	-1.35274	2.84699	-2.00861	-0.17729	3.67546	-0.40868	-0.27631	3.75598	-0.38925
H	-1.12150	4.31725	-1.15089	-2.09857	3.56032	-2.35189	-0.81899	4.55200	-0.36706	-0.90195	4.64432	-0.33914
C	-0.84874	2.23358	-1.50003	-1.47613	1.52388	-2.37865	-0.63536	2.53835	-1.03883	-0.73787	2.64757	-1.05966
H	-1.84212	2.13167	-1.90800	-2.33467	1.24197	-2.96702	-1.63247	2.54401	-1.45312	-1.73308	2.67089	-1.47707
C	4.72436	0.58962	2.22918	3.62050	0.41095	2.38029	4.79505	-0.15825	2.38625	4.52656	-0.36461	2.39103
H	4.80669	0.80128	3.28941	3.56151	0.13021	3.42610	4.84707	-0.31169	3.45857	4.51941	-0.63816	3.44109
C	3.40482	4.03537	0.55743	1.50288	3.93493	0.86354	3.63863	3.83000	1.30664	3.42691	3.72335	1.56235
H	4.41799	3.85782	0.92330	2.34495	3.89456	1.55806	4.64151	3.57732	1.65532	4.39453	3.42263	1.96976
H	2.76281	4.36524	1.38381	0.55663	3.89623	1.41557	3.00979	4.11730	2.15789	2.73906	3.97011	2.38182
H	3.42064	4.79615	-0.23324	1.57005	4.84945	0.25725	3.69140	4.65365	0.58425	3.55506	4.59808	0.90993
C	2.27620	1.02490	3.61035	1.26615	-1.06547	3.13971	2.31605	-0.42410	3.74487	1.91675	-0.87612	3.51815

H	2.73845	0.24095	4.22575	2.06928	-1.58805	3.67998	2.82774	-1.35246	4.03176	2.42455	-1.83177	3.71252
H	1.22435	1.13126	3.88631	0.37392	-1.69336	3.10345	1.25812	-0.49423	4.00827	0.83756	-0.99379	3.63863
H	2.79938	1.97679	3.77632	1.02709	-0.11046	3.62131	2.77121	0.42343	4.27464	2.29419	-0.11427	4.21565
C	5.48999	-0.51205	-2.65401	4.66397	2.44853	-2.12339	5.70638	0.56229	-2.54153	5.66758	0.93417	-2.36579
H	6.04571	-1.38288	-2.27984	5.69944	2.08095	-2.06699	6.34357	-0.33051	-2.48656	6.32471	0.05257	-2.38356
H	6.16330	0.35434	-2.71016	4.58502	3.39383	-1.56623	6.28938	1.44558	-2.24809	6.21861	1.78559	-1.94055
H	5.09595	-0.73090	-3.64959	4.40165	2.61955	-3.17136	5.34493	0.68888	-3.56499	5.36068	1.17627	-3.38703
C	3.88604	-3.51761	0.89856	4.53017	-2.82276	0.08826	4.04261	-3.71731	-0.02389	3.92070	-3.65764	-0.28659
H	4.68136	-3.16347	1.55724	5.31857	-2.19848	0.51540	4.89780	-3.53325	0.62878	4.83292	-3.47855	0.28651
H	4.32062	-4.04190	0.03816	4.96440	-3.51927	-0.64297	4.38960	-4.08355	-0.99773	4.17735	-4.07208	-1.27121
H	3.21709	-4.19090	1.44933	4.02664	-3.38438	0.88610	3.37332	-4.45359	0.43732	3.27332	-4.36061	0.25382

Table S8. XYZ coordinates of the DFT geometry optimized models of nickel **2b** out-of-plane of the carbocation moiety.

	Grimme Disperision Forces						No Dispersion Forces					
	Solvated			Gas-Phase			Solvated			Gas-Phase		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
Ni	-4.75991	-1.12251	-0.12693	-4.75991	-1.12251	-0.12693	-4.98939	-1.00763	-0.19985	-4.59536	-1.05000	-0.08400
Cl	-3.32967	-1.93110	-1.76588	-3.32967	-1.93110	-1.76588	-3.68505	-1.93319	-1.92713	-3.79779	-1.61897	-2.19857
Cl	-3.78706	-1.26496	1.97306	-3.78706	-1.26496	1.97306	-4.05202	-1.60632	1.85433	-4.03042	-1.28252	2.18361
Cl	-6.98730	-1.58789	0.07549	-6.98730	-1.58789	0.07549	-7.31219	-1.33926	0.07867	-6.83213	-1.71067	-0.17161
O	4.40136	2.29139	0.01057	4.40136	2.29139	0.01057	4.37356	2.31241	-0.39814	4.46923	2.14301	0.72975
O	3.28398	-2.68149	-0.08858	3.28398	-2.68149	-0.08858	3.45250	-2.70807	0.34171	3.10994	-2.59052	-0.82863
O	4.14521	-0.30996	2.31603	4.14521	-0.30996	2.31603	4.38749	0.09635	2.25845	3.98195	-1.40612	1.98975
O	3.80173	-0.12837	-2.31674	3.80173	-0.12837	-2.31674	3.76712	-0.55109	-2.32123	3.97876	0.84647	-2.09251
N	-4.73968	1.01309	-0.23680	-4.73968	1.01309	-0.23680	-4.74364	1.08779	-0.14341	-4.66282	1.03406	-0.15178
N	-0.12284	0.70207	0.42616	-0.12284	0.70207	0.42616	-0.05592	0.59646	0.45633	-0.09193	0.70508	0.55298
C	-1.55766	1.02871	0.65130	-1.55766	1.02871	0.65130	-1.49074	0.88930	0.71674	-1.51504	1.06449	0.75855
H	-1.59633	1.92794	1.26728	-1.59633	1.92794	1.26728	-1.53262	1.76261	1.36734	-1.54894	1.96511	1.37047
H	-2.02235	0.24617	1.25311	-2.02235	0.24617	1.25311	-1.91396	0.07259	1.29927	-2.00345	0.29510	1.35367
C	-3.67653	1.81885	-0.45567	-3.67653	1.81885	-0.45567	-3.61156	1.80602	-0.34898	-3.61242	1.85512	-0.39088
C	1.98011	-2.37032	0.04549	1.98011	-2.37032	0.04549	2.14240	-2.42449	0.31805	1.88698	-2.32876	-0.34896
C	4.05944	-0.24214	-0.00783	4.05944	-0.24214	-0.00783	4.15111	-0.24093	-0.03947	4.05235	-0.29941	-0.06217
C	-6.14155	2.95269	0.04675	-6.14155	2.95269	0.04675	-5.98562	3.13726	0.15494	-6.10511	2.94638	0.09733
H	-7.13427	3.34332	0.25121	-7.13427	3.34332	0.25121	-6.94336	3.60624	0.35876	-7.10353	3.32349	0.29640
C	2.18067	1.43863	0.16289	2.18067	1.43863	0.16289	2.22071	1.39134	0.08493	2.23571	1.38878	0.41031
C	-5.93976	1.57479	0.00990	-5.93976	1.57479	0.00990	-5.89541	1.75120	0.10324	-5.87477	1.57495	0.08913
H	-6.74986	0.87018	0.17685	-6.74986	0.87018	0.17685	-6.76996	1.12720	0.25429	-6.67403	0.86430	0.27095
C	1.64939	-0.95528	0.15691	1.64939	-0.95528	0.15691	1.76425	-1.01527	0.27257	1.61401	-0.95014	0.03133
C	4.82753	-0.44560	1.14290	4.82753	-0.44560	1.14290	4.99873	-0.20747	1.07669	4.73289	-1.04561	0.91089
C	1.22841	4.10606	0.14577	1.22841	4.10606	0.14577	1.20532	4.03737	0.16045	1.37754	4.07705	0.49401
H	0.86517	5.13091	0.11720	0.86517	5.13091	0.11720	0.81735	5.05237	0.19221	1.05095	5.11383	0.47840
C	6.18850	-0.76204	1.03721	6.18850	-0.76204	1.03721	6.36699	-0.47444	0.93535	6.08333	-1.37385	0.73586

H	6.79710	-0.92427	1.92009	6.79710	-0.92427	1.92009	7.03253	-0.45317	1.79123	6.62210	-1.94565	1.48299
C	2.61061	3.86985	0.06887	2.61061	3.86985	0.06887	2.56983	3.83594	-0.08208	2.75030	3.79650	0.57216
H	3.29171	4.70912	-0.00241	3.29171	4.70912	-0.00241	3.21388	4.69240	-0.23709	3.45788	4.61258	0.65168
C	3.08940	2.57128	0.07905	3.08940	2.57128	0.07905	3.08175	2.54916	-0.13518	3.18429	2.48120	0.56997
C	0.24943	-0.62384	0.31452	0.24943	-0.62384	0.31452	0.35393	-0.71831	0.36628	0.25068	-0.61877	0.36359
C	2.60597	0.08219	0.11279	2.60597	0.08219	0.11279	2.69010	0.04932	0.11484	2.61545	0.05001	0.13319
C	-3.81415	3.21263	-0.44273	-3.81415	3.21263	-0.44273	-3.64374	3.20668	-0.32823	-3.78041	3.24448	-0.40453
H	-2.94424	3.83317	-0.64724	-2.94424	3.83317	-0.64724	-2.73046	3.75936	-0.52907	-2.92447	3.88059	-0.61271
C	0.98595	-3.32954	0.06551	0.98595	-3.32954	0.06551	1.17491	-3.41517	0.34231	0.90677	-3.29990	-0.23301
H	1.23143	-4.38019	-0.03425	1.23143	-4.38019	-0.03425	1.45632	-4.46073	0.35692	1.11578	-4.33091	-0.49076
C	0.32265	3.07674	0.25642	0.32265	3.07674	0.25642	0.33645	2.98248	0.34068	0.42783	3.07624	0.47409
H	-0.73008	3.31224	0.29815	-0.73008	3.31224	0.29815	-0.70795	3.20284	0.49505	-0.61466	3.35602	0.44108
C	-2.31336	1.21075	-0.68306	-2.31336	1.21075	-0.68306	-2.28883	1.11232	-0.59275	-2.23603	1.26810	-0.59289
H	-1.73359	1.87311	-1.33859	-1.73359	1.87311	-1.33859	-1.69453	1.74513	-1.26172	-1.64449	1.95088	-1.21263
H	-2.41291	0.24285	-1.18555	-2.41291	0.24285	-1.18555	-2.44273	0.15816	-1.10394	-2.29409	0.31561	-1.12893
C	0.77632	1.73160	0.28497	0.77632	1.73160	0.28497	0.81722	1.65347	0.29979	0.83634	1.72215	0.47726
C	4.64892	-0.35187	-1.27189	4.64892	-0.35187	-1.27189	4.67664	-0.54345	-1.30412	4.72813	0.11667	-1.21850
C	-5.05546	3.79198	-0.18863	-5.05546	3.79198	-0.18863	-4.83219	3.88500	-0.07237	-5.03377	3.80124	-0.15925
H	-5.16993	4.87404	-0.17946	-5.16993	4.87404	-0.17946	-4.85509	4.97169	-0.05737	-5.16906	4.87973	-0.16986
C	6.75852	-0.87007	-0.23266	6.75852	-0.87007	-0.23266	6.87011	-0.77010	-0.33326	6.73486	-0.95333	-0.42552
H	7.81441	-1.11736	-0.32065	7.81441	-1.11736	-0.32065	7.93215	-0.97620	-0.44799	7.78271	-1.20862	-0.56732
C	-0.36016	-2.94828	0.20264	-0.36016	-2.94828	0.20264	-0.18395	-3.06937	0.34527	-0.37907	-2.94299	0.20126
H	-1.14376	-3.70093	0.18758	-1.14376	-3.70093	0.18758	-0.93060	-3.85960	0.33863	-1.13869	-3.71518	0.29593
C	-0.73206	-1.63049	0.33959	-0.73206	-1.63049	0.33959	-0.60267	-1.75621	0.36935	-0.72221	-1.63596	0.47716
H	-1.78477	-1.41919	0.43757	-1.78477	-1.41919	0.43757	-1.66404	-1.55727	0.36911	-1.73564	-1.43003	0.78423
C	6.00748	-0.66897	-1.39327	6.00748	-0.66897	-1.39327	6.04365	-0.80820	-1.45837	6.07585	-0.21258	-1.40919
H	6.47809	-0.76038	-2.36618	6.47809	-0.76038	-2.36618	6.46246	-1.04046	-2.43141	6.60762	0.09943	-2.30107
C	3.67720	-4.04060	-0.22988	3.67720	-4.04060	-0.22988	3.88193	-4.07239	0.36867	3.50860	-3.94168	-1.07151
H	4.76483	-4.01099	-0.32879	4.76483	-4.01099	-0.32879	4.97234	-4.02643	0.37929	4.55761	-3.87766	-1.36694
H	3.23385	-4.49318	-1.12771	3.23385	-4.49318	-1.12771	3.54007	-4.60987	-0.52409	2.91881	-4.38849	-1.88183
H	3.40011	-4.63064	0.65479	3.40011	-4.63064	0.65479	3.52160	-4.57969	1.27189	3.41391	-4.54597	-0.16060
C	4.29985	-0.28496	-3.63664	4.29985	-0.28496	-3.63664	4.22481	-0.85180	-3.63664	4.62589	1.42135	-3.22455
H	5.10427	0.43391	-3.85190	5.10427	0.43391	-3.85190	4.96374	-0.11555	-3.98006	5.44699	2.08366	-2.91766
H	3.45292	-0.09164	-4.29997	3.45292	-0.09164	-4.29997	3.34025	-0.80564	-4.27648	3.85864	2.00425	-3.73993
H	4.67102	-1.30599	-3.80683	4.67102	-1.30599	-3.80683	4.66102	-1.85831	-3.68744	5.01287	0.64768	-3.90162
C	4.83999	-0.53925	3.53240	4.83999	-0.53925	3.53240	5.18468	0.15064	3.43822	4.56717	-2.26163	2.96786
H	5.66539	0.17560	3.66555	5.66539	0.17560	3.66555	5.96119	0.92338	3.36066	5.41783	-1.77743	3.46670
H	5.23623	-1.56394	3.58218	5.23623	-1.56394	3.58218	5.65444	-0.81968	3.64745	4.89624	-3.20955	2.52035
H	4.10405	-0.39613	4.32781	4.10405	-0.39613	4.32781	4.49786	0.40490	4.24917	3.77973	-2.45678	3.69993
C	5.35408	3.33743	-0.12986	5.35408	3.33743	-0.12986	5.26713	3.40668	-0.62423	5.48307	3.15128	0.70526
H	6.31940	2.83041	-0.19526	6.31940	2.83041	-0.19526	6.23850	2.94437	-0.80823	6.42650	2.60485	0.75912
H	5.34354	4.00719	0.74126	5.34354	4.00719	0.74126	5.32423	4.05617	0.25751	5.39130	3.82448	1.56677
H	5.17572	3.91799	-1.04557	5.17572	3.91799	-1.04557	4.95959	3.98977	-1.50080	5.43824	3.72631	-0.22809

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