Supplementary Information for

Fluorinated Cobalt Catalysts and their use in forming Narrowly Dispersed Polyethylene Waxes of High Linearity and incorporating Vinyl Functionality

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Synthesis of 2,4-bis(bis(4-fluorophenyl)methyl)-6-fluoroaniline

A mixture of 2-fluoroaniline (5.60 g, 50 mmol) and bis(4-fluorophenyl)methanol (22.0 g, 100 mmol) was stirred and heated to 140 °C to form a melt. A mixture of $ZnCl_2$ (3.30 g, 25 mmol) and concentrated HCl solution (5 mL) was added as catalyst to the reaction vessel and the mixture stirred for 5 h at 140 °C until the reaction mixture had solidified and no further water formed. The resulting solid was dissolved in dichloromethane (100 mL) and washed with an aqueous solution of NH_4Cl solution (3 × 250 mL) and an aqueous solution of NaCl (2 × 250 mL). The organic phase was collected and dried over anhydrous Na_2SO_4. After filtering, the solvent weas evaporated under reduced pressure. The residue was recrystallized from petroleum ether and the product obtained as a white solid (20.6 g, 80%). ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 6.97−6.91 (m, 16H), 6.65 (d, J = 6.1 Hz, 1H), 6.03 (s, 1H, aryl-F), 5.40 (s, 1H, CH(p-FPh)$_2$), 5.26 (s, 1H, CH(p-FPh)$_2$), 3.46 (s, 2H, NH_2). ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 163.20, 162.90, 160.76, 160.46, 153.49, 151.11, 131.05, 130.87, 130.79, 130.74, 130.66, 115.87, 115.65, 115.42, 115.21, 114.51, 114.31, 54.53, 50.80, 50.77.

Two step synthesis of 4'-(phenylmethylene)bis(2-(bis(4-fluorophenyl)methyl)-6-fluoroaniline).

Step 1: Synthesis of 4,4'-(phenylmethylene)bis(2-fluoroaniline). Under a nitrogen atmosphere, benzaldehyde (10.6 g, 100 mmol) and 2-fluoroaniline (23.3 g, 210 mmol) were stirred and heated at 130 °C. Concentrated hydrochloric acid (10 mL) was then slowly added dropwise into the mixture. The mixture was stirred and heated at 130 °C for 6 h using a Dean-Stark apparatus. The reaction mixture was allowed to cool to room temperature and the residue dissolved in dichloromethane (100 mL) and then neutralized with ammonium hydroxide. The solution was then extracted with dichloromethane (3 × 50 mL) to afford an orange colored solution. The organic phase was washed with water and dried over $MgSO_4$. Following filtration, the dichloromethane was removed by rotary evaporation until approximately 10 mL was left. An excess of petroleum ether (*ca.* 100 mL) was added to initiate precipitation and the precipitate filtered and dried to give a white solid (19.5 g, 65%). ^{1}H NMR (400 MHz, $CDCl_3$. TMS): δ 7.28−7.23 (m, 2H, aryl-H), 7.20−7.17 (m, 1H, aryl-H), 7.07 (d, J = 8.1 Hz, 2H, aryl-H), 6.72 (s, 1H, aryl-H), 6.71-6.66 (m, 5H, aryl-H), 5.29 (s, 1H, $CHPh_2$), 3.62 (s, 4H, 2 × NH_2). ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 152.77, 150.39, 143.97, 135.00, 134.94, 132.69, 132.56, 129.20, 129.16, 128.35, 126.37, 125.15, 125.12, 116.74, 116.70, 116.23, 116.04, 54.92.

Step 2: Synthesis of 4,4'-(phenylmethylene)bis(2-(bis(4-fluorophenyl)methyl)-6-fluoroaniline). Under a nitrogen atmosphere, 4,4'-(phenylmethylene)bis(2-fluoroaniline) (6.20 g, 20.0 mmol) and bis(4-fluorophenyl)methanol (8.8 g, 40 mmol) were dissolved at 160 °C. A solution of zinc chloride in concentrated hydrochloric acid (3 mL) was then added dropwise to the solution resulting in the solution immediately becoming bluish violet in color. The mixture was stirred and heated for 6 h under an atmosphere of nitrogen. The mixture was then allowed to cool to room temperature, the residue dissolved in dichloromethane, neutralized with ammonium hydroxide and then extracted with dichloromethane. The organic phase was washed with water, dried over $MgSO_4$ and the solvent removed by rotary evaporation. The solid residue was loaded on a basic aluminum column and eluted with petroleum ether/ethyl acetate (50/1 v/v) forming the target compound as white powder (4.2 g, 30%). ^{1}H NMR (400 MHz, $CDCl_3$. TMS): δ 7.17−7.16 (m, 3H, aryl-H), 6.95−6.92 (m, 16H, aryl-H), 6.87 (d, J = 8.1 Hz, 2H, aryl-H), 6.57 (s, 1H, aryl-H), 6.53 (s, 1H, aryl-H), 5.98 (s, 2H, aryl-H), 5.37 (s, 2H, CH(p-FPh)$_2$), 5.04 (s, 1H, $CHPh_3$), 3.42 (s, 4H, 2 × NH_2). ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 157.63, 155.18, 147.89, 145.52, 138.28, 132.13, 128.69, 128.62, 125.36, 125.28, 123.61, 122.86, 120.94, 120.63, 110.28, 110.07, 108.91, 108.71, 49.61, 45.20, 45.18.

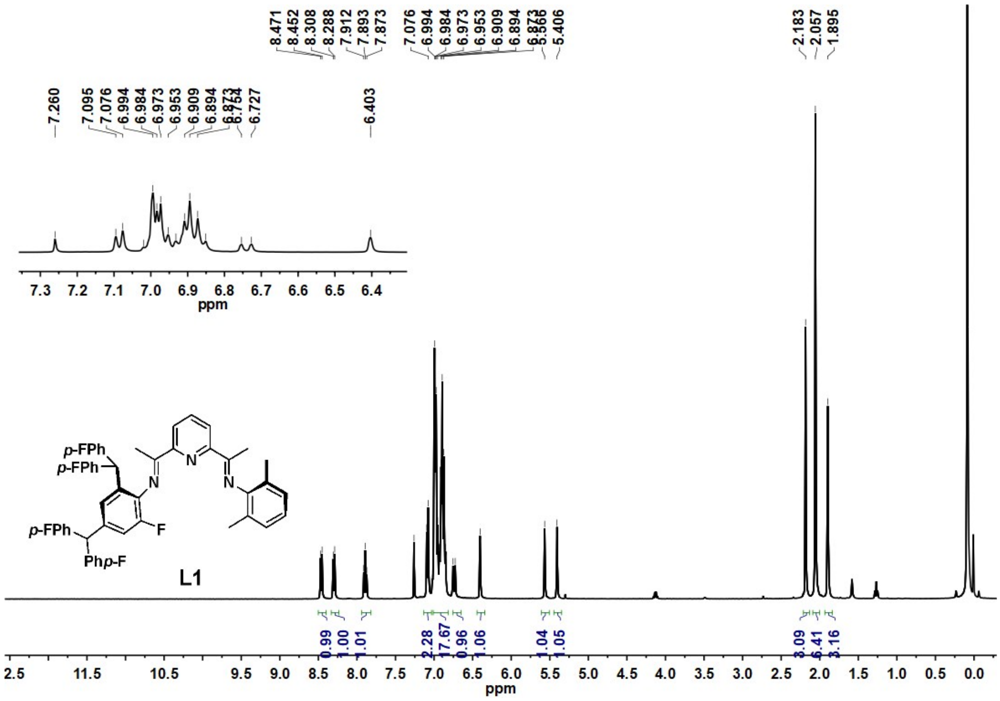
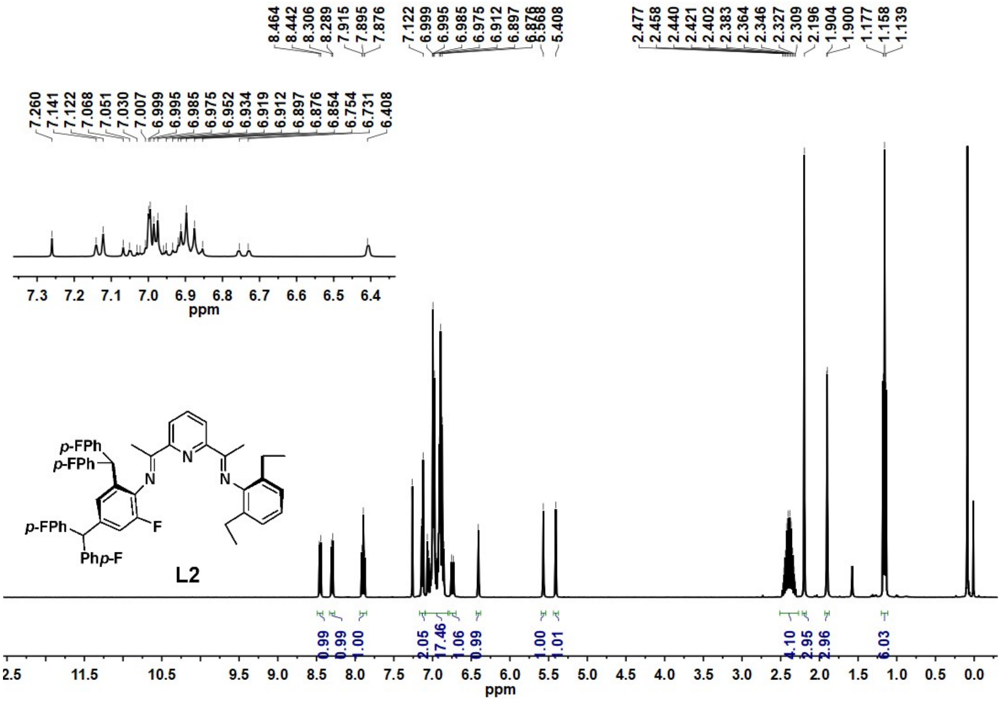


Figure S1 [1]H NMR spectrum of **L1** with an expansion of the δ 7.3 – 6.3 region; recorded in $CDCl_3$ at ambient temperature.



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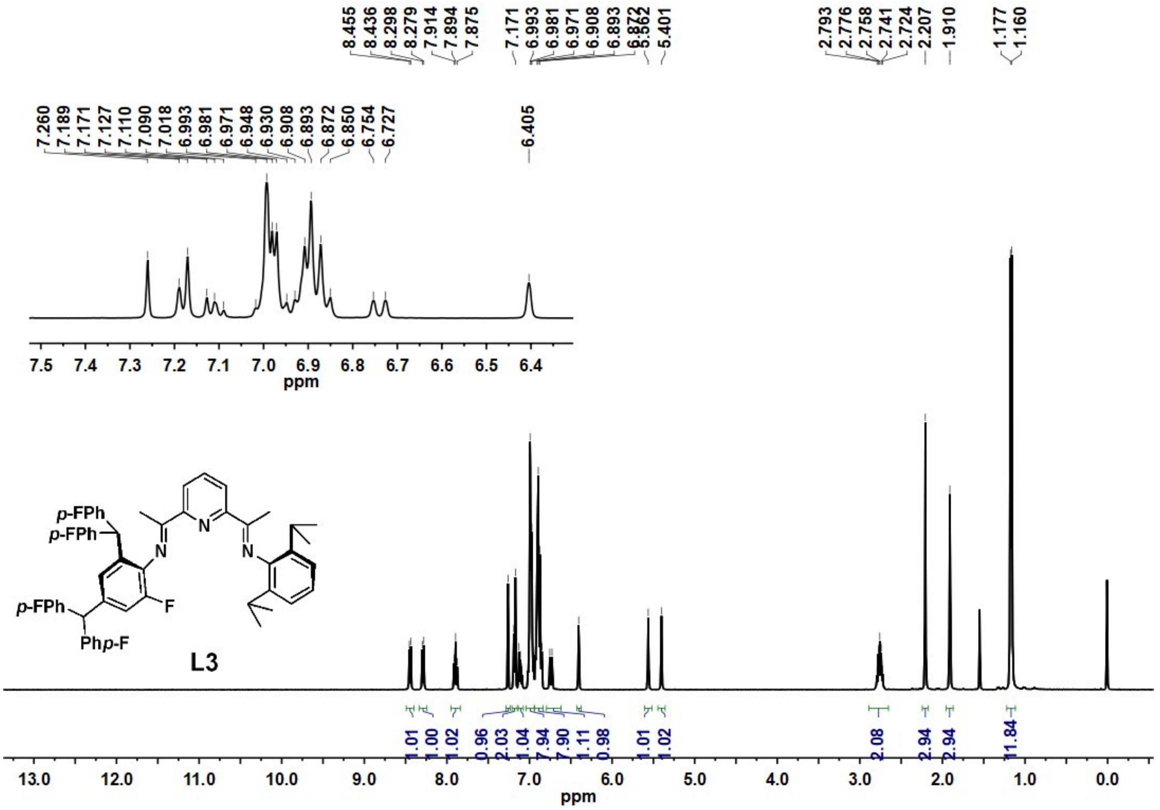


Figure S3 ^{1}H NMR spectrum of **L3** with an expansion of the δ 7.5 – 5.0 region; recorded in $CDCl_3$ at ambient temperature.

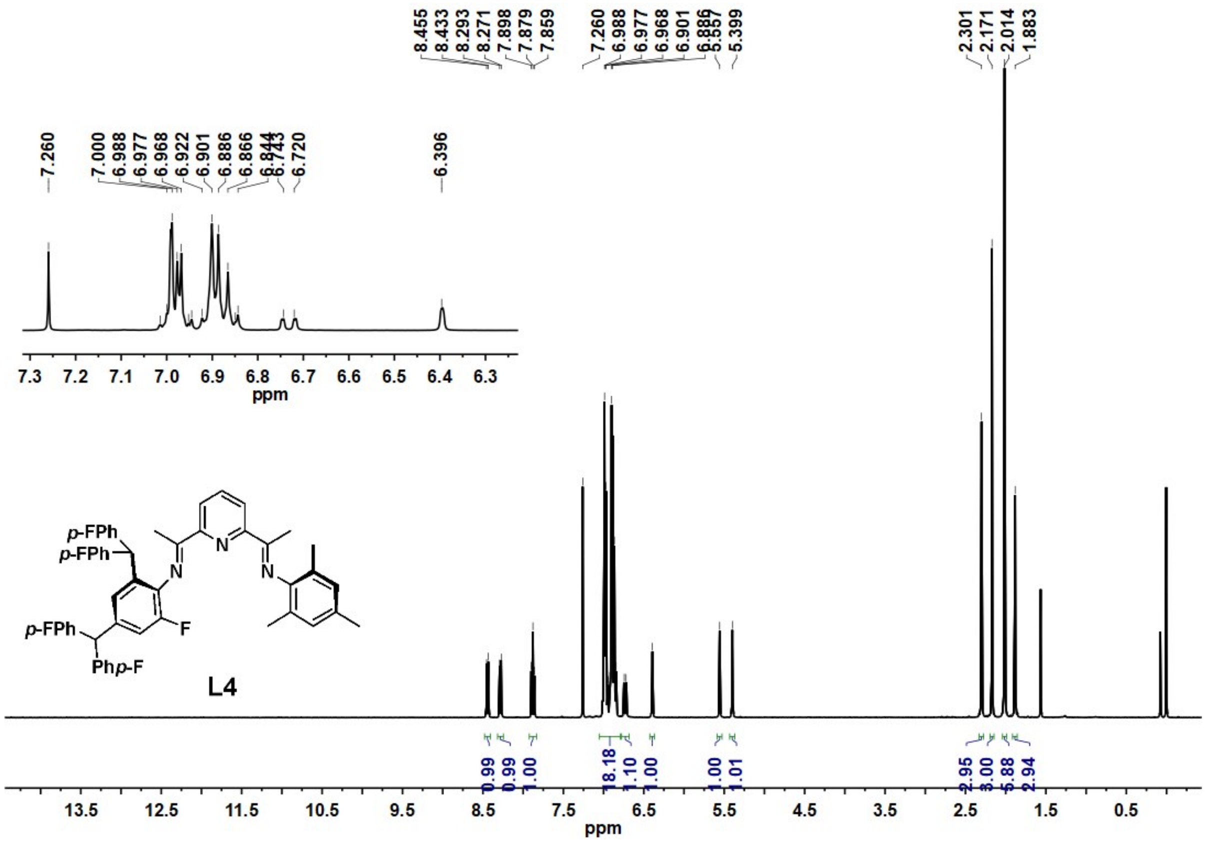


Figure S4 ^{1}H NMR spectrum of **L4** with an expansion of the δ 7.5 – 6.3 region; recorded in $CDCl_3$ at ambient temperature.

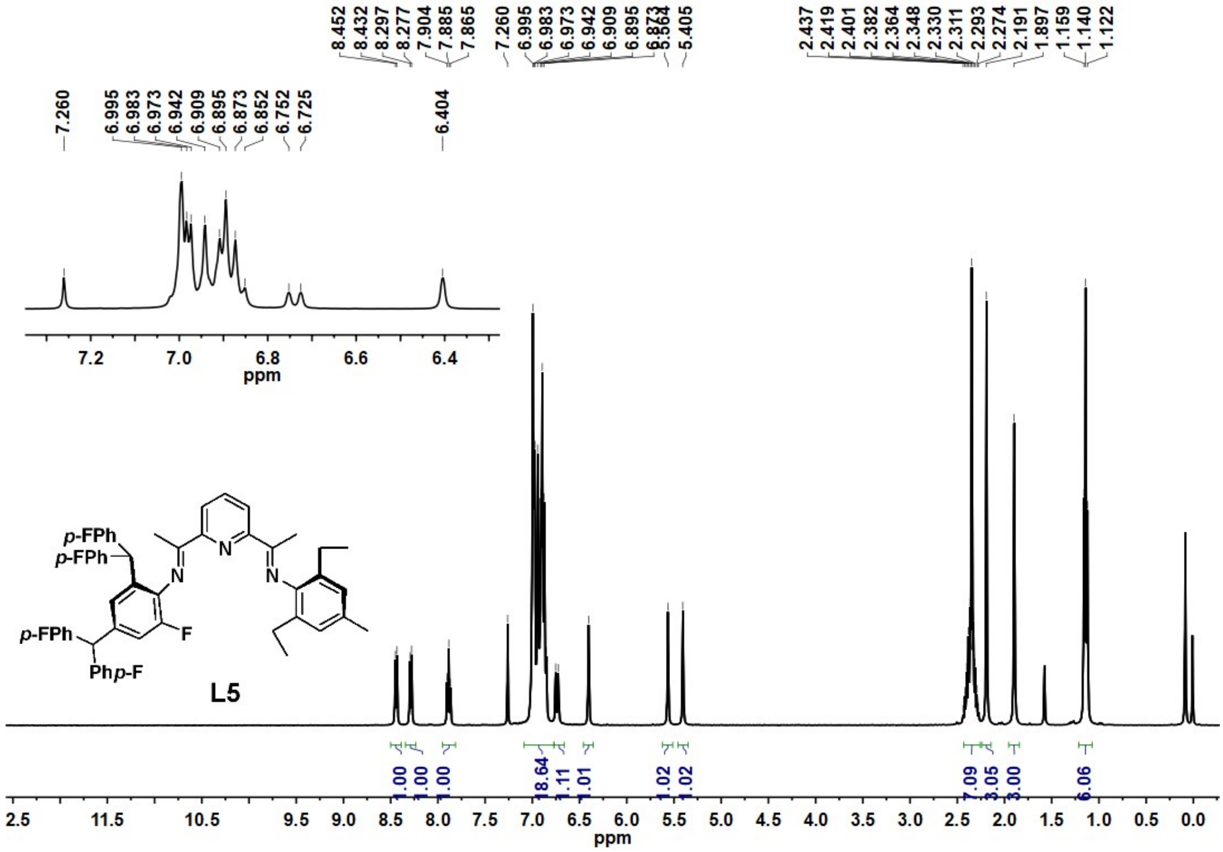


Figure S5 ^{1}H NMR spectrum of **L5** with an expansion of the δ 7.3 – 6.3 region; recorded in $CDCl_3$ at ambient temperature.

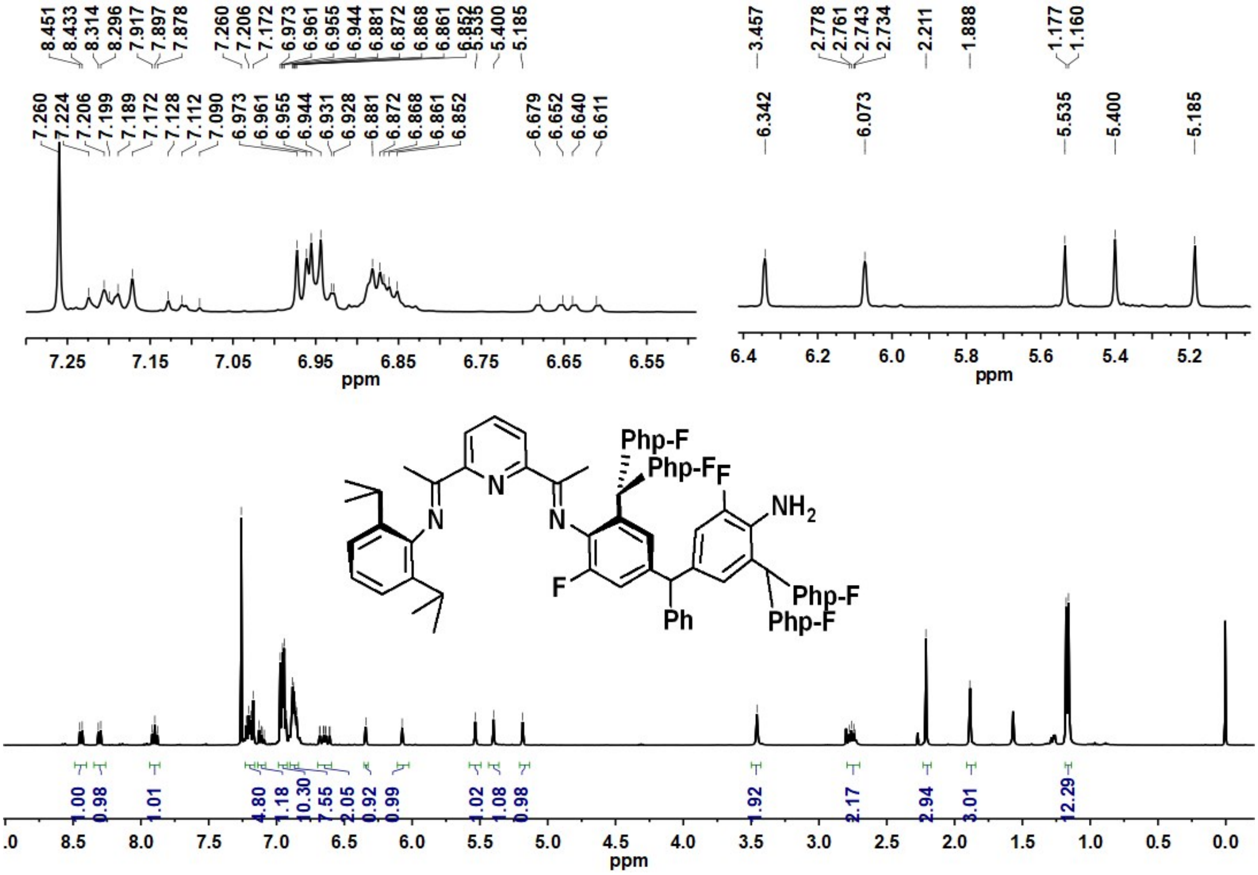


Figure S6 ^{1}H NMR spectrum of **L6** with expansions of the δ 7.3 – 6.5 and δ 6.4 – 5.1 regions; recorded in $CDCl_3$ at ambient temperature.

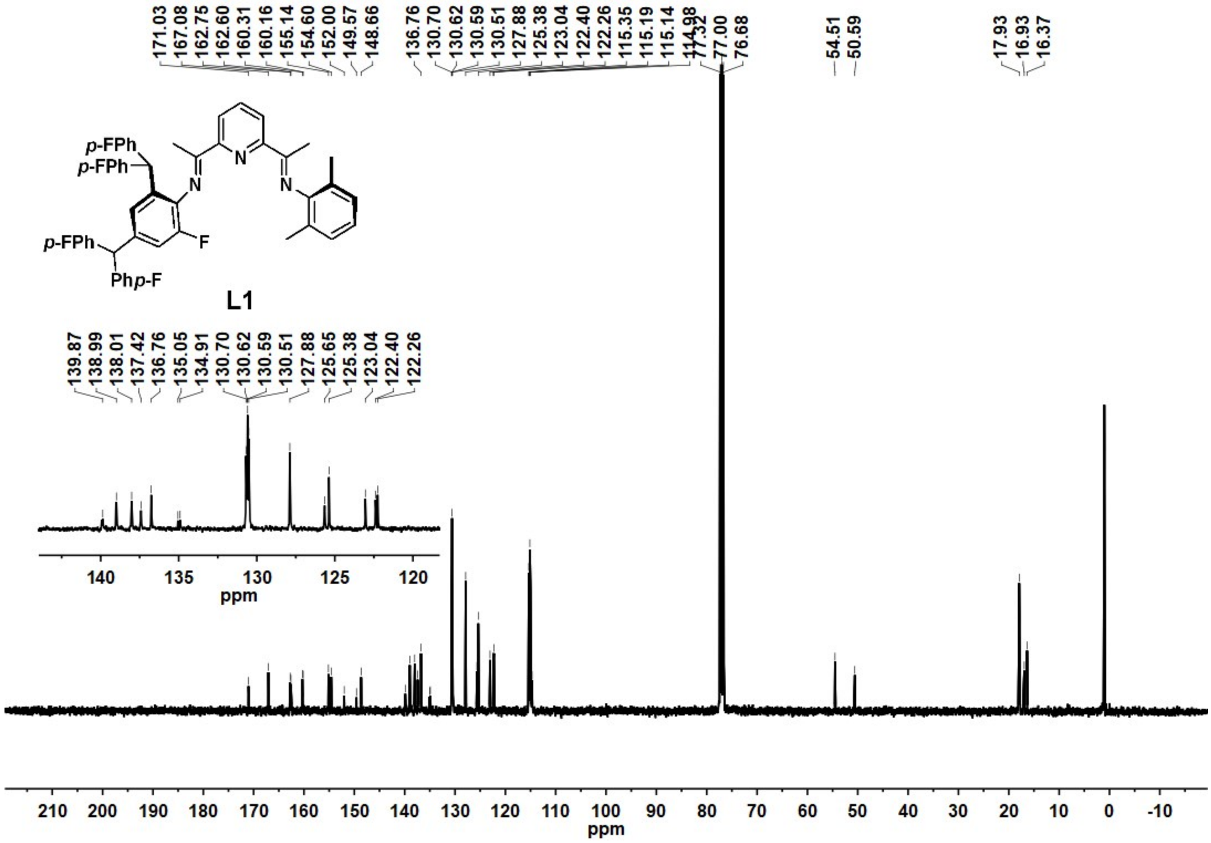


Figure S7 ^{13}C NMR spectrum of **L1**; recorded in $CDCl_3$ at ambient temperature.

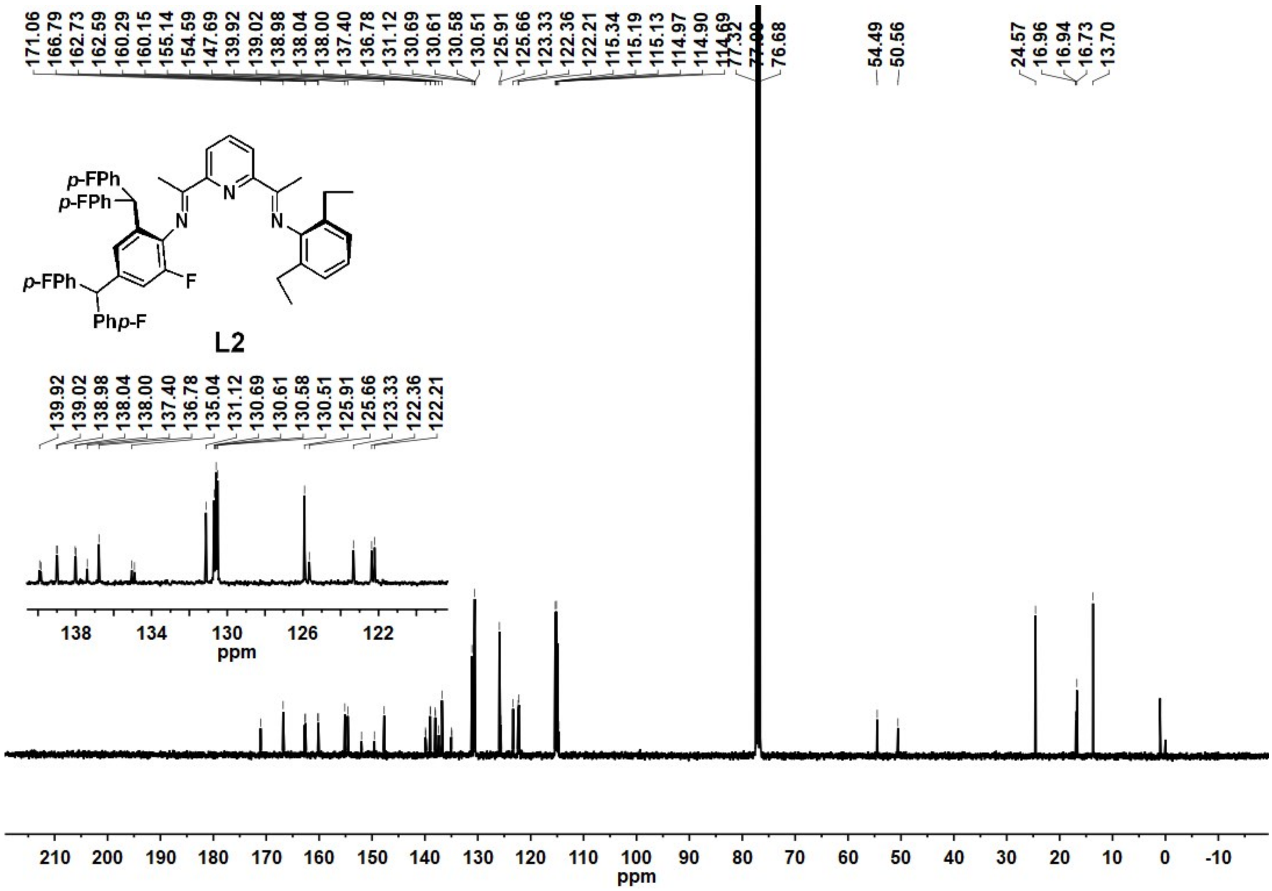


Figure S8 ^{13}C NMR spectrum of **L2**; recorded in $CDCl_3$ at ambient temperature.

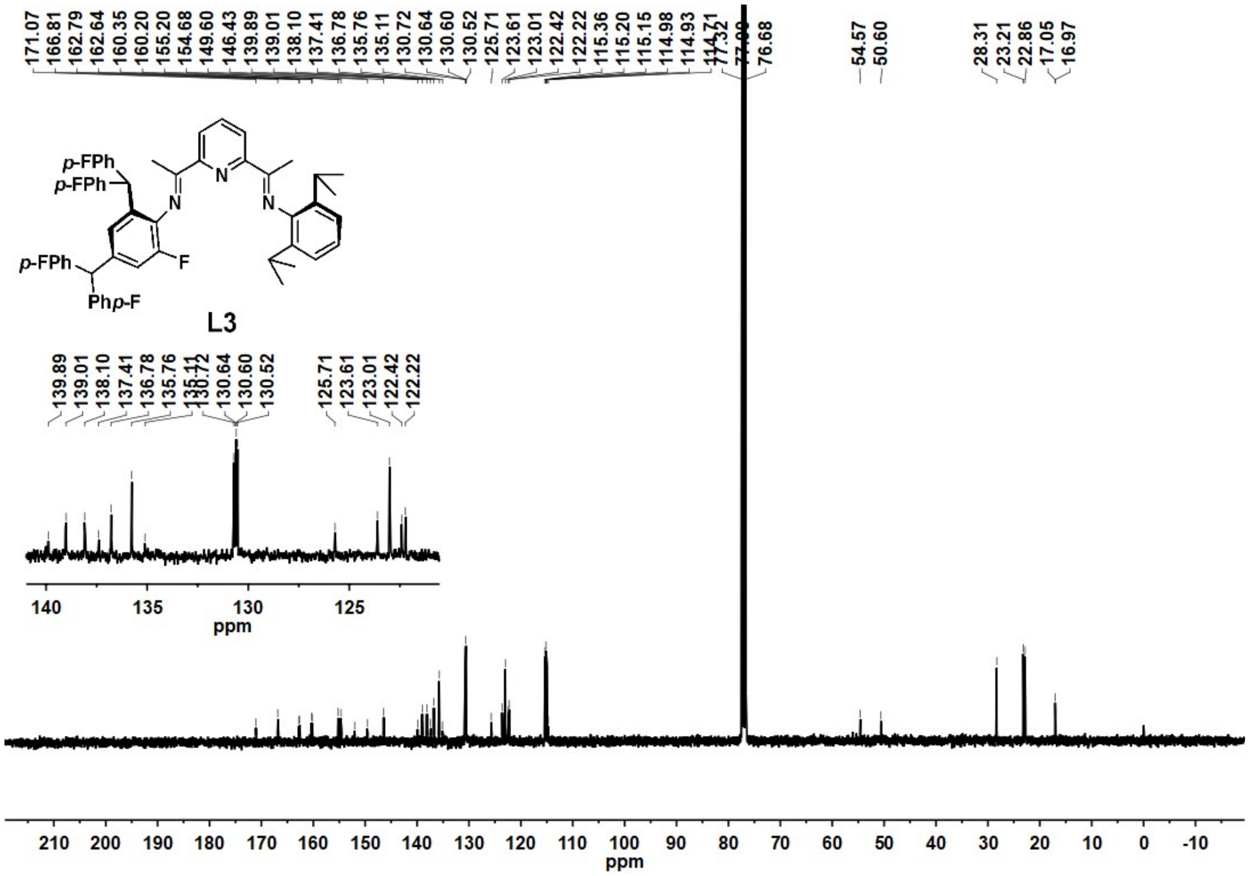


Figure S9 ^{13}C NMR spectrum of **L3**; recorded in $CDCl_3$ at ambient temperature.

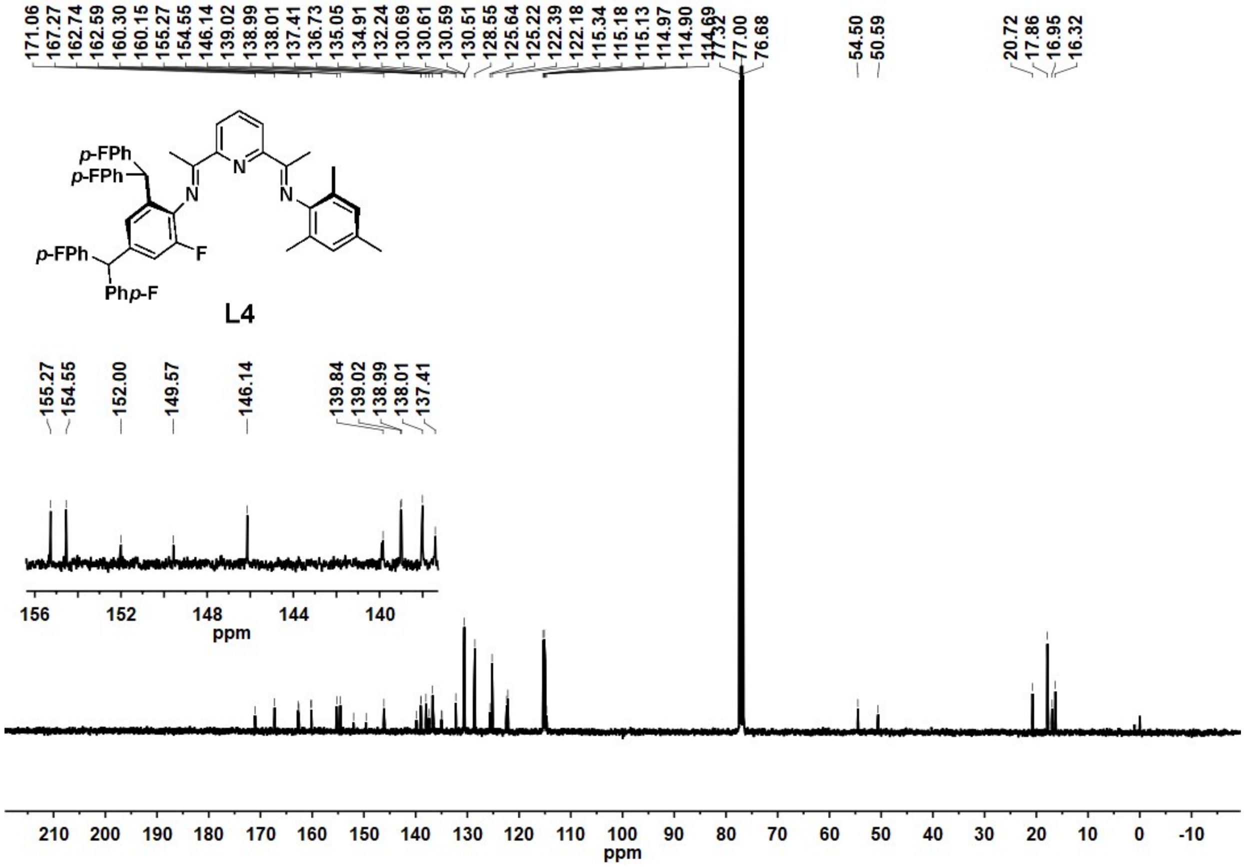


Figure S10 ^{13}C NMR spectrum of **L4**; recorded in $CDCl_3$ at ambient temperature.

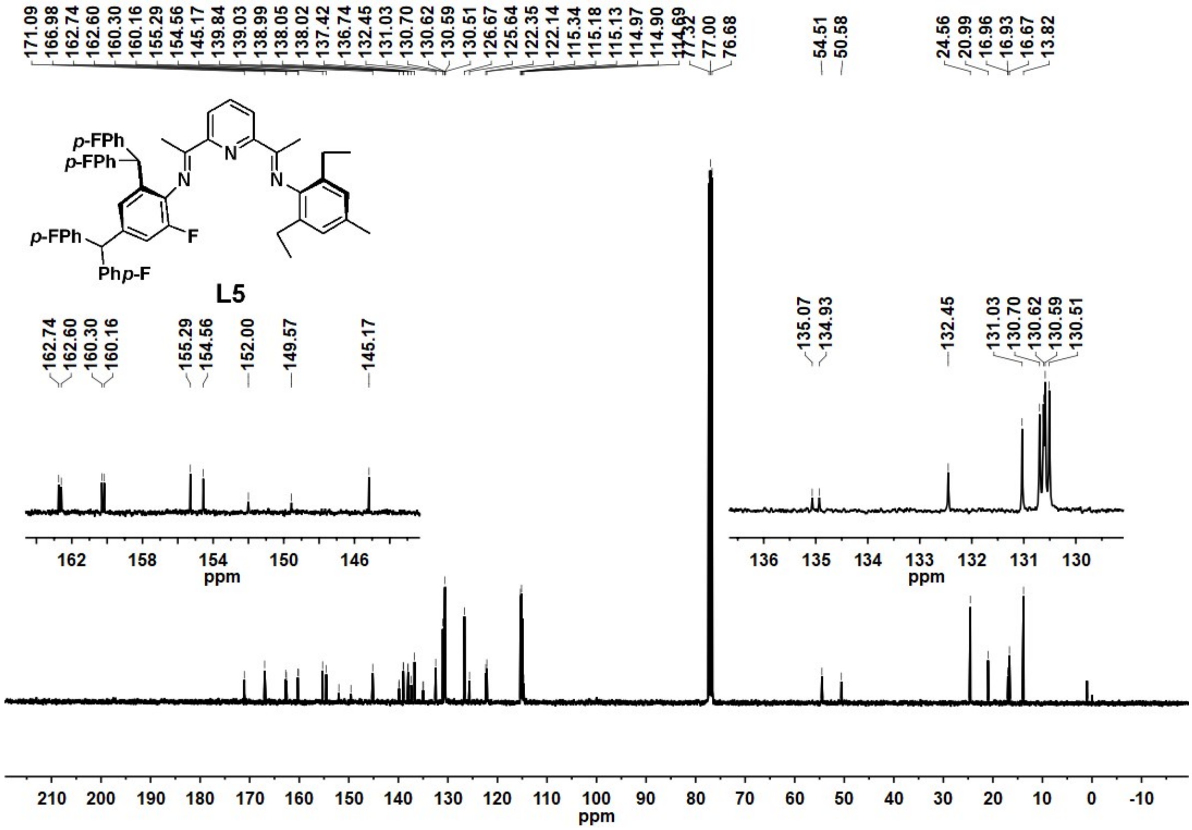


Figure S11 ^{13}C NMR spectrum of **L5**; recorded in $CDCl_3$ at ambient temperature.

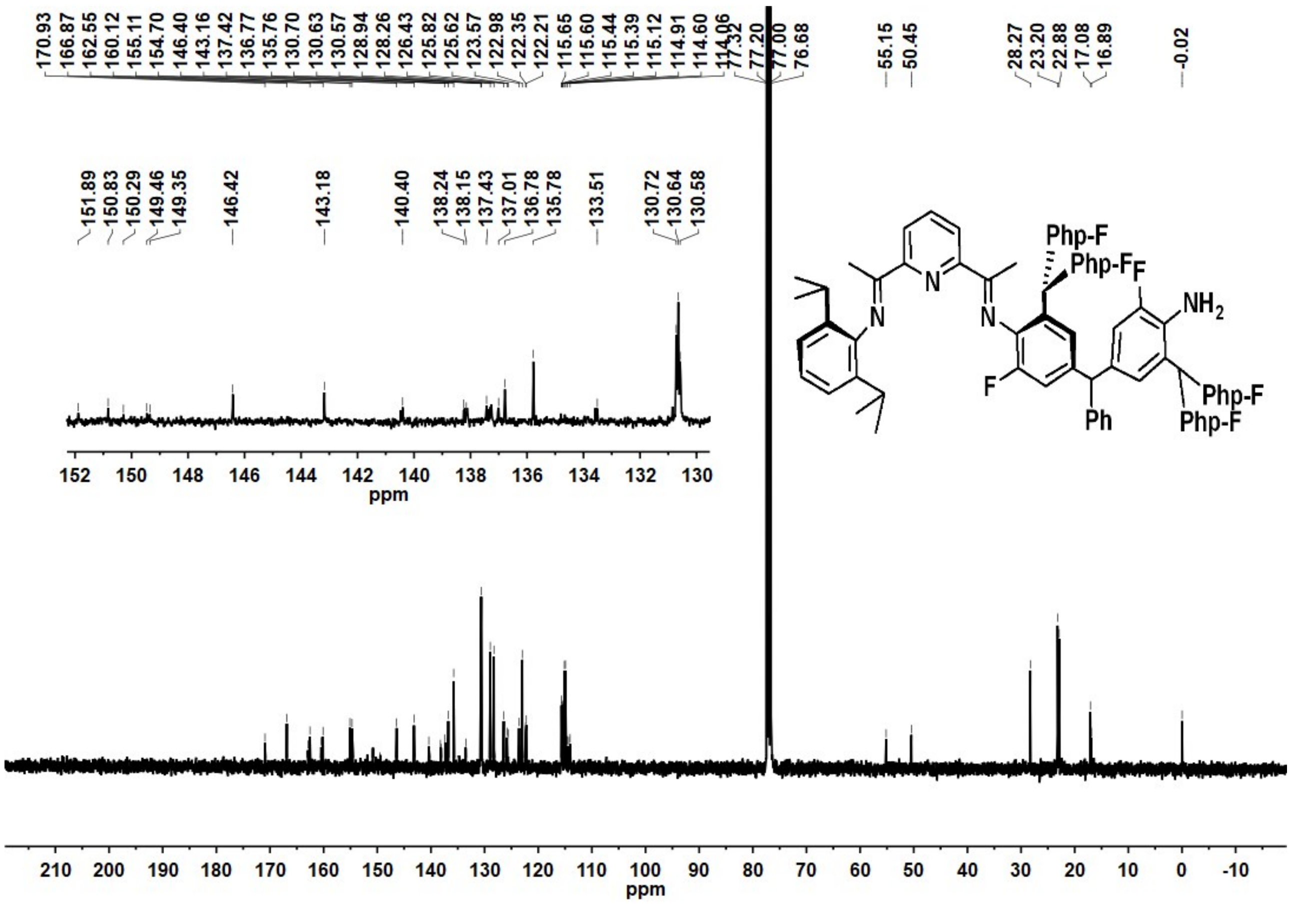


Figure S12 ^{13}C NMR spectrum of **L6**; recorded in $CDCl_3$ at ambient temperature.

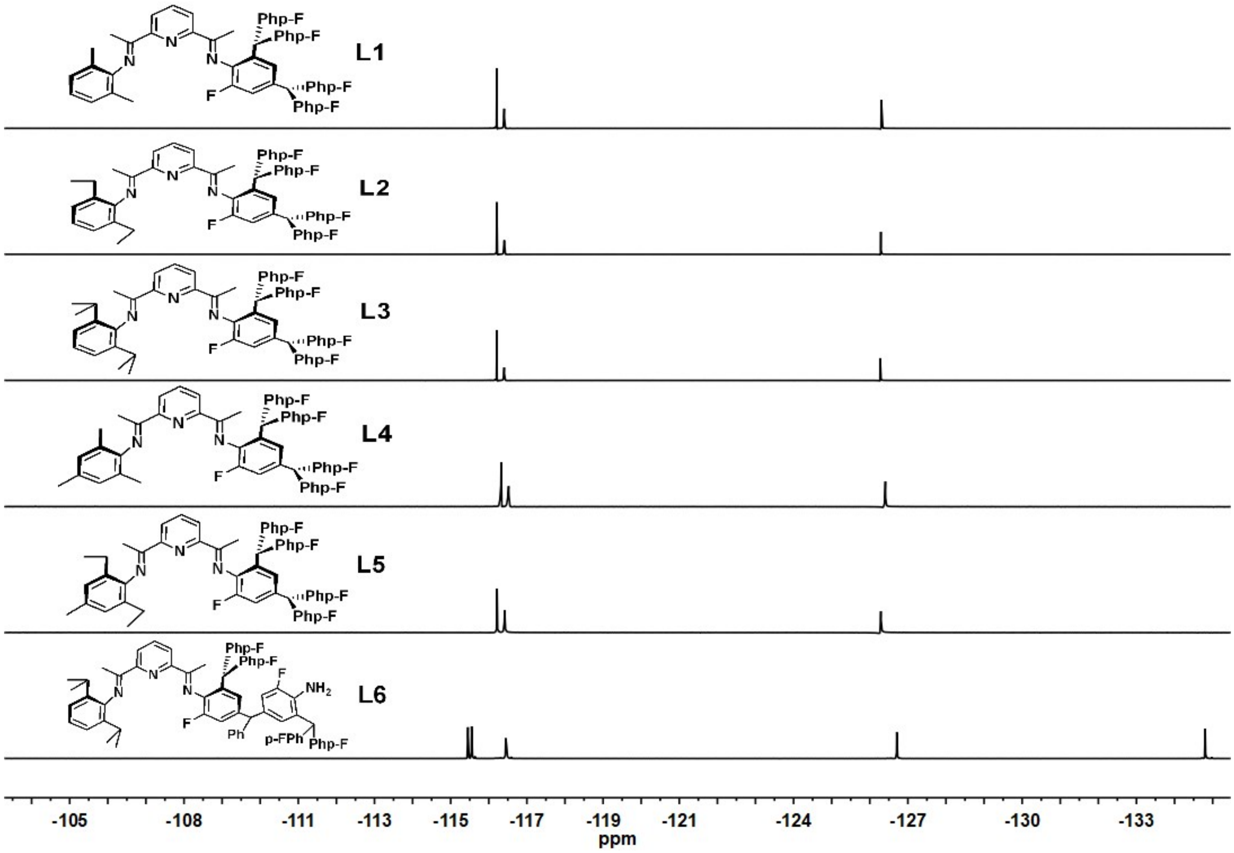


Figure S13 ^{19}F NMR spectra of **L1 – L6**; recorded in $CDCl_3$ at ambient temperature.

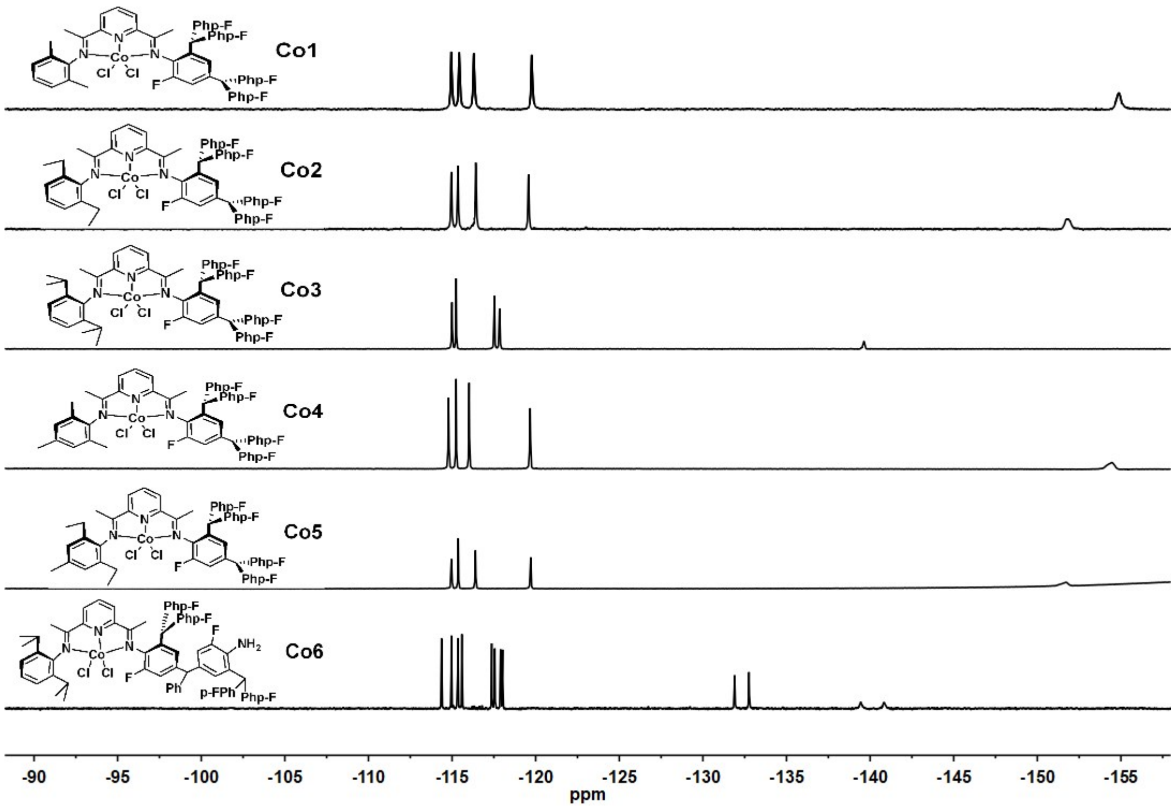


Figure S14 ^{19}F NMR spectra of **Co1 – Co6**; recorded in $CDCl_3$ at ambient temperature.

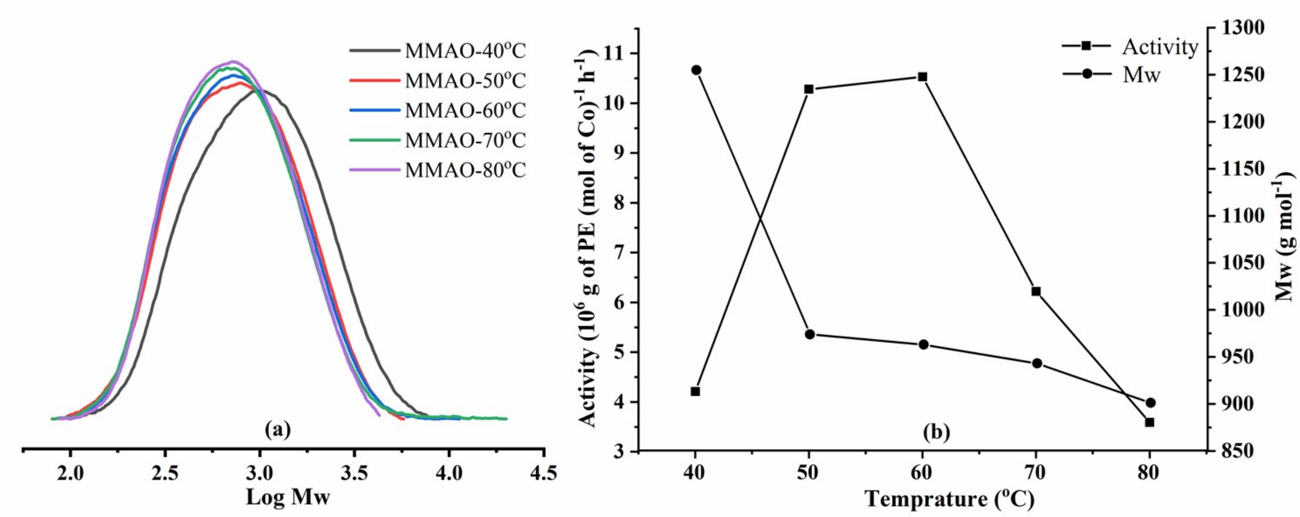


Figure S15 For **Co1**/MMAO (entries 1−5, Table 3): (a) GPC traces of the polyethylenes as a function of temperature; (b) plots of catalytic activity and polymer molecular weight *vs.* reaction temperature.

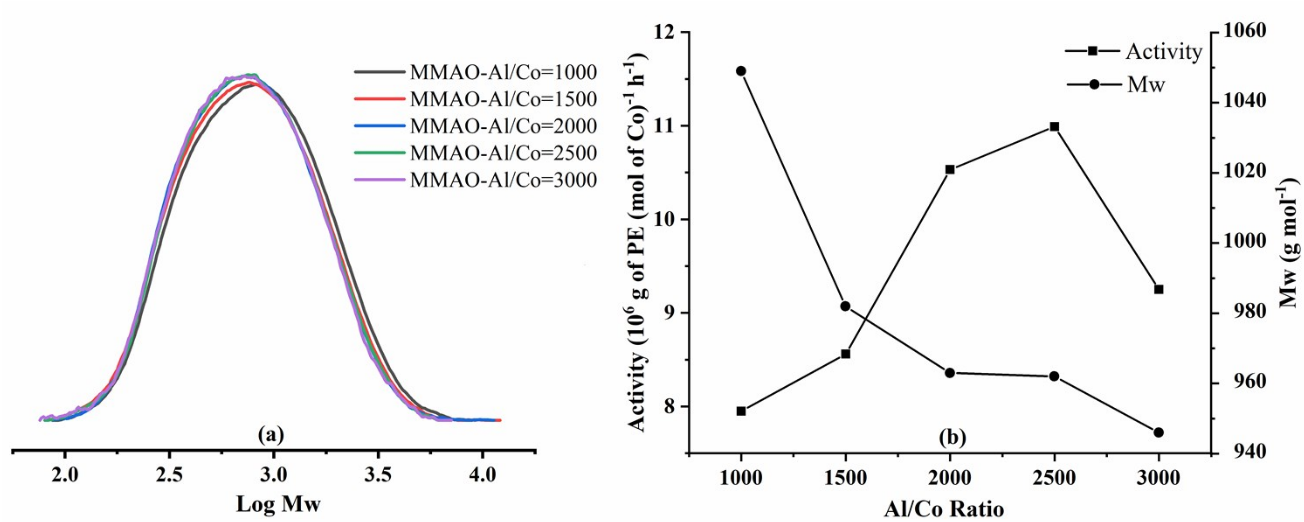


Figure S16 For **Co1**/MMAO (entries 3, 6–9, Table 3): (a) GPC traces of the polyethylenes as a function of Al:Co molar ratio; (b) plots of catalytic activity and polymer molecular weight *vs.* Al:Co molar ratio.

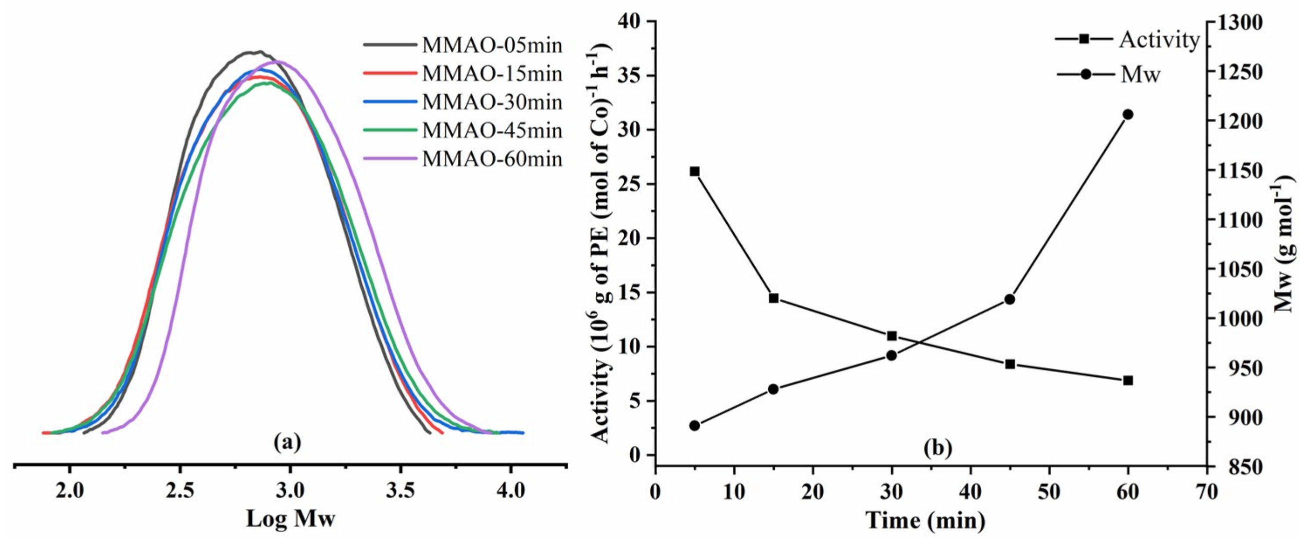


Figure S17 For **Co1**/MMAO (entries 8, 10–13, Table 3): (a) GPC traces of the polyethylenes as a function of run time (b) plots of catalytic activity and polymer molecular weight *vs*. run time.

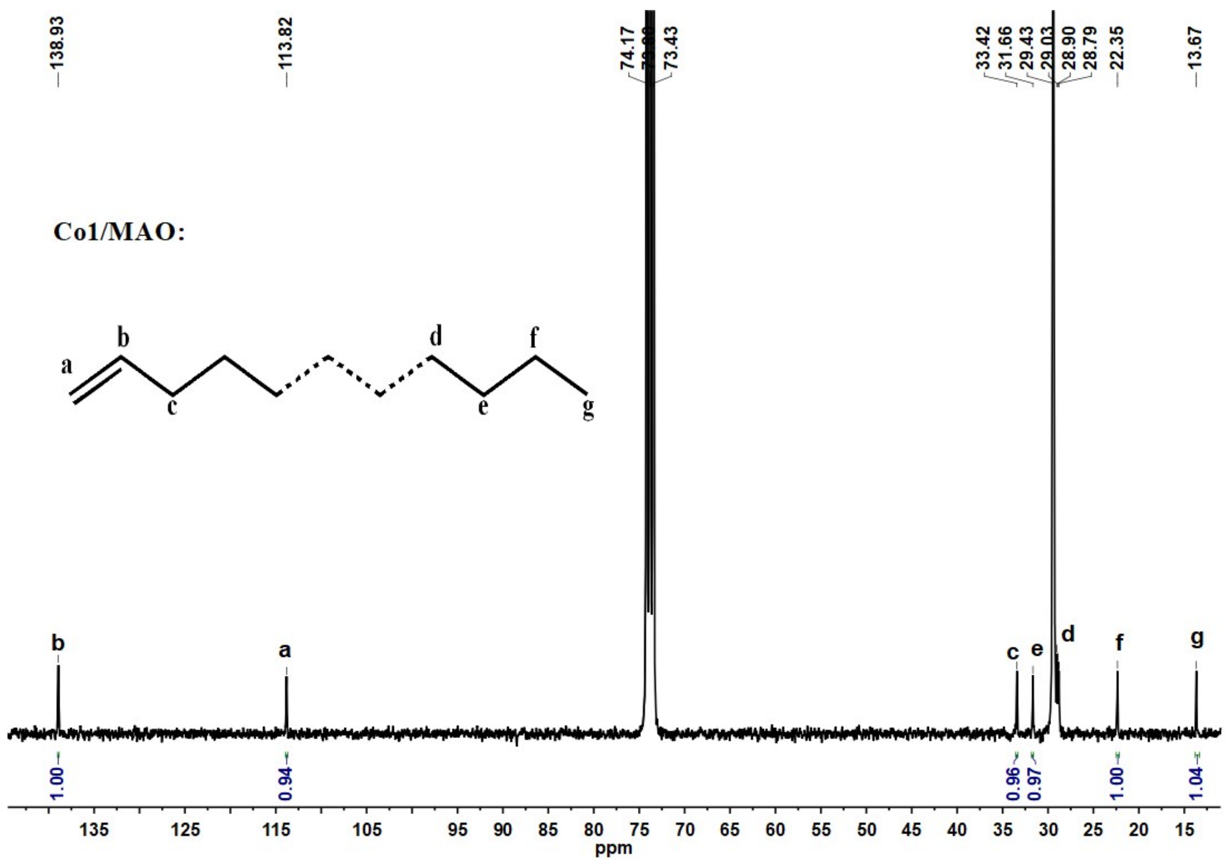


Figure S18. 1D sequence inverse-gated decoupled [13]C NMR spectrum of the polyethylene obtained using **Co1**/MAO at 70 °C **Co1**/MAO (entry 4, Table 2; δ C 73.8, tetrachloroethane-d_2)

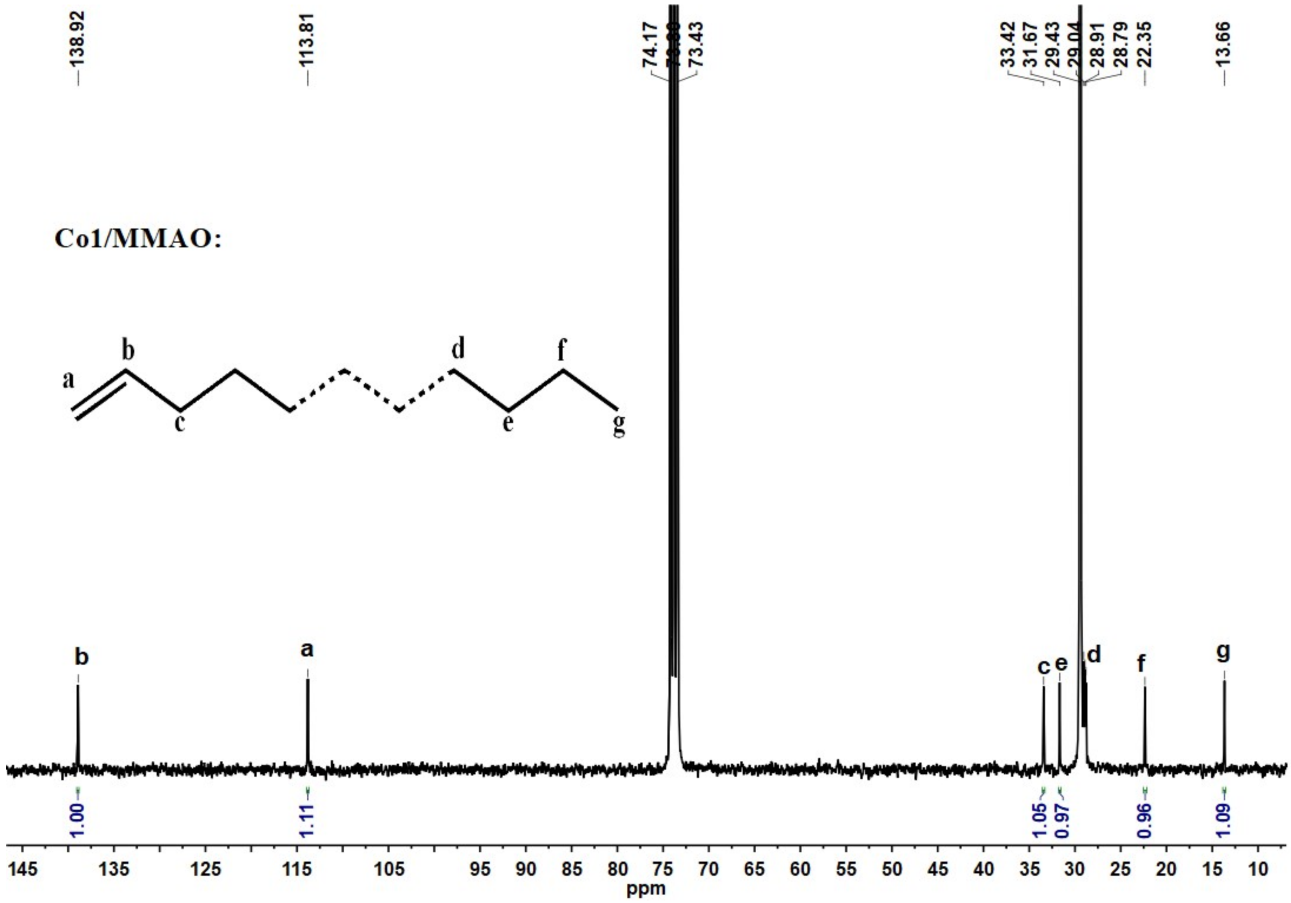


Figure S19. 1D sequence inverse-gated decoupled [13]C NMR spectrum of the polyethylene obtained using **Co1**/MAO at 70 °C **Co1**/MMAO (entry 8, Table 3; δ C 73.8, tetrachloroethane-d_2)

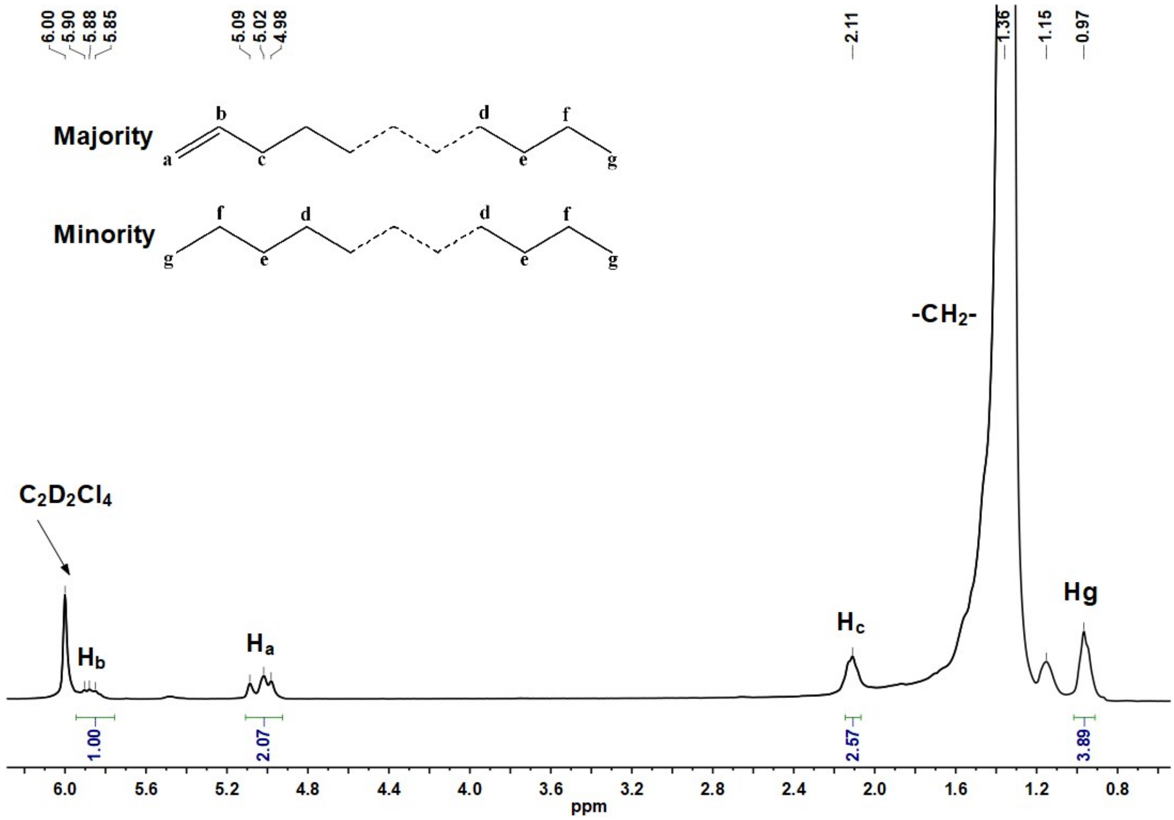


Figure S20. [1]H NMR spectrum of the polyethylene obtained using **Co6**/MAO at 70 °C; recorded in 1,1,2,2-tetrachloroethane-d_2 at 100 °C (entry 6, Table 4).

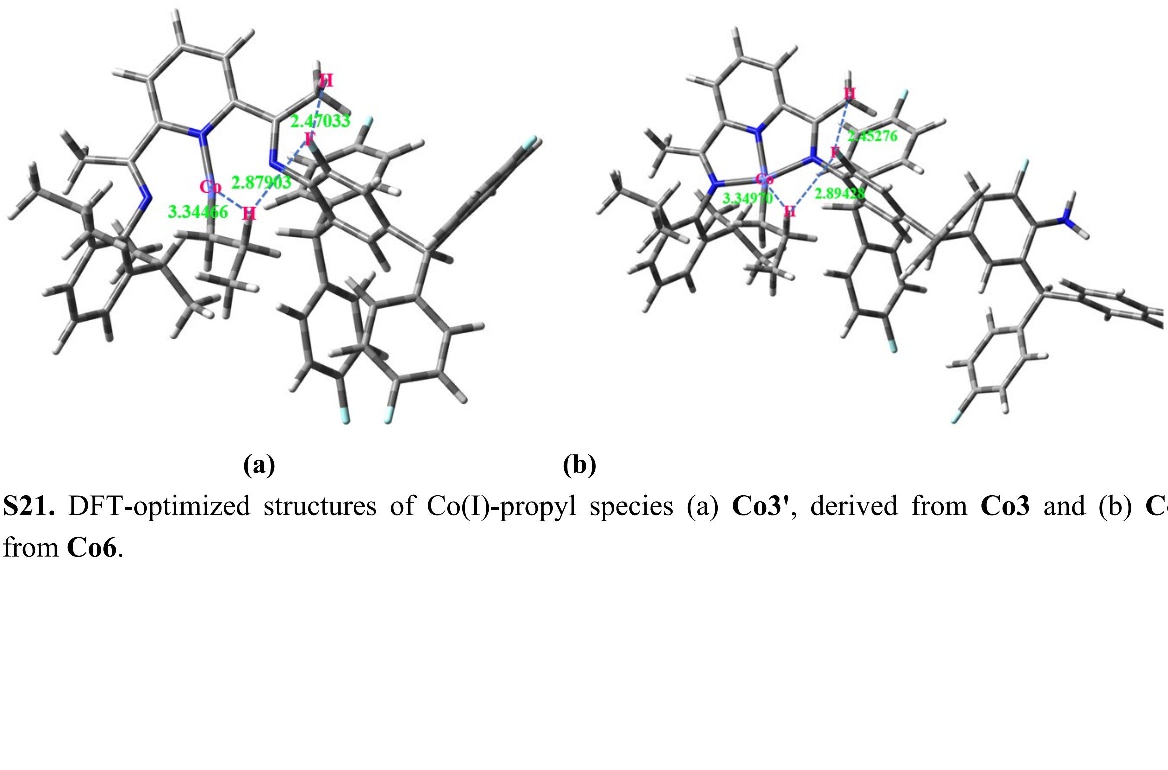


Figure S21. DFT-optimized structures of Co(I)-propyl species (a) **Co3'**, derived from **Co3** and (b) **Co6'**, derived from **Co6**.

Table 1 Crystal data and structure refinement for **Co1** and **Co5**.

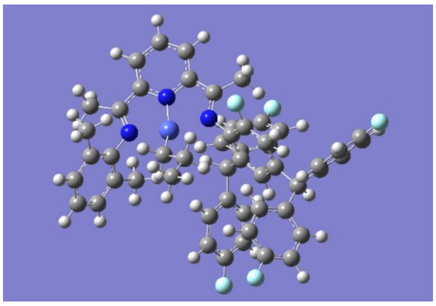
Identification code	**Co1**	**Co5**
CCDC Number	2023856	2023857
Empirical formula	$C_{49}H_{38}Cl_2CoF_5N_3$	$5(C_{52}H_{44}Cl_2CoF_5N_3)$
Formula weight	893.65	4678.65
Temperature/K	170.00(10)	169.99(14)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	11.8773(6)	20.2887(2)
b/Å	12.8721(5)	22.5854(2)
c/Å	14.5308(6)	30.0093(2)
α/°	97.115(3)	94.0520(10)
β/°	92.063(4)	105.3480(10)
γ/°	98.641(4)	102.8980(10)
Volume/Å^3	2176.04(17)	12802.4(2)
Z	2	2
ρ_{calc}g/cm^3	1.364	1.214
μ/mm^{-1}	0.576	4.030
F(000)	918.0	4830.0
Crystal size/mm^3	0.32 × 0.251 × 0.123	0.23 × 0.19 × 0.15
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.874 to 61.724	4.742 to 151.234
Index ranges	$-14 \le h \le 16$, $-17 \le k \le 18$, $-19 \le l \le 20$	$-22 \le h \le 25$, $-28 \le k \le 28$, $-37 \le l \le 36$
Reflections collected	35166	172540
Independent reflections	11961 [R_{int} = 0.0416, R_{sigma} = 0.0609]	50851 [R_{int} = 0.1038, R_{sigma} = 0.0791]
Data/restraints/parameters	11961/0/545	50851/59/2881
Goodness-of-fit on F^2	1.021	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0515, wR_2 = 0.1174	R_1 = 0.0759, wR_2 = 0.1702
Final R indexes [all data]	R_1 = 0.1013, wR_2 = 0.1438	R_1 = 0.1308, wR_2 = 0.2049
Largest diff. peak/hole / e Å^{-3}	0.57/-0.41	0.92/-0.50

Supporting information for the DFT optimization studies on Co1', Co3' and Co6'.

Computational details

All computations were carried out using density functional theory (DFT) making use of the Gaussian 09 program[1]. The DFT calculation was performed using B3LYP functional group[2], and the electrons in the inner layer of cobalt atom are described by equivalent potential fields in combination with the Stuttgart/Dresden (SDD) pseudopotential[3]. It is assumed that the cobalt center adopts a low spin state (S = 0), and the spin state of the entire structure is a singlet state. The basis set 6-31G* is used for the other atoms.

Optimized Structure of Co1'



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C	4.80896200	3.95019500	-2.00969400
C	5.48583000	2.73935000	-1.81505300
C	4.77326600	1.61133800	-1.41656500
N	3.41715800	1.67845400	-1.18280100
H	5.35083300	4.83510100	-2.32682000
H	2.88767500	4.92961800	-1.98675900
H	6.55640400	2.67494700	-1.98304900
C	5.26685400	0.26995500	-1.21470900
C	1.32955400	2.69013200	-1.17211000
C	6.74069100	-0.03253900	-1.26701100
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C	0.36843500	3.84610700	-1.19461900
H	-0.34476000	3.76837700	-0.36807700
H	0.89613000	4.79700500	-1.09422900
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N	0.98679300	1.43372300	-0.91054300
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C	-0.77756400	0.63457100	0.62596700
C	-2.68072400	0.91367500	-1.43051900
C	-2.11779000	0.28762700	0.82048300
C	-3.08259300	0.41710300	-0.18827000
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C	0.09092400	-1.92465500	2.30552300
C	-0.72376900	-1.43570800	4.92707700
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F	-0.97480800	1.69315700	-2.84998900
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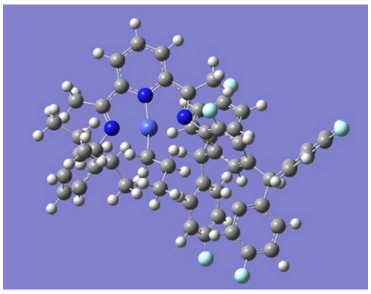
Optimized Structure of Co3'



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C	5.44060800	-4.14314400	0.27681200
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C	-6.22640100	-3.56098800	0.94761100
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F	-8.57672400	2.29250600	-3.63072200
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Co	2.18239000	0.31078300	-0.92277400
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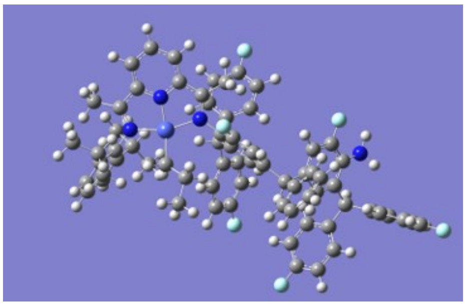
Optimized Structure of Co6'



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N	-6.50153000	-1.98485300	-2.25333700
H	-6.45342500	-2.96263500	-2.51781400
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H	1.44412800	1.91008900	4.27571400

References

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