Electronic Supplementary Information

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1 General Information

All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques or an MBraun UniLab Glovebox.

Chemicals and Solvents: Solvents were dried and degassed with an *MBraun SPS800* solvent-purification system. THF, diethyl ether were stored over molecular sieves (3 Å). *n*-hexane was stored over a potassium mirror. 1,2-Dimethoxyethane was stirred over K/benzophenone, distilled and stored over molecular sieves (3 Å). All chemicals were purchased from commercial suppliers and used as received, if not stated otherwise.

Cyclic Voltammetry: Cyclic voltammetry experiments were performed in a single-compartment cell inside a nitrogen-filled glovebox using a CH Instruments CH1600E potentiostat. The cell was equipped with a platinum disc working electrode (2 mm diameter) polished with 0.05 µm alumina paste, a platinum wire counter electrode and an $Ag/AgNO_3$ reference electrode. The supporting electrolyte, tetra-*n*-butylammonium hexafluorophosphate, was dried *in vacuo* at 110 °C for three days. All redox potentials are reported vs. the ferrocenium/ferrocene (Fc^+/Fc) couple.

Elemental Analyses: CHN analyses were recorded by the analytical department of the University of Regensburg with a Micro Vario Cube (Elementar).

ESI-MS: ESI mass spectra carried out by the analytical department of the University of Regensburg, *Agilent Q-TOF 6549 UHD*.

EPR spectroscopy: The experimental X-band EPR spectrum of **Int-A** was recorded on a Bruker EMX spectrometer (Bruker BioSpin Rheinstetten) equipped with a He temperature-control cryostat system (Oxford Instruments). The *g* values were calculated with the ORCA software package[1,2] at the B3LYP[3]/def2-TZVP[4] level of theory. The spectrum was analysed and simulated using the W95EPR program of Prof. Frank Neese.

NMR spectroscopy: ^{1}H, $^{13}C\{^{1}H\}$, $^{13}C\{^{1}H,^{31}P\}$, $^{11}B\{^{1}H\}$, ^{11}B, $^{31}P\{^{1}H\}$, and ^{31}P NMR spectra in solutions were recorded on *Bruker Avance 300* (300 MHz) and *Bruker Avance 400* (400 MHz) if not stated otherwise. These chemical shifts are given relative to solvents resonances on the tetramethylsilane scale. The following abbreviations have been used for multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets.

Melting point: Melting points were measured on samples in sealed capillaries on a Stuart SMP10 melting point apparatus.

UV/vis spectra: UV/vis spectra were recorded on an Ocean Optics Flame spectrometer (Varian Cary 50 spectrometer) in a Quartz cuvette with a layer thickness of 1 cm at room temperature with a concentration of 10^{-4} to 10^{-6} M.

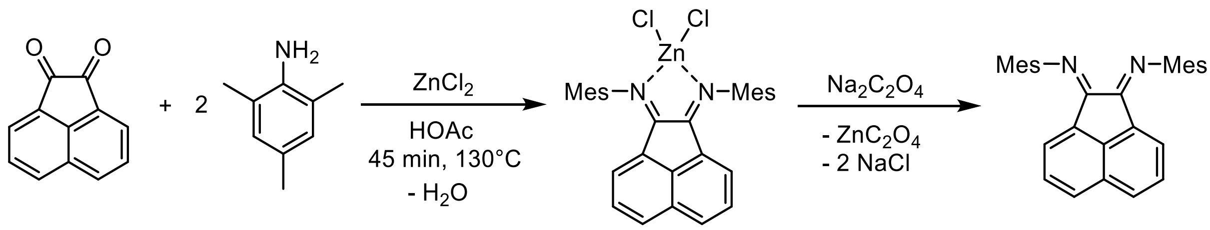
Single-crystal X-ray crystallography: The single crystal X-ray diffraction (XRD) data were recorded on an Agilent GV1000 with a Titan S2 CCD detector (for **2**) and an Agilent Super Nova diffractometer with an Atlas CCD detector (for **Int-A** and **3**). Microfocus Cu K_α radiation (λ = 1.54184 Å) was used in each measurement. Empirical multi-scan[5] and analytical absorption corrections[6] were applied to the data. The structures were solved with SHELXT[7] and least-square refinements on F^2 were carried out with SHELXL[8].

CCDC 1943845 (**2**), 1943847 (**Int-A**), 1943848 (**3**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre (https://www.ccdc.cam.ac.uk/).

2 Synthesis of Starting Materials

Synthesis of Bis[*N*,*N'*-(2,4,6-trimethylphenyl)imino]acenaphthene (^{Mes}BIAN)

^{Mes}BIAN was synthesised according to a procedure of *Gasperini* and co-workers.[9]



Acenaphthenquinone (5.5 g, 30.0 mmol, 1.0 equiv.) and zinc(II) chloride (10.95 g, 80.3 mmol, 2.7 equiv.) were mixed in 85 mL acetonitrile and stirred for 10 minutes at 60 °C before 2,4,6-trimethylaniline (9.7 mL, 69.2 mmol, 2.3 equiv.) was added to the yellow suspension. The reaction mixture immediately turned orange and was heated to reflux for 45 min. The formed solid was filtered hot and washed with diethyl ether (3 x 50 mL). [(^{Mes}BIAN)$ZnCl_2$] was dried *in vacuo* and dissolved in 500 mL dichloromethane in a separating funnel. After addition of 150 mL saturated sodium oxalate solution, the mixture was shaken for five minutes until white zinc(II) oxalate was formed.

The organic phase was separated and dried over magnesium sulfate. After filtration, the solvent was evaporated and ^{Mes}BIAN was obtained as orange powder (9.1 g, 72.9%).

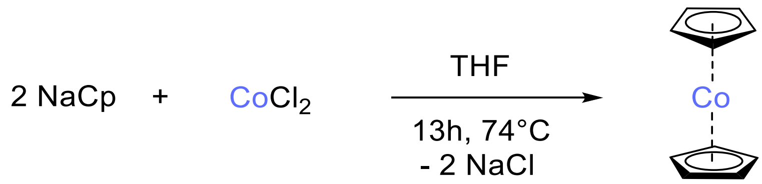
Yield: 9.1 g (21.8 mmol, 73%)

Chemical formula: $C_{30}H_{28}N_2$ (MW = 416.57 g mol^{-1})

^{1}H NMR (300.13 MHz, 300 K, $CDCl_3$) δ[ppm]: 7.89 (d, *J* = 8.2 Hz, 2H, CH_{BIAN}), 7.36 (dd, *J* = 8.2 Hz, 7.2 Hz, 2H, CH_{BIAN}), 6.97 (s, 4H, CH_{Ar}), 6.77 (d, *J* = 7.2 Hz, 2H, CH_{BIAN}), 2.38 (s, 6H, *p*-CH_3), 2.38 (s, 12H, *o*-CH_3)

Synthesis of Cobaltocene

Cobaltocene was synthesised according to a procedure of *King* and co-workers.[10]



Cobalt(II) chloride (3.0 g, 23.1 mmol, 1 equiv.) was dissolved in 70 mL THF and added dropwise to a solution of sodium cyclopentadienide (4.8 g, 46.2 mmol, 2 equiv.) in 50 mL THF. The resulting mixture was stirred at reflux for 13 h. After cooling to room temperature, the solvent was evaporated and the residue dried *in vacuo*. Sublimation (120 °C, 10^{-3} mbar) afforded cobaltocene as purple crystals.

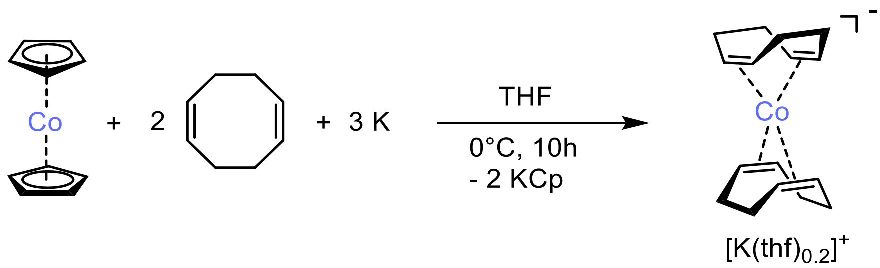
Yield: 1.83 g (9.7 mmol, 42%)

Chemical formula: $C_{10}H_{10}Co$ (M = 189.12 g mol^{-1})

^{1}H NMR (300.13 MHz, 300 K, C_6D_6) δ[ppm]: -51.74 (s, 10H, Cp)

Synthesis of potassium bis(1,5-cyclooctadiene)cobaltate

[K(thf)$_{0.2}${Co(η^4-cod)$_2$}] was synthesised according to *Jonas* and co-workers.[11]



Cobaltocene (9.0 g, 47.8 mmol, 1.0 equiv.) and distilled 1,5-cyclooctadiene (17.7 mL, 144 mmol, 3.0 equiv.) were transferred to elemental potassium (7.5 g, 191.8 mmol, 4.0 equiv.) at 0 °C. The reaction mixture was stirred at 0 °C for 10 h with exclusion of light. The reaction mixture turned yellow-brown while stirring. The mixture was stored at -80 °C overnight. Subsequently, the suspension was filtered at -80 °C, the filtrate was concentrated and layered with diethyl ether. Dark yellow crystals were isolated after four days at -30 °C and dried *in vacuo* (7.5 g, 48.0%). The isolated compound may contain a variable amount of THF. This sample contained 0.2 THF molecules per formula unit based on elemental analysis.

Yield: 7.5 g (22.8 mmol, 48%)

Chemical formula: $C_6H_{18}BN$ (M = 115.03 g mol^{-1})

^{1}H NMR (300.13 MHz, 300 K, THF-d_8) δ[ppm]: 2.20 (s, 16H, cod-CH_2), 1.88 (s, 8H, cod-CH); elemental analysis calcd. for $C_{16}H_{24}Co\cdot(C_4H_8O)_{0.2}$ (328.82): C: 61.37 H: 7.85; found: C 61.44 H 7.77

Synthesis of potassium graphite (KC_8)

$$K + 8\,C_{Graphit} \xrightarrow[3\text{ h, }130\text{ °C}]{\textit{in vacuo}} KC_8$$

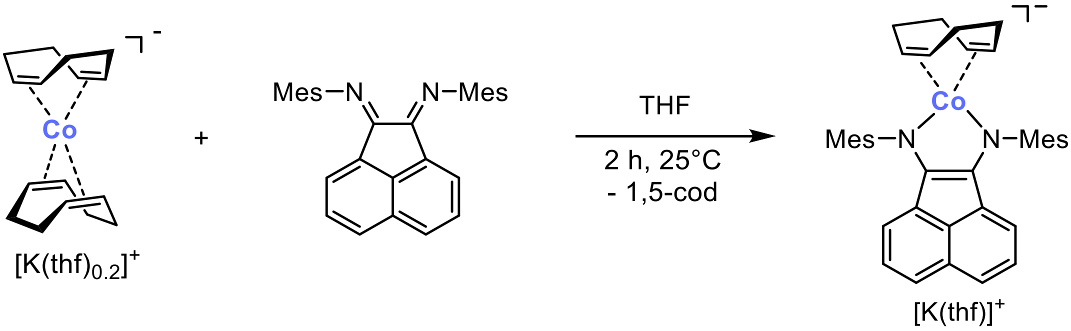
Freshly cut potassium chunks (6.55 g, 168 mmol, 1.0 equiv.) and graphite (16.1 g, 1.34 mol, 8.0 equiv.) were mixed as solids and heated for three hours at 130 °C *in vacuo*. Potassium graphite was formed as gold-brown powder in quantitative yield and used without further analytics.

Yield: 22.5 g (166.5 mmol, >99%)

Chemical formula: KC_8 (M = 135.18 g mol^{-1})

Synthesis of [K(thf){(^{Mes}BIAN)Co(η^4-cod)}] (1)

[K(thf){(^{Mes}BIAN)Co(η^4-cod)}] (**1**) was synthesised by a procedure of *Wolf* and co-workers.[12,13]



1

A solution of ^{Mes}BIAN (1.15 g, 2.8 mmol, 1.0 equiv.) in 200 mL THF was added to a solution of [$K(thf)_{0.2}Co(\eta^4\text{-cod})_2$] (0.9 g, 2.8 mmol, 1.0 equiv.) in 100 mL THF. An immediate colour change to dark green was observed. After stirring the reaction mixture for two hours, the solvent was removed and the residue was washed with 100 mL *n*-hexane. The crude product was dissolved in 40 mL THF and filtered. The filtrate was concentrated and layered with *n*-hexane. Dark green crystals were isolated after storage at room temperature upon storing for one week (0.85 g, 43%). The crystals still contained 0.1 equiv. of *n*-hexane after drying the crystalline solid *in vacuo* according to ^{1}H NMR spectroscopy.

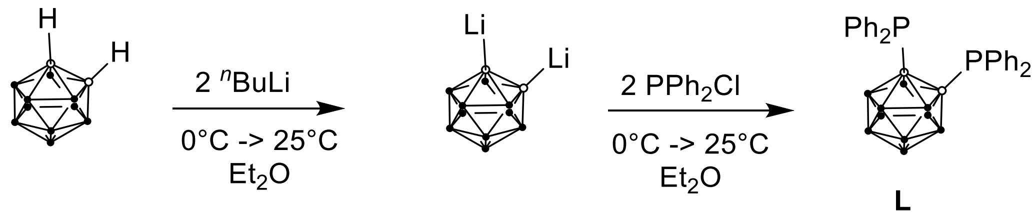
Yield: 0.85 g (1.2 mmol, 43%)

Chemical formula: $C_{38}H_{40}N_2CoK$ (C_4H_8O) $(C_6H_{14})_{0.1}$ (M = 703.51 g mol^{-1})

^{1}H NMR (300.13 MHz, 300 K, THF-d_8) δ[ppm]: 6.08 (m, 4H, CH_{Ar}), 6.28 (m, 2H, CH_{BIAN}), 6.37 (m, 4H, CH_{BIAN}), 5.21 (m, 2H, CH_{BIAN}), 2.65 (m, 4H, cod-CH), 2.45 (m, 12H, *o*-CH_3), 2.33 (m, 4H, cod-CH_2), 2.25 (m, 6H, *p*-CH_3), 1.02 (m, 4H, cod-CH_2)

Synthesis of 1,2-bis(diphenylphosphino)-*ortho*-carborane (L)

1,2-bis(diphenylphosphino)-*ortho*-carborane (**L**) was synthesised by an adapted procedure of *Schröder* and co-workers.[14]



o-Carborane (2.54 g, 17.6 mmol, 1.0 equiv.) was dissolved in 100 mL Et_2O and cooled to O °C. *n*-BuLi (15.0 mL, 37.5 mmol, 2.1 equiv., 2.5 M in *n*-hexane) was added dropwise within 5 minutes. A colourless precipitate was formed, and the solution was stirred at 0 °C for 30 min and 2 h at room temperature. Freshly distilled PPh_2Cl (6.8 mL, 37.5 mmol, 2.1 equiv.) in 10 mL Et_2O was added dropwise again at 0 °C. The resulting reaction mixture was stirred overnight and the bright yellow solution was filtered over a pad of silica. The solvent was removed from the clear filtrate and the raw material recrystallised from high-boiling petroleum ether (b.p. 130 °C). 1,2-bis(diphenylphosphino)-*ortho*-carborane (**L**) was obtained as white crystalline solid.

Yield: 1.103 g (2.15 mmol, 12.2%)

Chemical formula: $C_{26}H_{30}P_2B_{10}$ (M = 512.57 g mol^{-1})

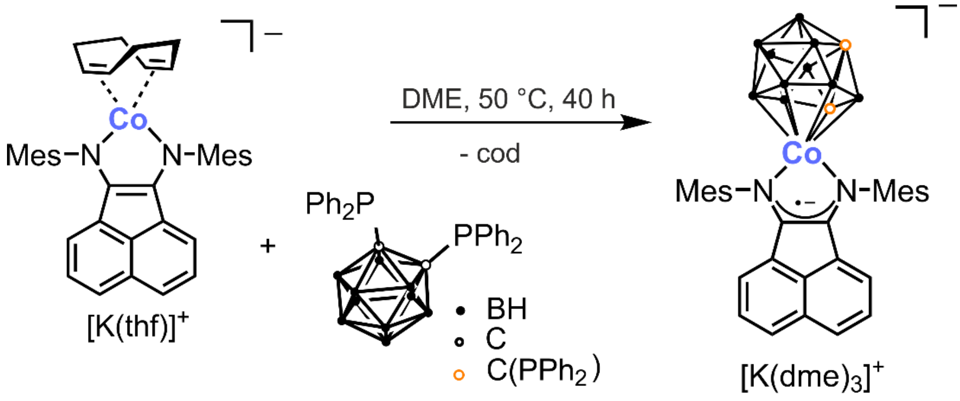
^{1}H NMR (400.13 MHz, 300 K, THF-d_8) δ[ppm]: 7.90 (m, 8H, CH_{Ar}), 7.46 (m, 10H, CH_{Ar}), 2.17 (br s, 10H, $B_{10}H_{10}$)

^{11}B{^{1}H} NMR (128.4 MHz, 300 K, THF-d_8) δ[ppm]: 1.16 (br s), -5.72 (br s), -8.12 (br s), -10.33 (br s)

^{31}P{^{1}H} NMR (162 MHz, 300 K, THF-d_8) δ[ppm]: 10.1 ppm

3 Synthesis and Characterisation of 2

3.1 Synthesis



1 **L** **2** (59%)

[K(thf){(^{Mes}BIAN)Co(η^4-cod)}] (274 mg, 0.39 mmol, 1.0 equiv.) (**1**) was dissolved in 10 mL THF and added dropwise to a solution of 1,2-bis(diphenylphosphino)-*ortho*-carborane (200 mg, 0.39 mmol, 1.0 equiv.) (**L**) in 10 mL THF. The solution immediately turned red-orange and was stirred for 40 h at 50 °C. During that time the colour of the reaction mixture became dark violet. After the reaction the solvent was removed and the residue dissolved in 15 mL DME. The solution was filtered, and the solid residue washed with 3 mL DME. The filtrate was layered with 30 mL *n*-hexane and stored at -35 °C. Dark violet microcrystals were obtained upon storing for one week and isolated by decanting the mother liquor. The crystals still contained three molecules of DME after drying the powder *in vacuo* according to ^{1}H NMR spectroscopy. Analytically pure, crystalline samples of **2**, suitable for single-crystal X-ray crystallography were obtained by diffusion of *n*-hexane into a concentrated DME solution.

Yield: 286 mg (0.23 mmol, 59%)

Chemical formula: $C_{56}H_{70}KCoN_2P_2B_{10}\cdot(C_4H_8O_2)_3$ (M = 1244.5 g mol^{-1})

^{1}H NMR (400.13 MHz, 300 K, THF-d$_8$) δ[ppm]: 7.90 (m, 2H, $CH_{Ar(Phosphine)}$) 7.69 (m, 2H, $CH_{Ar(Phosphine)}$), 7.50 (m, 4H, $CH_{Ar(Phosphine)}$), 7.10 (m, 4H, $CH_{Ar(Phosphine)}$), 7.10 (m, 2H, CH_{BIAN}), 7.05 (m, 8H, $CH_{Ar(Phosphine)}$), 6.83 (m, 2H, $CH_{Ar(BIAN)}$), 6.80 (s, 1H, $CH_{Ar(Mes)}$), 6.75 (s, 1H, $CH_{Ar(Mes)}$),6.71 (s, 1H, $CH_{Ar(Mes)}$), 6.65 (s, 1H, $CH_{Ar(Mes)}$), 5.73 (d, J = 7.2 Hz), 1H, CH_{BIAN}), 5.64 (d, J = 7.2 Hz, 1H, CH_{BIAN}), 3.43 (DME, CH_2), 3.27 (DME, CH_3) 2.40 (two overlapping singlets, 6H, *o*-CH_3), 2.32 (s, 3H, *p*-CH_3), 2.19 (s, 3H, *p*-CH_3), 1.90 (s, 3H, *o*-CH_3), 1.88 (s, 3H, *o*-CH_3)

^{11}B NMR (128.4 MHz, 300 K, THF-d$_8$) δ[ppm]: 13.3 (br s), 0.4 (br s), -9.6 (br d), -20.9 (br d)

^{11}B{^{1}H} NMR (128.4 MHz, 300 K, THF-d$_8$) δ[ppm]: 13.3 (br s), 0.4 (br s), -9.6 (br s), -20.9 (br s)

$^{13}C\{^1H\}$ NMR (100.6 MHz, 300 K, THF-d_8) δ[ppm]: 153.5, 152.0, 151.4, 145.1 (d, J_{CP} = 21.3 Hz), 143.9 (d, J_{CP} = 21.0 Hz), 139.8 (d, J_{CP} = 25.3 Hz), 137.8 (dd, J_{CP} = 7.0 Hz, 7.8 Hz), 136.5 (d, J_{CP} = 5.5 Hz), 136.4 (d, J_{CP} = 5.8 Hz), 135.8 (dd, J_{CP} = 3.8 Hz, 25.3 Hz), 135.0(d, J_{CP} = 22.6 Hz), 134.4, 134.2, 133.8, 133.6, 132.8, 132.3, 131.6, 130.8 (d, J_{CP} = 2.6 Hz), 130.5 (d, J_{CP} = 2.5 Hz), 129.1, 128.9, 128.7, 128.4, 128.3, 128.1, 128.0, 127.9 (d, J_{CP} = 8.0 Hz), 127.6, 127.4 (d, J_{CP} = 3.2 Hz), 127.3(d, J_{CP} = 2.6 Hz), 124.2, 124.0, 118.2, 118.0, 72.5 (DME), 58.7 (DME), 21.5 (CH_3), 21.1 (CH_3), 20.7 (d, J_{CP} = 12.1 Hz, CH_3), 20.2 (d, J_{CP} = 9.4 Hz, CH_3), 19.5 (CH_3), 19.2 (CH_3)

$^{13}C\{^1H,^{31}P\}$ NMR (100.6 MHz, 300 K, THF-d_8) δ[ppm]:153.5, 152.0, 151.4, 145.1, 143.9, 139.8, 137.8, 136.5, 136.4, 135.8, 135.0, 134.4, 134.2, 133.8, 133.6, 132.8, 132.3, 131.6, 130.8, 130.5, 129.1, 128.9, 128.7, 128.4, 128.3, 128.1, 128.0, 127.9, 127.6, 127.4, 127.3, 124.2, 124.0, 118.2, 118.0, 72.5 (DME), 58.7 (DME), 21.5 (CH_3), 21.1 (CH_3), 20.7 (CH_3), 20.2 (CH_3), 19.5 (CH_3), 19.2 (CH_3)

$^{31}P\{^1H\}$ NMR (162 MHz, 300 K, THF-d_8) δ[ppm]: 28.9 (s, 1P), 24.2 (s, 1P)

CHN analysis: calcd. For $C_{68}H_{88}B_{10}CoKN_2O_6P_2$: found (calc.): C: 63.20 (62.95) H: 6.70 (6.84) N: 2.02 (2.16)

Melting point: T > 285 °C: decomposition to a black oil

UV-Vis-spectroscopy: measured in THF: λ_{max} (nm) / ε (L·mol^{-1}·cm^{-1}): 320 (34000), 504 (51000), 605 (11000)

Cyclic Voltammogram (CV): The CV of complex **2** (13.5 mg) was recorded in 10 mL THF and with the addition of 380 mg $^{n}Bu_4NPF_6$ as electrolyte.

3.2 NMR spectra

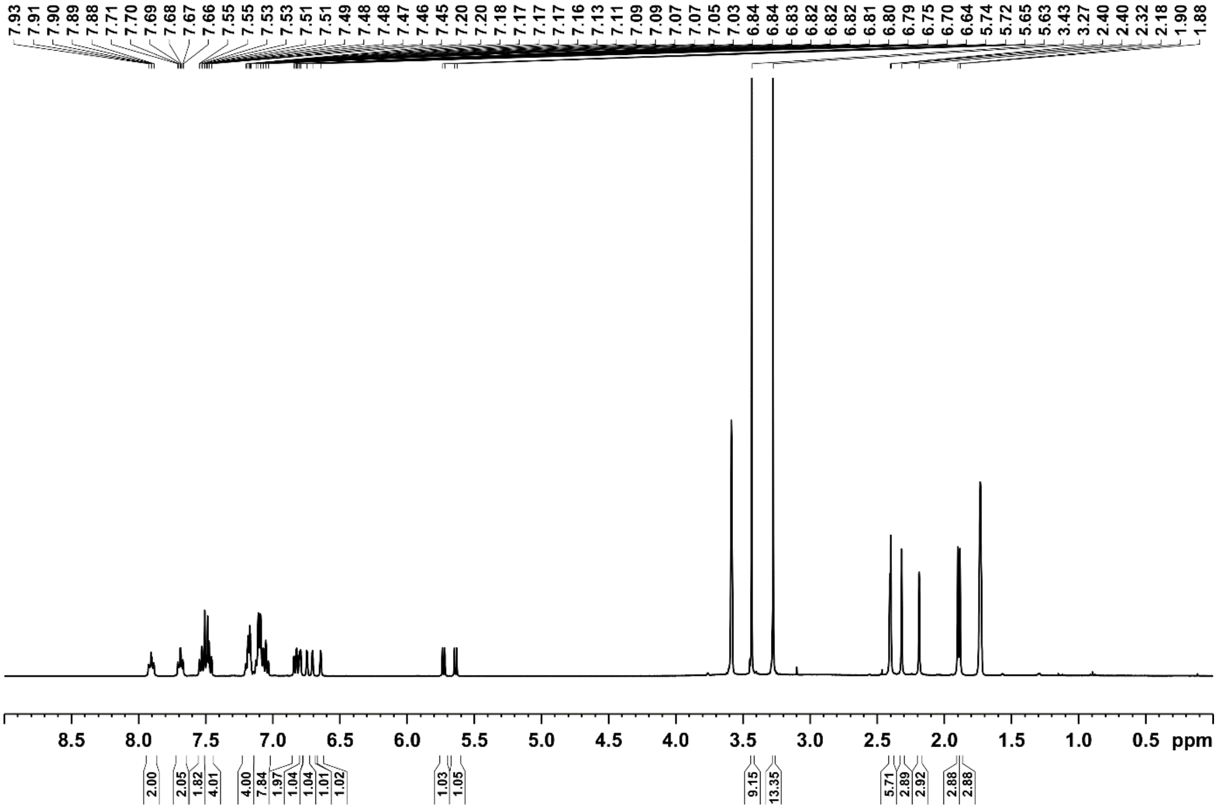
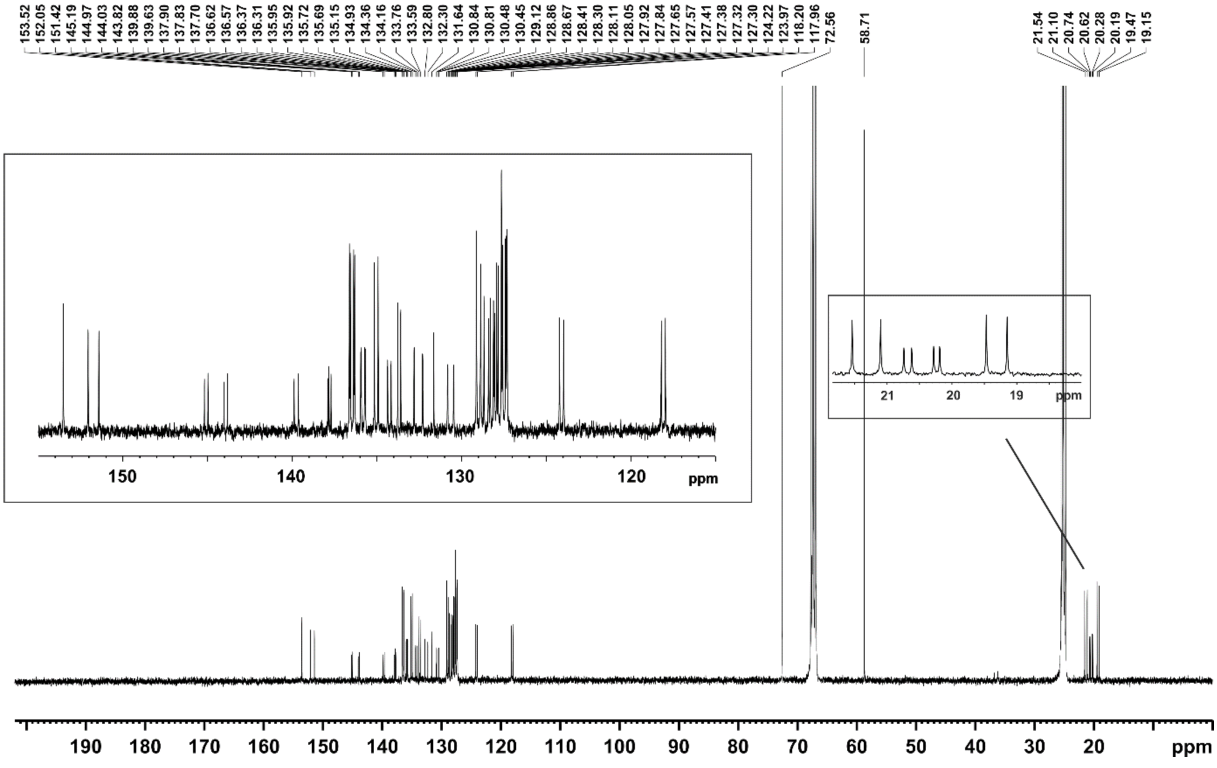


Figure S1. ^1H NMR spectrum (400.13 MHz, 300 K, THF-d_8) of **2**.



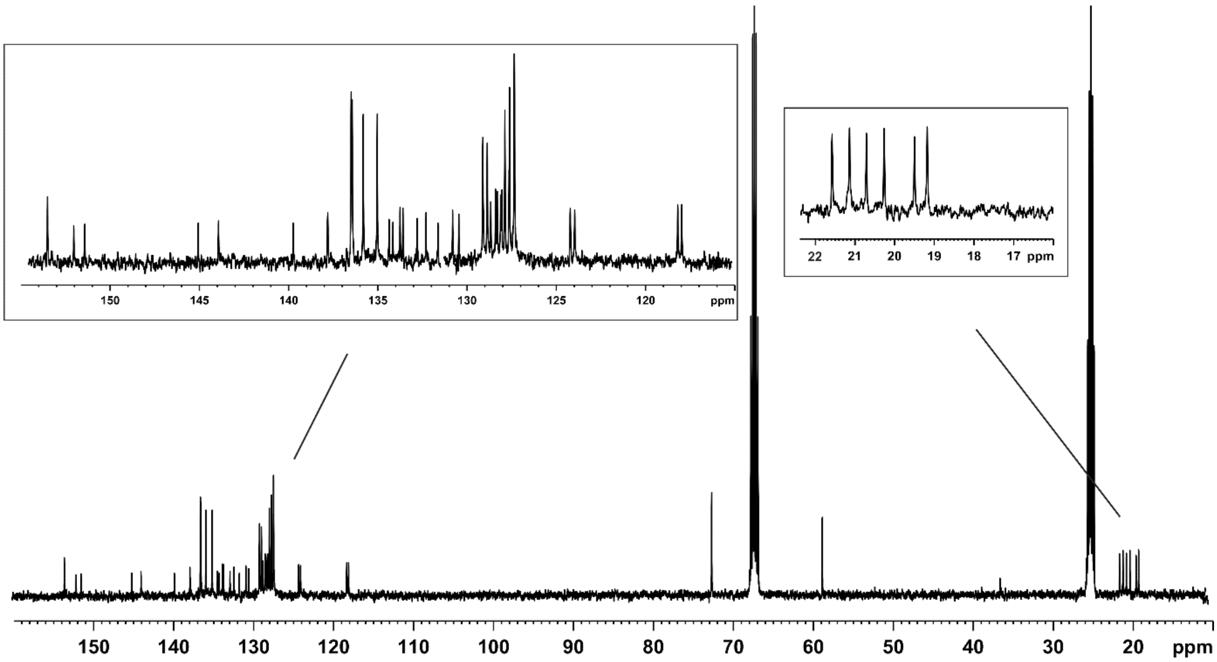


Figure S2. $^{13}C\{^{1}H\}$ and $^{13}C\{^{1}H,^{31}P\}$ NMR spectra (100.6 MHz, 300 K, THF-d_8) of **2**.

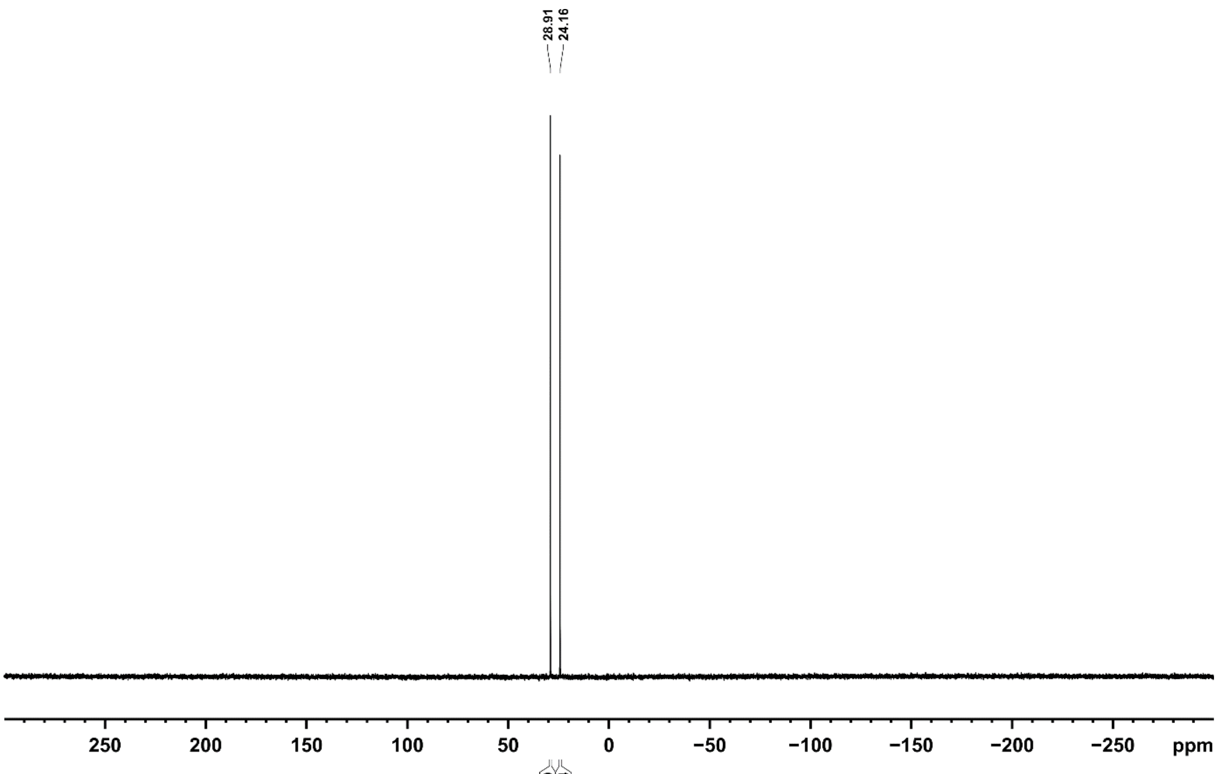


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum (161 MHz, 300 K, THF-d_8) of **2**.

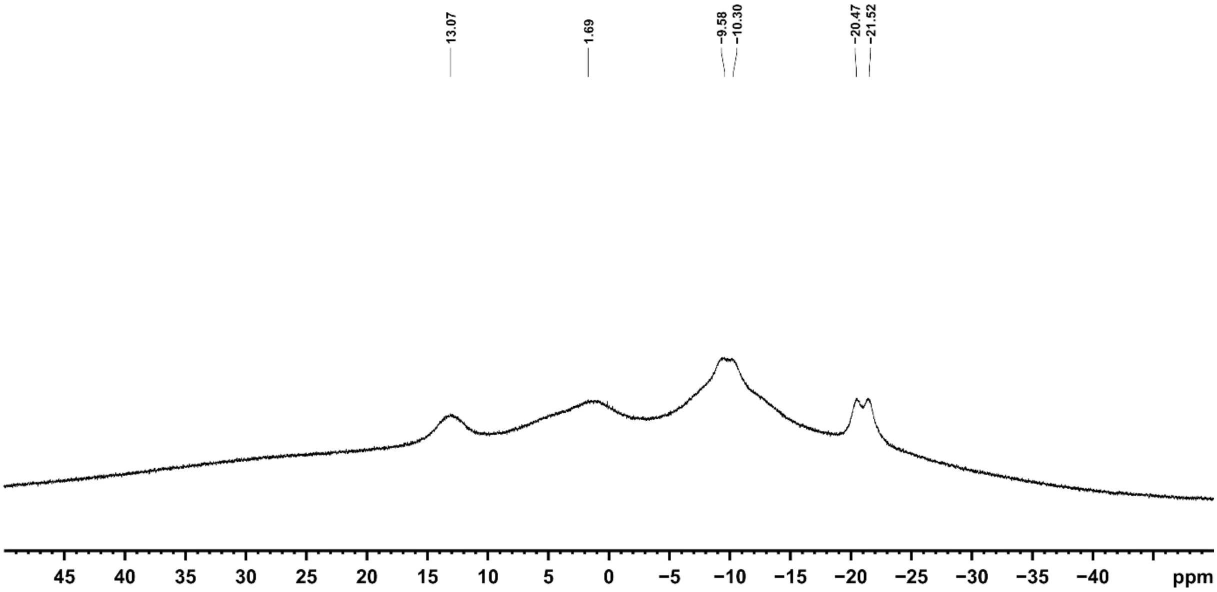


Figure S4. ^{11}B NMR spectrum (128.4 MHz, 300 K, THF-d_8) of **2**.

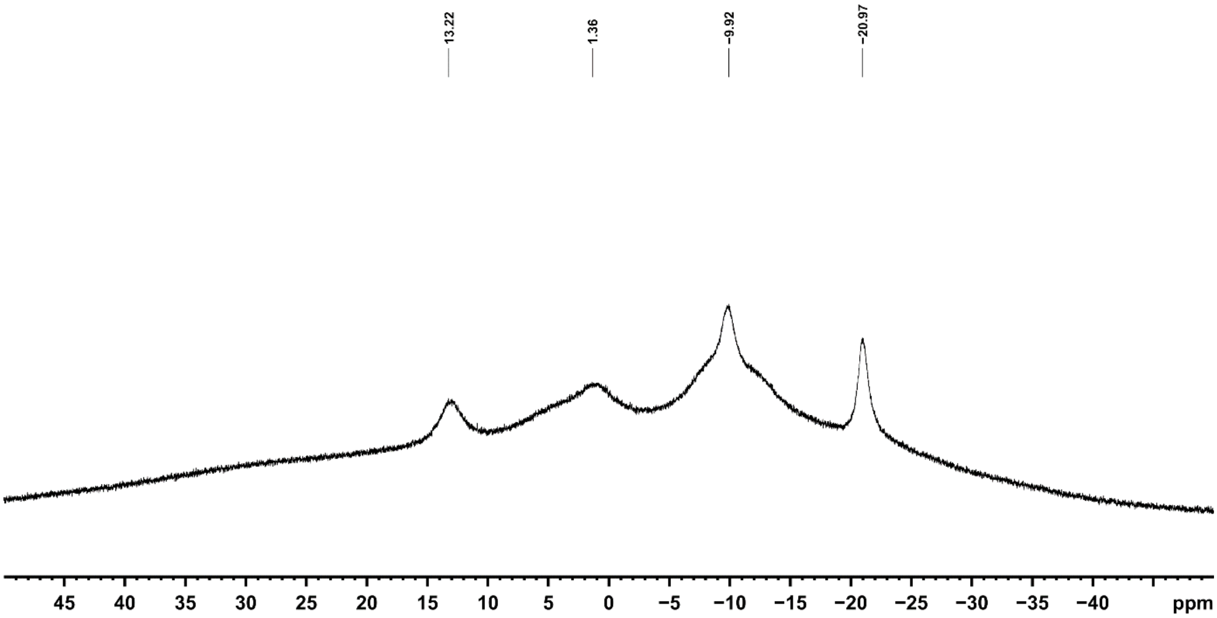


Figure S5. $^{11}B\{^1H\}$ NMR spectrum (128.4 MHz, 300 K, THF-d_8) of **2**.

3.3 Cyclic Voltammetry

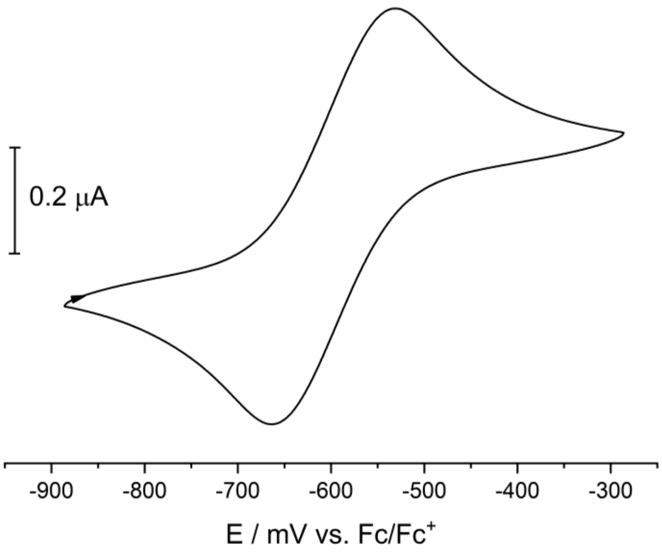


Figure S6. Cyclic voltammogram of **2** in THF/$^{n}Bu_4NPF_6$; scan rate: 50 mV/s.

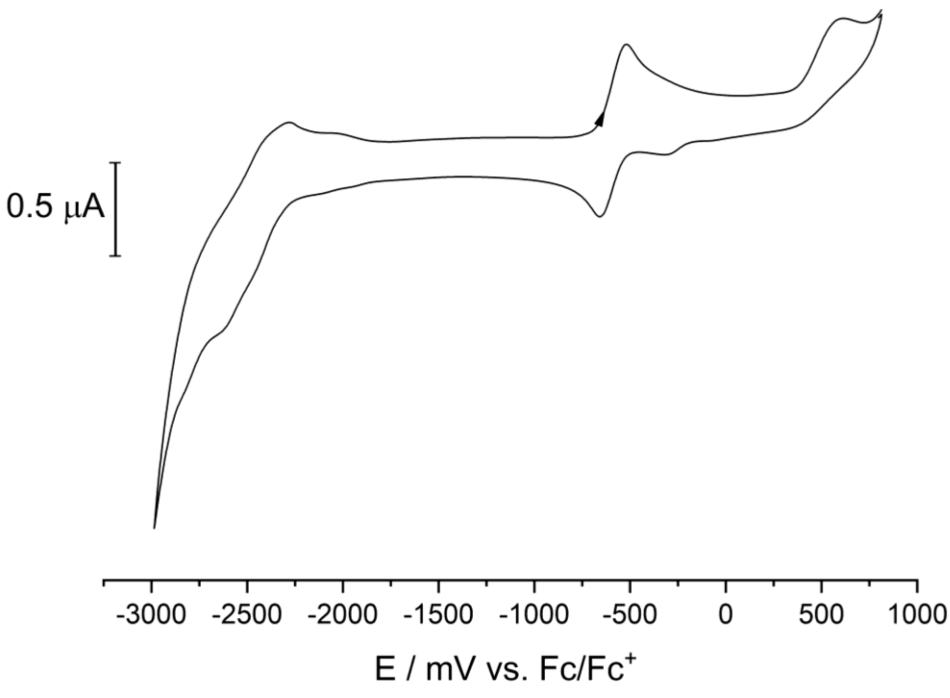


Figure S7. Cyclic voltammogram of **2** in THF/$^{n}Bu_4NPF_6$; scan rate: 50 mV/s.

3.4 UV/vis spectrum

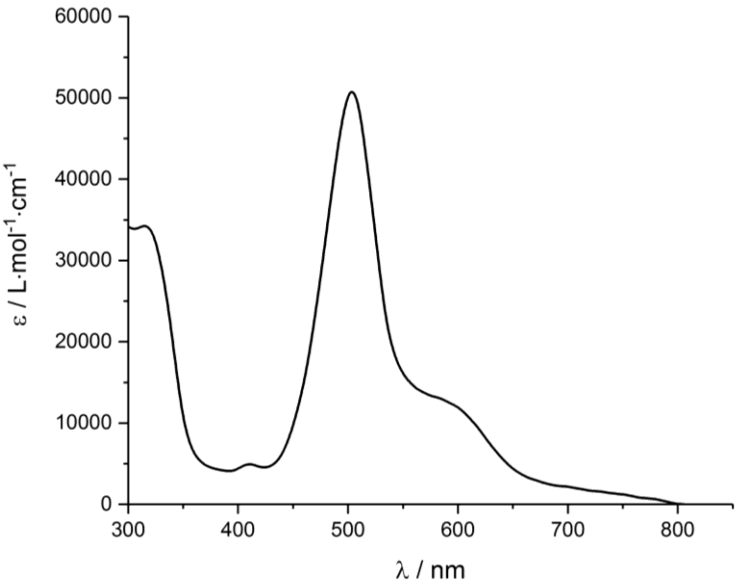


Figure S8. UV/Vis spectrum of **2** in THF.

3.5 Single-crystal X-ray crystallography

Table 1 Crystal data and structure refinement for 2

Empirical formula	$C_{68}H_{88}B_{10}CoKN_2O_6P_2$
Formula weight	1297.47
Temperature/K	123(1)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.9629(1)
b/Å	13.7270(2)
c/Å	36.1365(4)
α/°	90
β/°	95.597(1)
γ/°	90
Volume/Å^3	6893.2(1)
Z	4
ρ_{calc}g/cm^3	1.250
μ/mm^{-1}	3.326
F(000)	2736.0
Crystal size/mm^3	0.526 × 0.294 × 0.161

Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.892 to 147.778
Index ranges	-17 ≤ h ≤ 13, -16 ≤ k ≤ 16, -44 ≤ l ≤ 39
Reflections collected	32794
Independent reflections	13569 [R_{int} = 0.0282, R_{sigma} = 0.0332]
Data/restraints/parameters	13569/49/858
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0365, wR_2 = 0.0892
Final R indexes [all data]	R_1 = 0.0423, wR_2 = 0.0926
Largest diff. peak/hole / e Å^{-3}	0.28/-0.30

Table 2. Crystal data and structure refinement for [(^{Mes}BIAN)Co(η^4-cod)] (Int-A)

Empirical formula	$C_{41}H_{47}CoN_2$
Formula weight	626.73
Temperature/K	123(1)
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	8.1878(9)
b/Å	10.6068(9)
c/Å	19.841(1)
α/°	102.644(6)
β/°	95.457(7)
γ/°	97.860(8)
Volume/Å^3	1651.5(3)
Z	2
ρ_{calc} g/cm^3	1.260
μ/mm^{-1}	4.294
F(000)	668.0
Crystal size/mm^3	0.423 × 0.216 × 0.135
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.658 to 148.162
Index ranges	-10 ≤ h ≤ 9, -12 ≤ k ≤ 12, -18 ≤ l ≤ 24
Reflections collected	9999

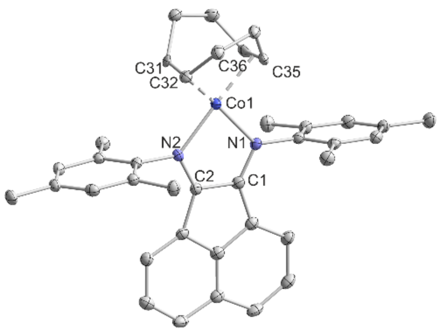
Independent reflections	6275 [R_{int} = 0.0618, R_{sigma} = 0.0826]
Data/restraints/parameters	6275/0/404
Goodness-of-fit on F^2	1.098
Final R indexes [I>=2σ (I)]	R_1 = 0.0683, wR_2 = 0.1661
Final R indexes [all data]	R_1 = 0.0790, wR_2 = 0.1728
Largest diff. peak/hole / e Å^{-3}	0.98/-0.85

Table°3. Crystal data and structure refinement for [(^{Mes}BIAN)Co(L)] (3)

Empirical formula	$C_{56}H_{58}B_{10}CoN_2P_2$
Formula weight	988.01
Temperature/K	123(1)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.2578(2)
b/Å	24.1038(4)
c/Å	19.6169(3)
α/°	90
β/°	96.950(2)
γ/°	90
Volume/Å^3	5284.0(2)
Z	4
ρ_{calc}g/cm^3	1.242
μ/mm^{-1}	3.406
F(000)	2060.0
Crystal size/mm^3	0.292 × 0.259 × 0.176
Radiation	CuK_α (λ = 1.54184)
2Θ range for data collection/°	7.336 to 147.688
Index ranges	$-13 \le h \le 13$, $-29 \le k \le 28$, $-24 \le l \le 24$
Reflections collected	20536
Independent reflections	10282 [R_{int} = 0.0325, R_{sigma} = 0.0418]
Data/restraints/parameters	10282/0/646
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0459, wR_2 = 0.1189
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.1230
Largest diff. peak/hole / e Å^{-3}	0.58/-0.54

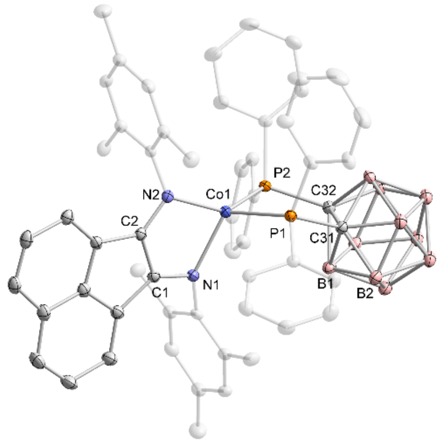
4 Characterisation of Intermediate Species

4.1 [(^{Mes}BIAN)Co(η^4-cod)] (**Int-A**) and [(^{Mes}BIAN)Co(**L**)] (**3**)



Int-A

- paramagnetic
- ligand centered radical
- monoanionic BIAN ligand
- cobalt(I) species
- fully characterised



3

- paramagnetic
- monoanionic BIAN ligand
- presumably cobalt(I)
- only characterised by XRD

[K(thf){(^{Mes}BIAN)Co(η^4-cod)] (**1**) (126 mg, 0.179 mmol, 1.0 equiv.) was dissolved in 3 mL THF and added to a solution of 1,2-bis(diphenylphosphino)-*ortho*-carborane (**L**) (93 mg, 0.181 mmol, 1.01 equiv.) in 3 mL THF. The solution turned orange immediately upon addition and was stirred for 30 min. After solvent evaporation, the dark orange residue was dried *in vacuo* and was subsequently extracted with *n*-hexane (8 mL). Storage of the solution at room temperature afforded dark orange crystals of [(^{Mes}BIAN)Co(η^4-cod)] (**Int-A**) as the major component and a minor amount of dark orange, almost black crystals of [(^{Mes}BIAN)Co(**L**)] (**3**), which were both characterised by single-crystal X-ray crystallography. **3** could not be further characterised due to the small amount of isolated compound, which is formed as a mixture with **Int-A** and **L**. **3** is presumably formed by reaction of ligand **L** and **Int-A**.

Characterisation data for Int-A:

Yield: 20.3 mg (0.031 mmol, 17%)

Chemical formula: $C_{38}H_{40}N_2Co$ (M = 583.69 g mol^{-1})

^{1}H NMR (400.13 MHz, 300 K, THF-d_8) δ[ppm]: Paramagnetic compound with broad signals at 10.5, 7.8, 0.7 and -2 ppm (see Figure S9). An assignment of these signals was not possible and no other resonances were observed from -100 to +100 ppm.

EPR: The sample was prepared in a nitrogen-filled glovebox in degassed, dry toluene and measured in a glass at 20 K. The signal shows very slightly axial symmetry (nearly isotropic) with calculated *g* values: g_x = 1.998, g_y = 1.994, g_z = 2.003 and simulated *g* values: $g_{\|}$ = 2.011, $g_{\perp}$ = 1.996 (see Figure S10)

CHN analysis: calcd. For $C_{38}H_{40}N_2Co$: found (calc.): C: 76.26 (78.20) H: 6.95 (6.91) N: 4.09 (4.80). The found CHN values are not consistent with the calculated CHN values. This is likely due to contamination of the major species **3** with complex **6** and ligand **L** as shown by single-crystal X-ray crystallography.

Magnetic moment (Evans' method): μ_{eff} = 1.8(1) μ_B

Melting point: > 210 °C: decomposition to a black oil

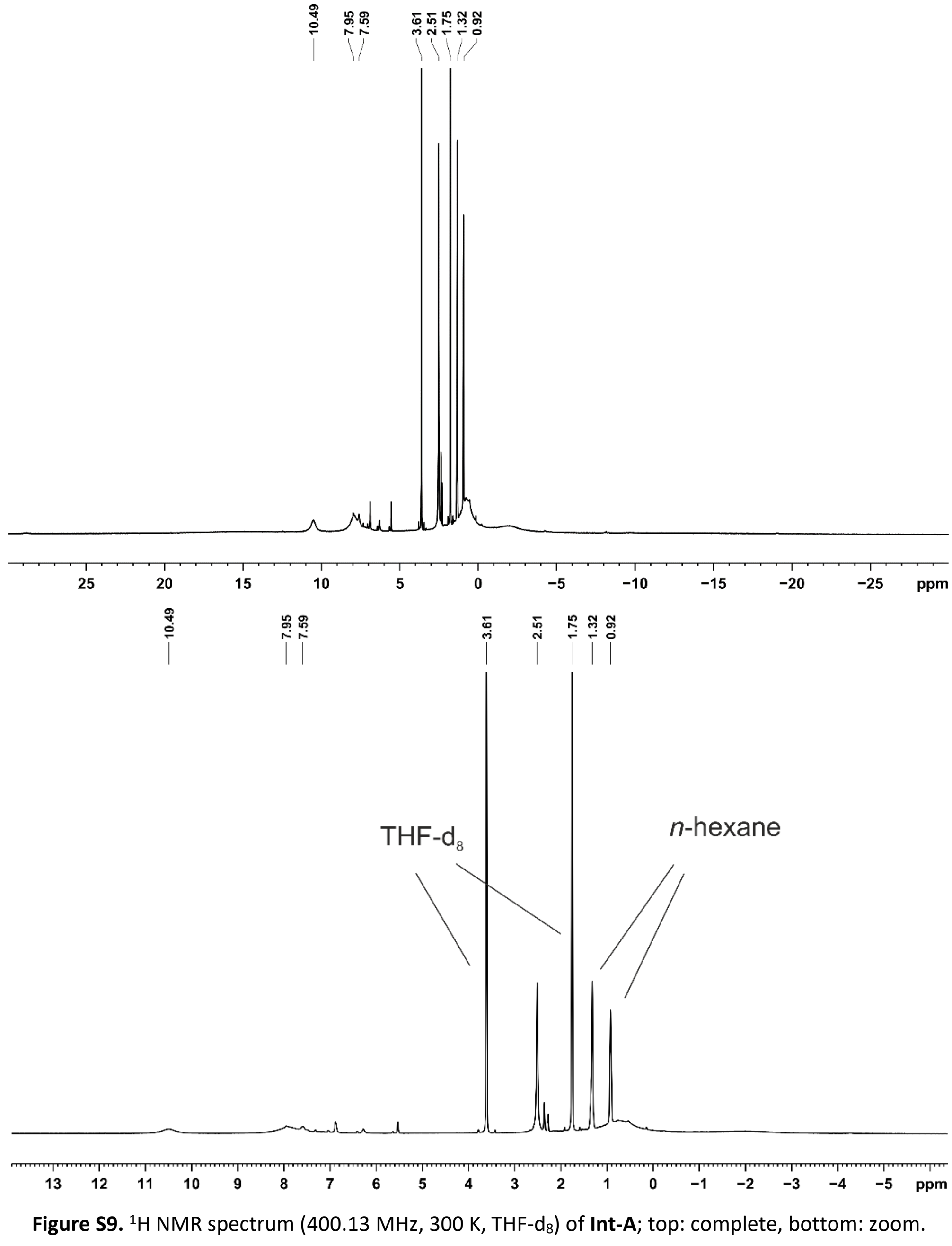


Figure S9. ^1H NMR spectrum (400.13 MHz, 300 K, THF-d_8) of **Int-A**; top: complete, bottom: zoom.

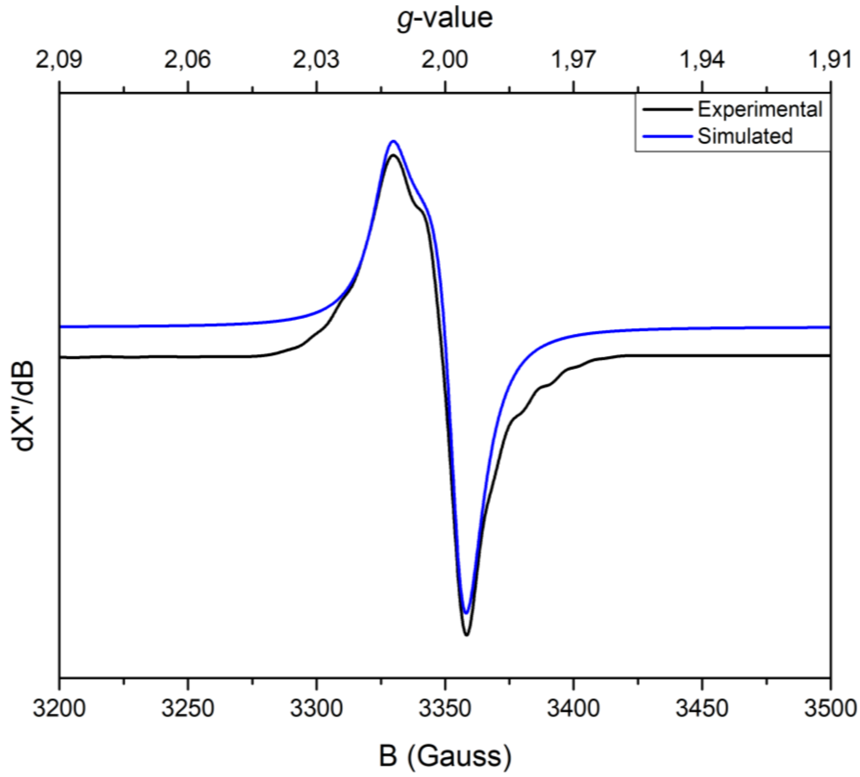


Figure S10. Experimental (black) and simulated (blue) X-band EPR spectrum of **Int-A** at 20 K (Microwave (frequency: 9.370555 GHz, Power: 0.6325 mW, Modulation amplitude: 1.000 G).

Spin density plot: M06-D3(0)-def2-TZVP CPCM(THF); isosurface value: 0.05: Ligand-centred radical

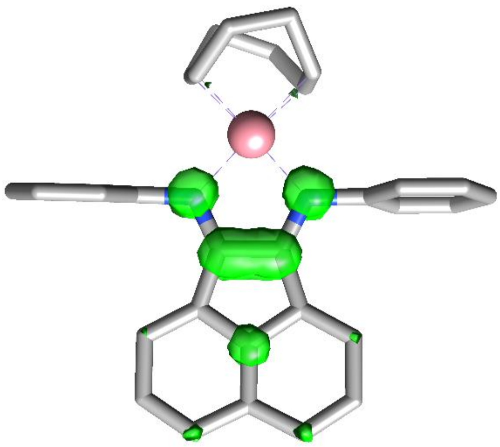


Figure S11. Spin density plot of **Int-A**.

5 Mechanistic Studies

5.1 $^{31}P\{^1H\}$ NMR monitoring

[K(thf){(^{Mes}BIAN)Co(η^4-cod)] (15 mg, 0.021 mmol, 1.0 equiv.) (**1**) and 1,2-bis(diphenylphosphino)-*ortho*-carborane (10.8 mg, 0.021 mmol, 1.0 equiv.) (**L**) were dissolved in THF (0.7 mL) in a J. Young NMR tube and a few drops of C_6D_6 were added.

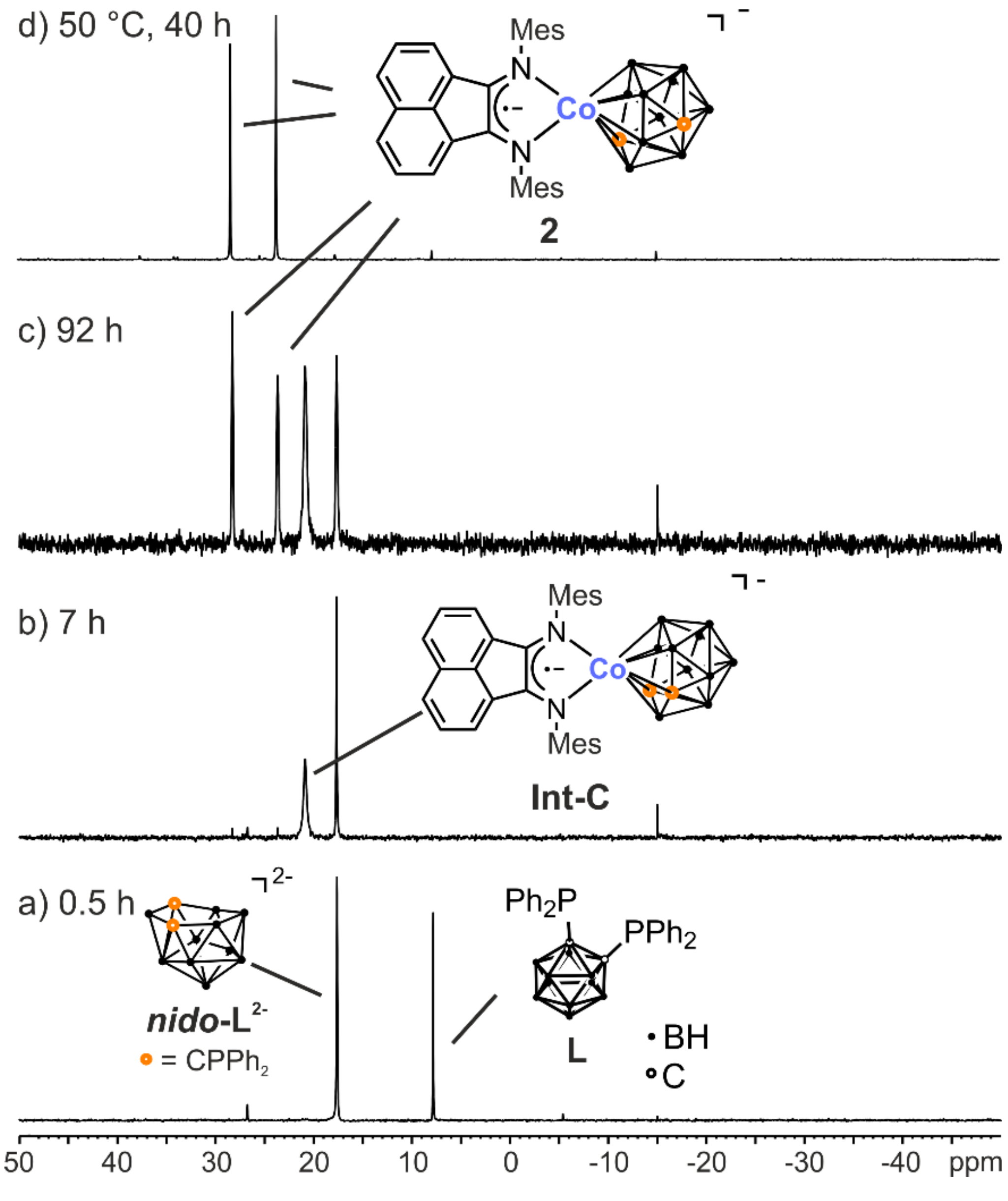
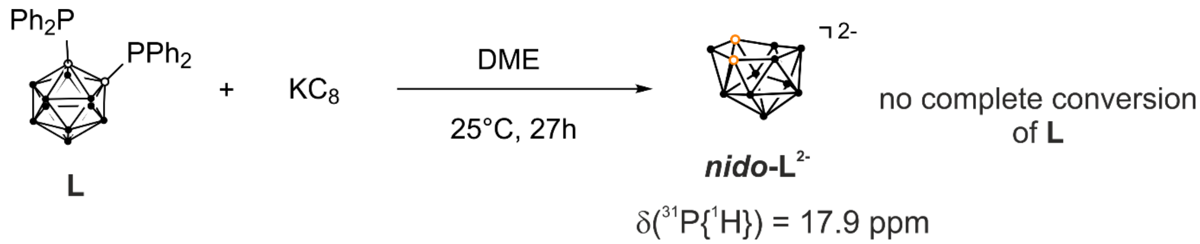


Figure S12. $^{31}P\{^1H\}$ NMR spectra (161 MHz, 300K, C_6D_6) of a 1:1 reaction of **1** and **L** in THF at 25 °C; reaction NMR at 50 °C in THF (top).

5.2 Stoichiometric reductions with potassium graphite

a) 1:1 reaction



Potassium graphite (KC_8, 5.3 mg, 0.039 mmol, 1.0 equiv.) was added to a solution of 1,2-bis(diphenylphosphinocarborane) (**L**) (19.2 mg, 0.037 mmol, 1.0 equiv.) in 1.0 mL DME at ambient temperature. The solution turned light yellow and was stirred for 27 h. After addition of a few drops C_6D_6 the reaction mixture was analysed by ^{11}B and ^{31}P NMR spectroscopy.

$^{31}P\{^1H\}$ NMR (162 MHz, 300 K, C_6D_6 in DME) δ[ppm]: main signals at: 17.8 (***nido*-L^{2-}**, integral: 1), 8.0 (**L**, integral 0.94), -15.1 (P_2Ph_4)

^{11}B NMR (128.4 MHz, 300 K, C_6D_6 in DME) δ[ppm]: 20.8 (br s), -1.5 (m), -9.4 (m), -18.5 (m), -22.0 (m)

$^{11}B\{^1H\}$ NMR (128.4 MHz, 300 K, C_6D_6 in DME) δ[ppm]: 20.1 (br s), -0.9 (s), -2.2 (s), -7.7 (s), -9.9 (s), -18.4 (s), -21.9 (s)

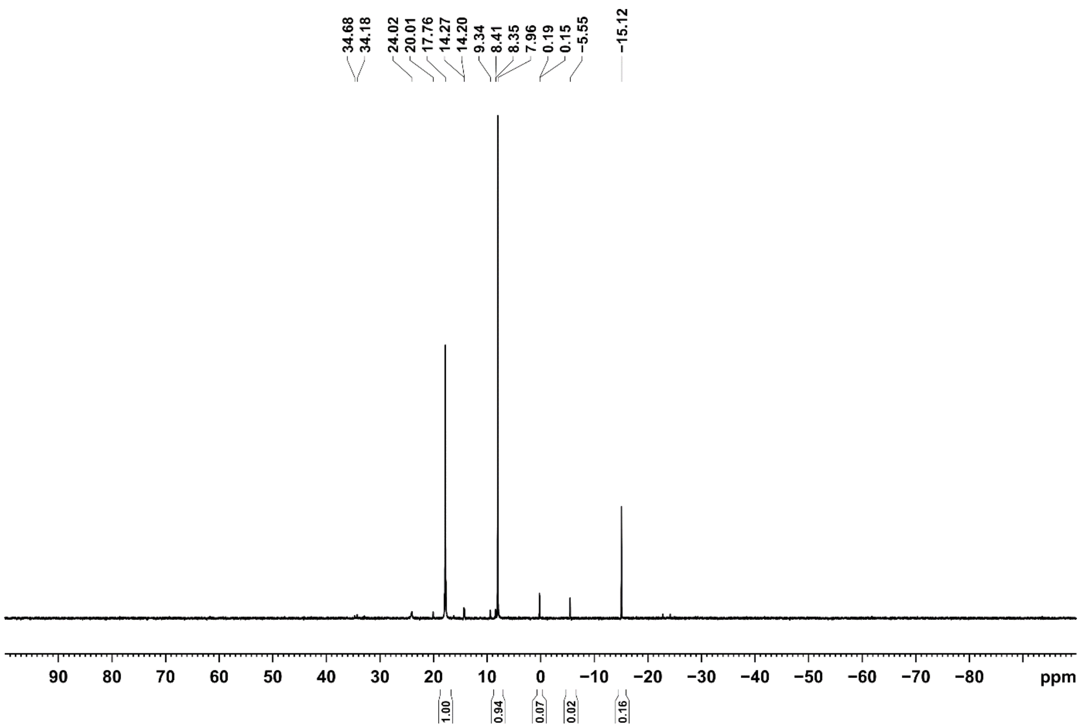


Figure S13. $^{31}P\{^1H\}$ NMR spectrum (161 MHz, 300 K, C_6D_6) of **L** and 1.0 equiv. KC_8 in DME.

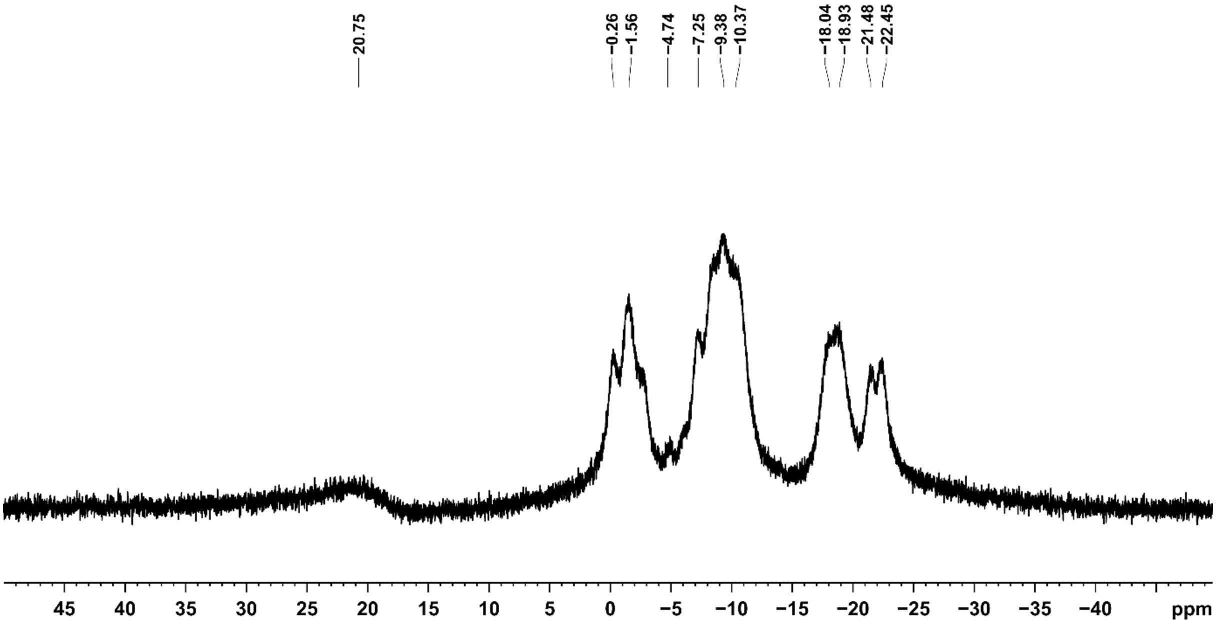


Figure S14. ^{11}B NMR spectrum (128.4 MHz, 300 K, C_6D_6) of **L** and 1.0 equiv. KC_8 in DME.

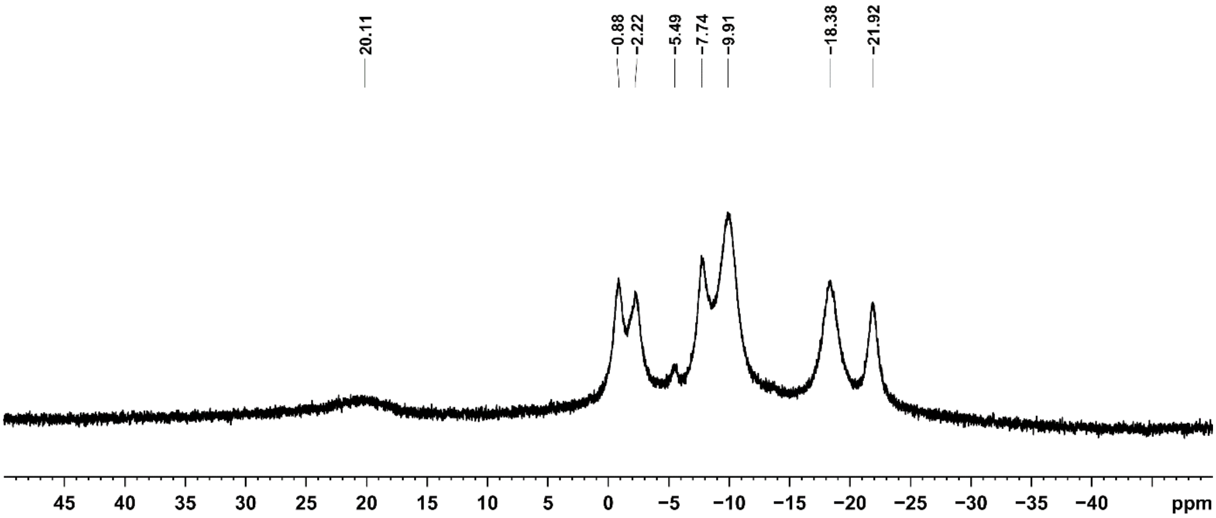
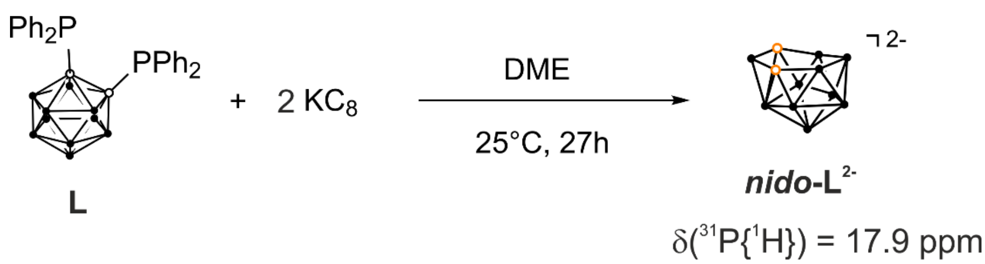


Figure S15. $^{11}B\{^1H\}$ NMR spectrum (128.4 MHz, 300 K, C_6D_6) of **L** and 1.0 equiv. KC_8 in DME.

b) 2:1 reaction



Potassium graphite (KC_8, 10.7 mg, 0.079 mmol, 2.0 equiv.) was added to a solution of 1,2-bis(diphenylphosphino)-*ortho*-carborane (**L**) (20.2 mg, 0.04 mmol, 1.0 equiv.) in 1.5 mL DME at ambient temperature. The solution turned yellowish and was stirred for 16 h. After addition of a few drops C_6D_6 the reaction mixture was analysed by ^{11}B and ^{31}P NMR spectroscopy.

$^{31}P\{^1H\}$ NMR (162 MHz, 300 K, C_6D_6 in DME) δ[ppm]: main signals at: 17.8 (*nido*-L^{2-}, integral: 1), -15.2 (P_2Ph_4, integral 0.05)

^{11}B NMR (128.4 MHz, 300 K, C_6D_6 in DME) δ[ppm]: 20.9 (br s), -2.4 (m), -18.5 (m), -22.0 (m)

$^{11}B\{^1H\}$ NMR (128.4 MHz, 300 K, C_6D_6 in DME) δ[ppm]: 20.9 (br s), -2.4 (s), -18.5 (s), -22.0 (s)

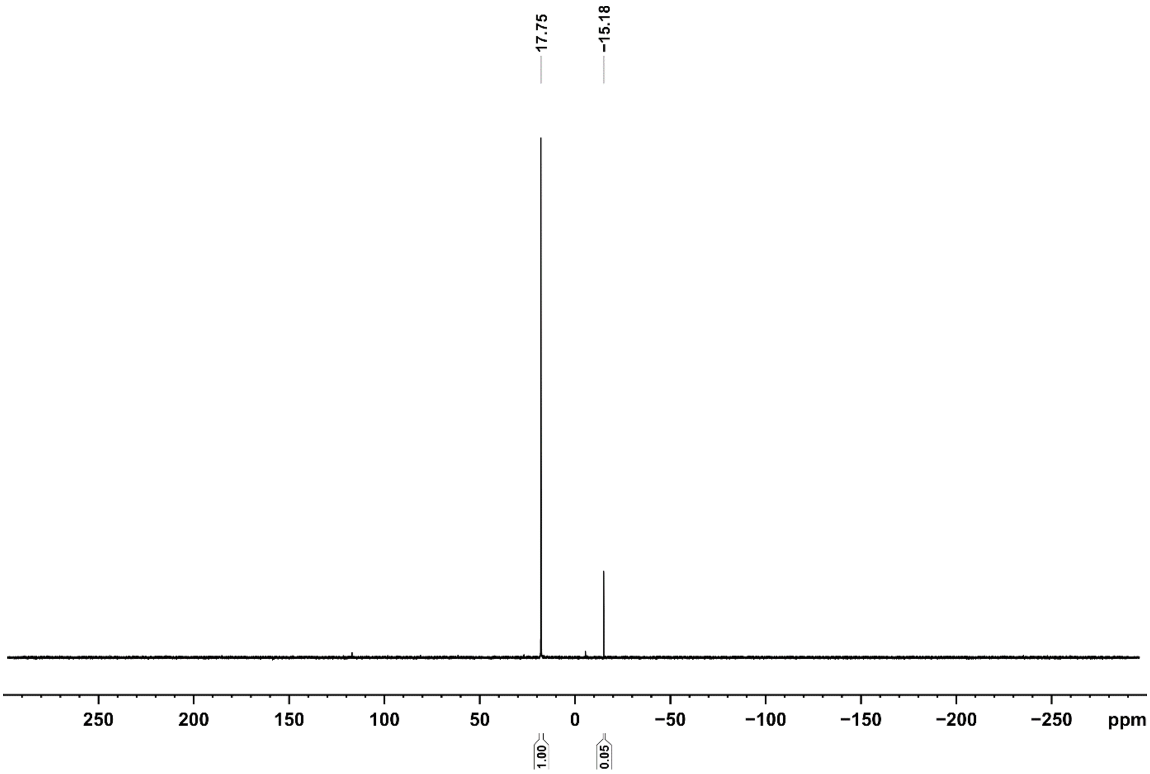


Figure S16 $^{31}P\{^1H\}$ NMR spectrum (161 MHz, 300 K, C_6D_6) of **L** and 2 equiv. KC_8 in DME.

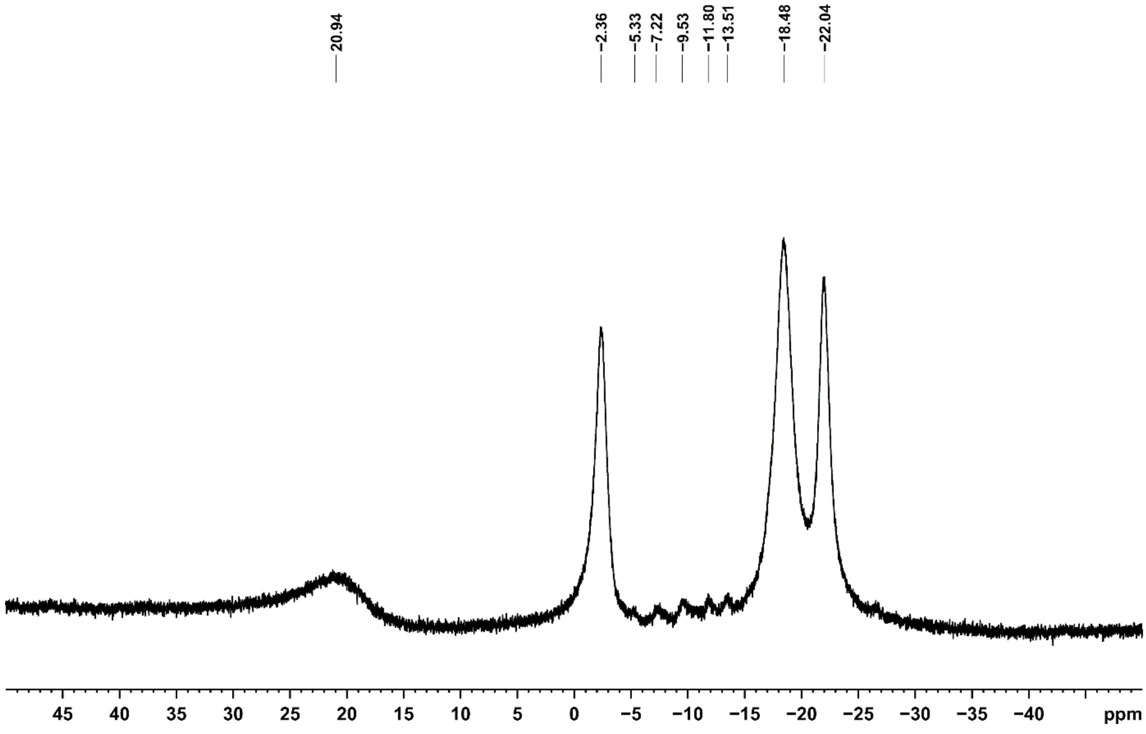


Figure S17. $^{11}B\{^1H\}$ NMR spectrum (128.4 MHz, 300 K, C_6D_6) of **L** and 2 equiv. KC_8 in DME.

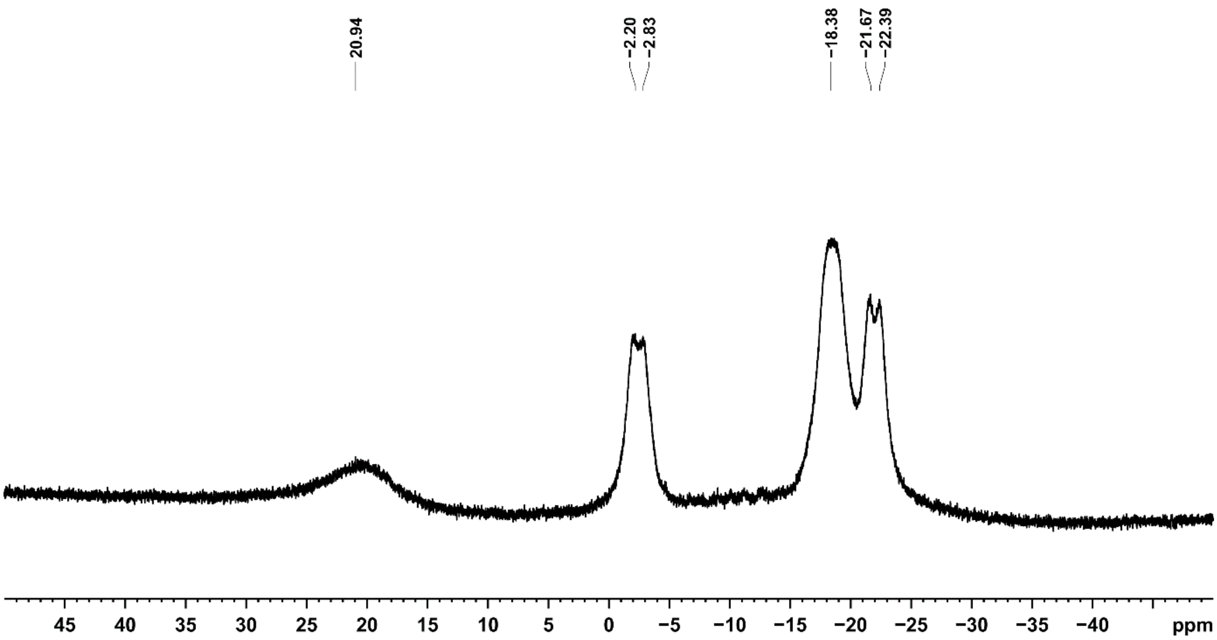
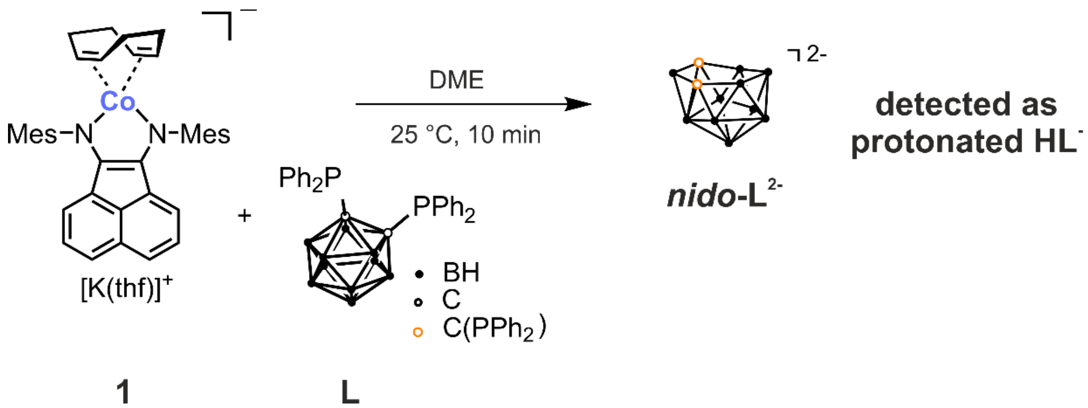


Figure S18. ^{11}B NMR spectrum (128.4 MHz, 300 K, C_6D_6) of **L** and 2 equiv. KC_8 in DME.

5.3 ESI-MS Analysis



In an inert atmosphere, [K(thf){(^{Mes}BIAN)Co(η^4-cod)] (**1**) (5 mg, 0.0071 mmol, 1.0 equiv.) and 1,2-bis(diphenylphosphino)-*ortho*-carborane (**L**) (3.6 mg, 0.0071 mmol, 1.0 equiv.) were dissolved in DME (1 mL). The solution was added dropwise to the cobaltate solution. The solution immediately turned orange and was diluted to a concentration of around 10^{-4} mol·L^{-1}. The solution was injected into the ESI-MS spectrometer with a Hamilton syringe. The sample was analysed using a negative fragmentator potential (-120 V). The simulation suggests that the observed species has the molecular formula $B_{10}C_{26}H_{31}P_2$ (***nido*-HL**$^-$) This means that ligand **L** was reduced by two electrons and subsequently protonated, which underlines the hypothesis that a dianionic *nido*-carborane (***nido*-L^{2-}**) is initially formed.

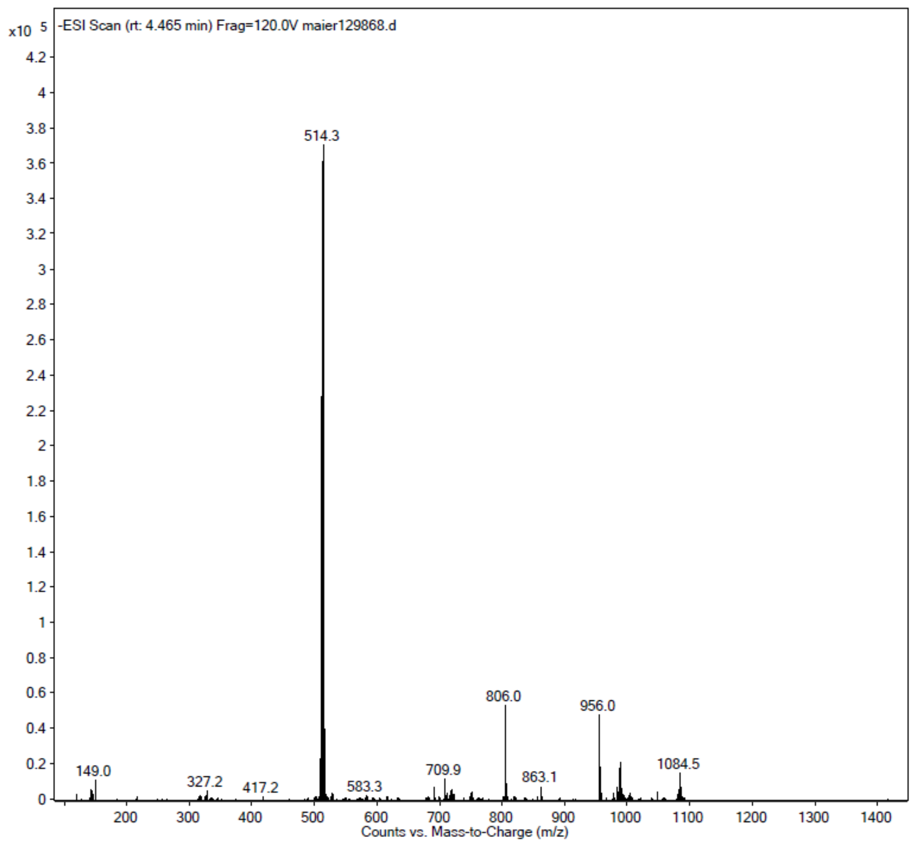


Figure S19. ESI Scan (4.465 min) Frag = 120.0 V.

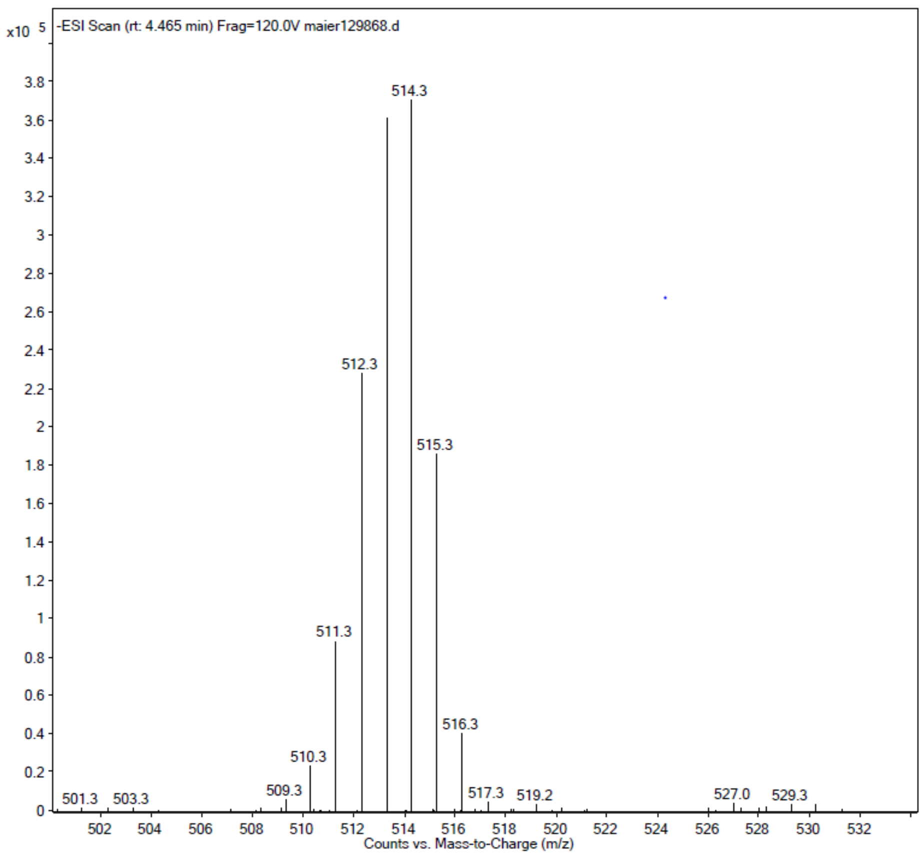


Figure S20. ESI Scan (4.465 min) Frag=120.0 V (zoom).

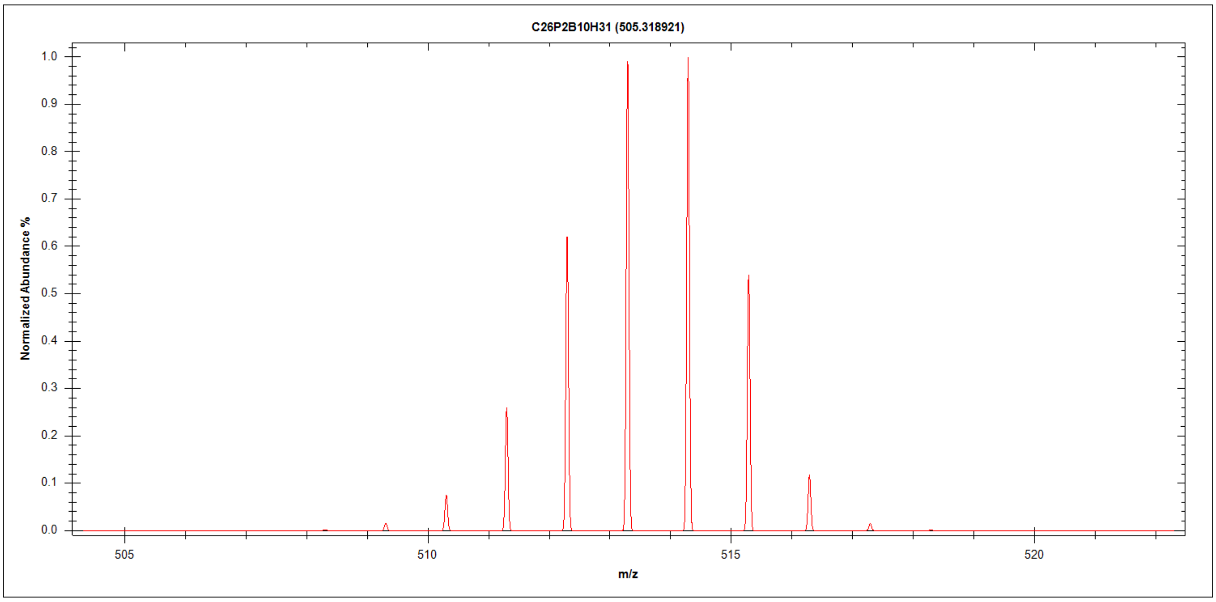


Figure S21. Simulation of mass spectrum of $C_{26}P_2B_{10}H_{31}$.

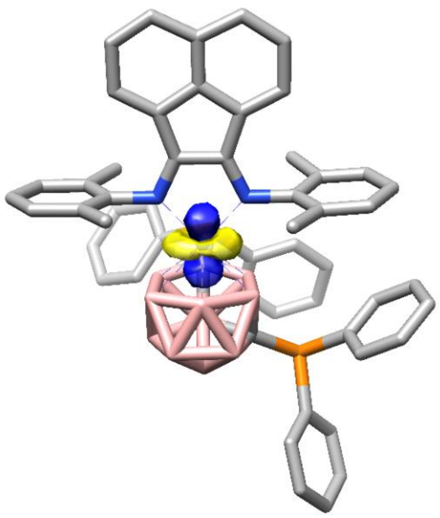
6 Computational details

General Methods

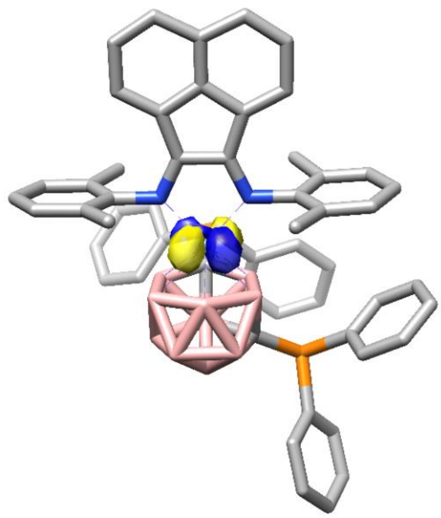
All calculations were carried out with the ORCA program package.[1,2] All geometry optimisations were performed at the BP86-D3BJ/def2-TZVP[4,15-18] level of theory in the gas phase. Frequency calculations were carried out to confirm the nature of stationary points found by geometry optimisations. Density fitting techniques, also called resolution-of-identity approximation (RI),[19] were used for GGA calculations, whereas the RIJCOSX[20] approximation was used for all other calculations. To save computational cost, all mesityl groups on the BIAN ligand were replaced by phenyl groups, except for the calculations presented in the CASSCF and TD-DFT sections where only the methyl groups in the *para*-position were replaced by hydrogen atoms. Final-single point energies for the mechanistic investigations have been obtained at the M06-D3(0)/def2-TZVP[4,16,21,22] CPCM(THF)[23,24] level of theory.

CASSCF calculations

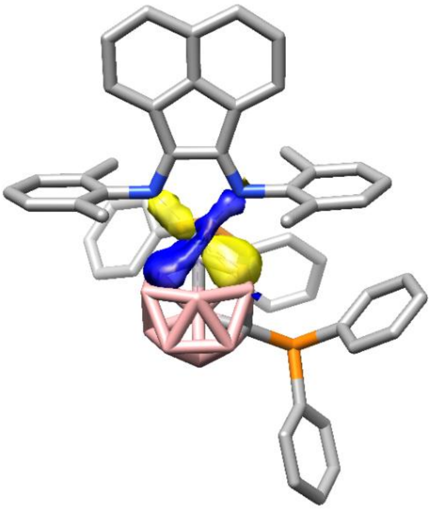
α-Diimine complexes potentially exhibit open-shell singlet character (or broken-symmetry character in the framework of density functional theory) due to the non-innocent ligand system.[25] This behaviour imposes challenges to single-reference methods. Therefore, we conducted CASSCF-DLPNO-NEVPT2/cc-pVTZ[26-28] calculations to get an insight into the electronic structure of **2**. The initial guess orbitals were chosen from a PBE/def2-SVP calculation. Thereby, the active-space was constructed to contain the 3d orbitals on cobalt as well as the bonding-interaction between cobalt and the ligands. Additionally, three orbitals of the second d-shell (containing the 4d orbital on cobalt) were included to aid convergence. In total, this led to an active space of 10 electrons in 10 orbitals. Analysis of the natural orbitals of the active space reveals six 3d electrons on cobalt (245, 246, 248), two metal−ligand bonding orbitals (247, 249) and their correlating antibonding orbitals (251, 250) and finally three 4d orbitals on cobalt (252, 253, 254), which present the above-mentioned double-shell of the occupied 3d orbitals on Co. The orbitals 247 and 250 are almost equally distributed over the metal atom and the BIAN ligand framework, which indicates a strong covalent interaction between the metal atom and the ligand. For this reason, an assignment of an oxidation state to Co remains ambiguous (see the main text). As discussed in the main text, partial reduction of the BIAN ligand can be deduced from the orbitals 249 and 250, which resemble the Co-BIAN π-bonding and π-antibonding orbitals. Their respective occupations, 1.776 and 0.231, indicate dominant closed-shell character of **2** (occupations of 2.00 and 0.00 would account for an ideal closed-shell compound, whilst equal occupations of 1.000 would account for an ideal open-shell singlet species). This can also be deduced by looking at the composition of the CASSCF wavefunction: The contribution of the ground state configuration state function is 80%, whilst higher configuration state functions (corresponding to excited states in a single-reference framework) contribute the remaining 20%, indicating some multi-reference character of **2.** The configuration state function where 250 is doubly occupied and 249 is empty shows the most significant contribution of all higher configuration state functions to the overall wavefunction (8%, a contribution of 50% would indicate an ideal open-shell singlet species).



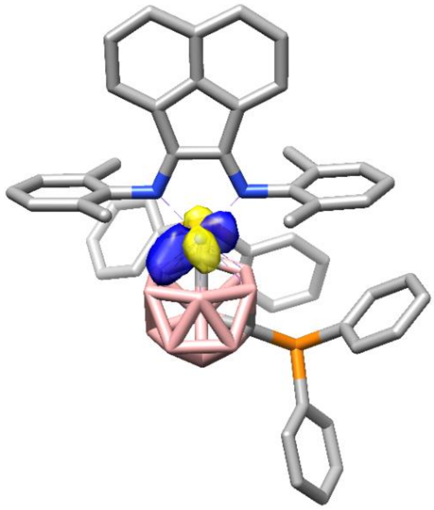
245 (occ.: 1.971, 69% $3d_{x^2-y^2}$, 12% $3d_{yz}$)



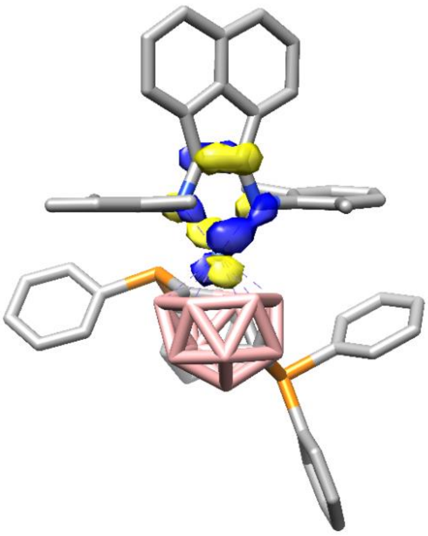
246 (occ.: 1.954, 58% $3d_{xz}$, 16% $3d_{z^2}$)



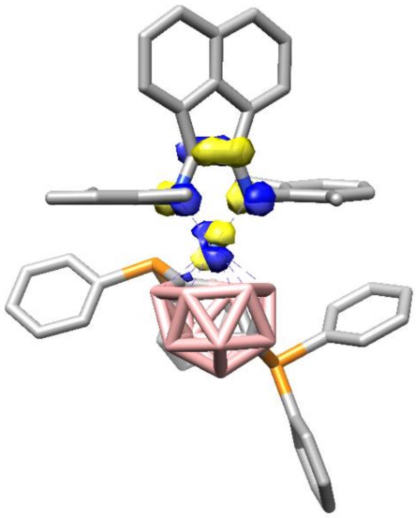
247 (occ.: 1.930, 41% 3d)



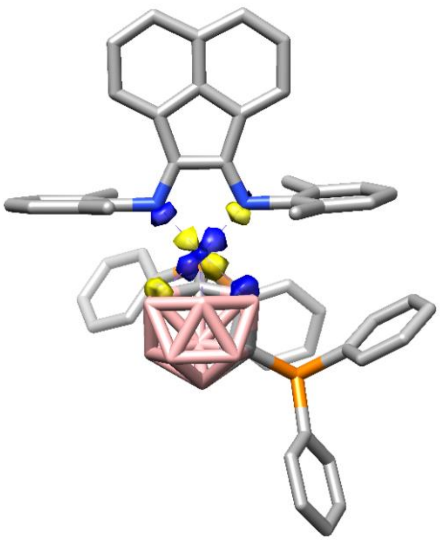
248 (occ.: 1.928, 47% $3d_{z^2}$, 13% d_{xz}, 10% d_{xy})



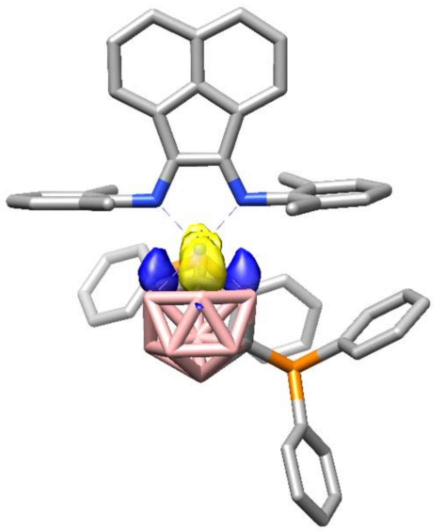
249 (occ.: 1.776, 42% $3d_{yz}$)



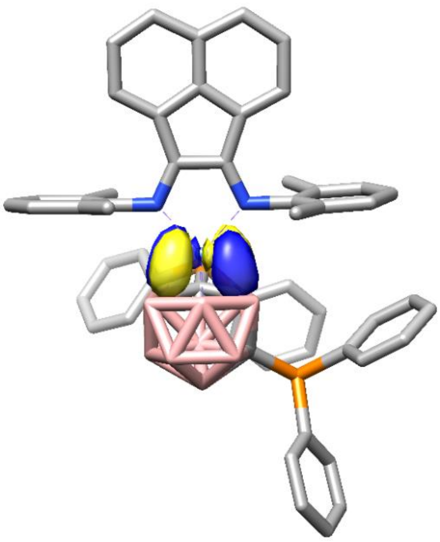
250 (occ.: 0.231, 37% $3d_{yz}$)



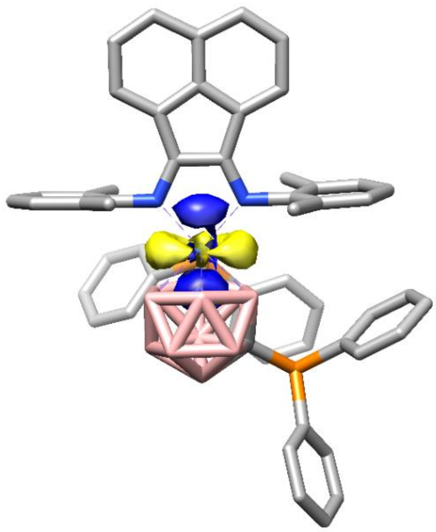
251 (occ.: 0.087, 59% $3d_{xy}$)



252 (occ.: 0.063, 30% $4d_{z^2}$, 12% $4d_{xz}$)



253 (occ.: 0.035, 10% $4d_{z^2}$, 37% $4d_{xz}$)

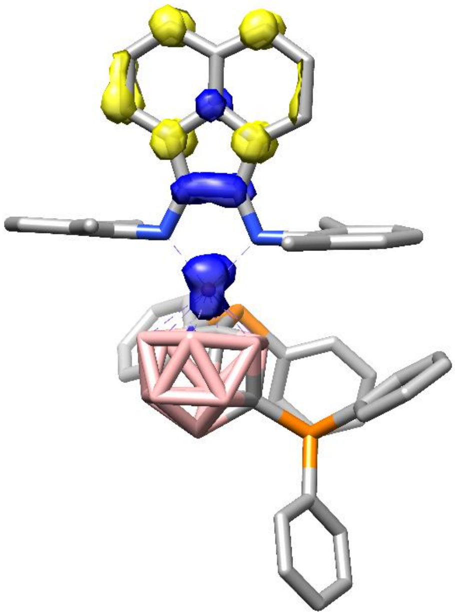


254 (occ.: 0.025, 47% $4d_{x^2-y^2}$)

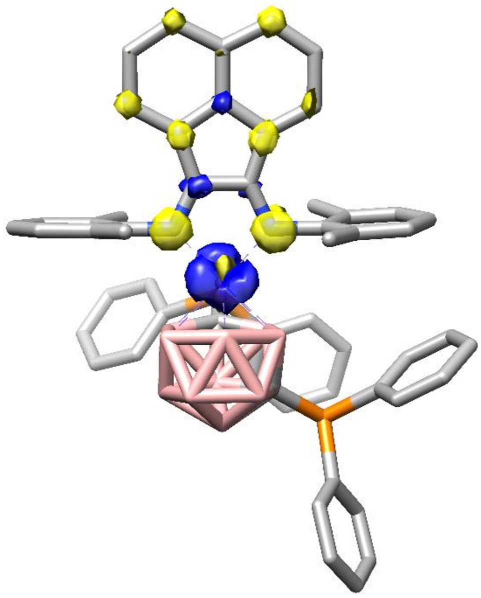
Figure S22. CASSCF natural orbitals of **2**. For each orbital, the occupation (occ.) and the highest contribution of d orbitals on cobalt as derived from Löwdin population analysis are given. For orbital 247, the sum of all contributions is given, since all 3d orbitals atomic orbitals of Co contribute significantly to this orbital. Surface isovalue = 0.06.

TD-DFT calculations on 2

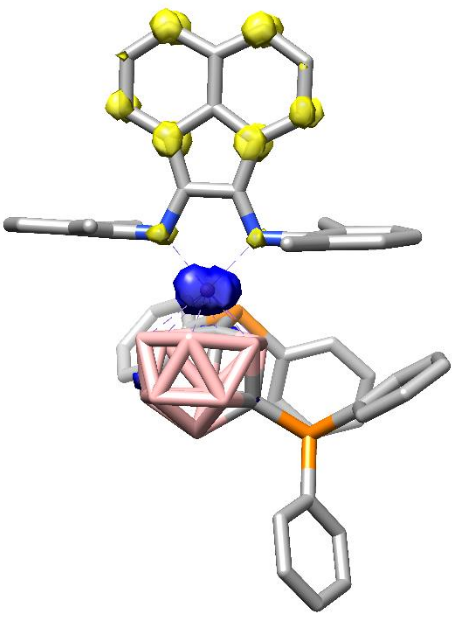
TD-DFT calculations on **2** have been conducted at the M06/def2-TZVP level in the gas phase. Compared to the experimental absorption spectrum, the calculated absorption spectrum is blue-shifted, however, the overall shape agrees reasonably well (Figure S24). Looking at the difference densities of the most intense transitions (as judged by the calculated oscillator strengths f_{osc}) in the visible region of the spectrum allowed for the assignment of these transitions as MLCT (d−π*) bands (Figure S23).



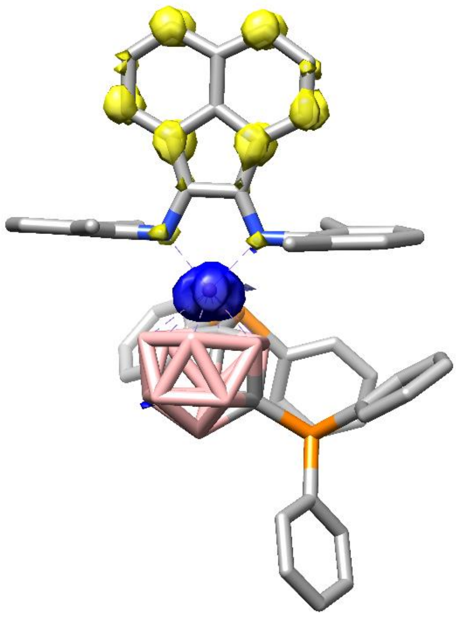
3 (652 nm, f_{osc} = 0.016355562)



6 (502 nm, f_{osc} = 0.314564984)



10 (428 nm, f_{osc} = 0.412937032)



12 (417 nm, f_{osc} = 0.173695227)

Figure S23. Difference densities for selected excited states of **2** (transitions proceed from blue to yellow). Surface isovalue = 0.004 (0.002 for state 6) together with calculated wavelengths of the transitions and oscillator strengths.

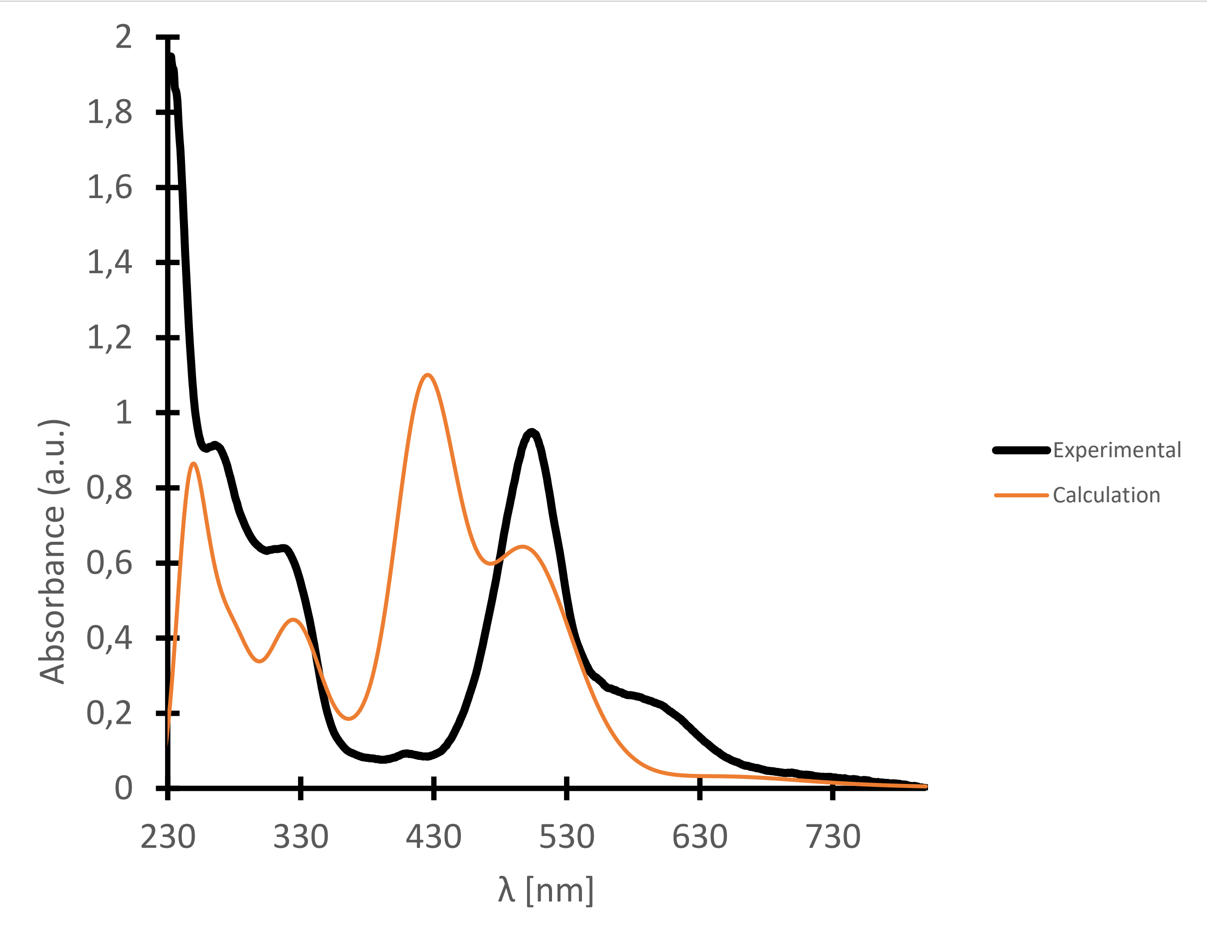


Figure S24. Calculated (orange) and measured UV-vis spectrum of **2**.

Cartesian Coordinates of optimised structures

1,2-bis(diphenylphosphino)-*ortho*-carborane (**L**)

P	2.65421812827846	7.37367936317896	2.78173969969008
P	3.53792233623493	6.82168171269276	5.86861568339196
C	1.62794338499846	5.86772146188883	0.71383297497796
H	1.25145405334320	5.25661069314031	1.53582479807679
C	3.50482871751196	4.61880010358639	7.52445185444037
H	2.70869167948196	4.30149714390811	6.84747205798437
C	4.13646668442575	5.85537221217030	7.31088996442934
C	5.13979060170252	6.27190645772864	8.19565343200451
H	5.61755173831239	7.24188826194006	8.06470385563254
C	3.94880568920122	8.55409006036635	6.30887974614204
C	2.37880505817515	7.02004766272085	1.00021236831990
C	4.00710841794903	9.91173258793522	2.30532494622536
H	4.83969251743492	9.39001749138482	1.83831269554040
C	2.58791468138369	7.44249763635032	-1.37852499764891
H	2.95878805797633	8.06389929989575	-2.19472720134997
C	2.82268562654551	9.35719401229529	6.55245250444069
H	1.82752654515217	8.92213273346985	6.44052786829250
C	1.85964628262676	9.89728874656466	3.41286269852417
H	1.01369266398171	9.34033209857496	3.82113407570257
C	2.91601762544916	9.18936839332278	2.81569832749948
C	4.04293104474799	11.30253597161177	2.40761516506161
H	4.90316240445037	11.84863313275646	2.01761096514557
C	5.22464466757606	9.12802423405939	6.43473060839706
H	6.11476218122891	8.53134478833964	6.24464536624530

C	4.23512728705153	11.25811732210594	7.02737298154846
H	4.34946539494722	12.30837341432243	7.29852571156967
C	4.36810584592864	6.60120533681744	2.97794624626085
C	4.82882851304501	6.30042952179625	4.59220173402316
C	1.88685635067438	11.28958098855894	3.49852826036296
H	1.05776735617714	11.82096018978326	3.96744615268843
C	2.84544070445746	7.81191704895525	-0.05741707025910
H	3.40672771117707	8.72302603678663	0.14602564361602
C	1.86099334174220	6.28149652367122	-1.65623364028814
H	1.66468616083083	5.99380525530339	-2.68993712095068
B	6.63900717404658	5.30621247165283	2.05237475543443
H	7.28165522171954	4.95474078105675	1.11242145350078
C	4.91056343265526	4.21062854196673	9.44717184417400
H	5.21641642084850	3.57100218917654	10.27625287597001
C	3.89529126879862	3.79656096366799	8.58137156161590
H	3.40413475001513	2.83440938063756	8.73046168245222
B	7.14057075431222	6.66052359873432	3.09713554700303
H	8.13509176578877	7.29596883249055	2.93267305199981
B	7.12049400522332	4.99361588991841	3.73227626836761
H	8.11884292123169	4.41509886132926	4.03072964337238
C	5.52536681530506	5.45108229207229	9.25642985211772
H	6.31135685320181	5.78108821888734	9.93762162454328
C	1.37814948207683	5.49526586872721	-0.60699283661161
H	0.80369593543358	4.59222046437131	-0.81739878087299
C	2.98490643040274	11.99476386967591	3.00384974921794
H	3.01969810588065	13.08241006627796	3.08443822067002
B	5.67574737158347	7.47185836106992	3.66810644342107
H	5.53013513110651	8.61342107736588	3.92640718274682
B	5.64816669037003	4.79852520954694	4.69947746568914
H	5.50827516224039	4.15638102704097	5.68571765154592
C	5.36430538707936	10.47050947597156	6.78510760198997
H	6.36187291447794	10.90418975734894	6.86931247162482
B	6.52549895626849	6.33272689941659	4.72972564417357
H	6.99233237374000	6.73869017527642	5.74440428837198
B	4.86893000655181	5.30264371207403	1.97844379907883
H	4.19086738326003	5.00851391532215	1.05227693166114
B	5.74649307202835	6.83880637081438	2.01124452741327
H	5.65922598667361	7.60145731725574	1.10265428959927
C	2.96257344054461	10.69690899655798	6.91655775239368
H	2.07577368293290	11.30481429693753	7.09838106678239
B	5.69518629969760	4.16194388156621	3.04846628578558
H	5.65089244946001	2.98915377401615	2.84332318938023
B	4.25283926862194	5.00124948977591	3.61715176051994
H	3.16478764392036	4.58527666617886	3.85281601118934

Dianionic ligand L^{2-} (*ortho*-L^{2-})

P	2.270395	6.978628	1.786529
P	3.608758	7.161786	6.189151
C	3.140017	6.393960	-0.816587
H	3.451494	5.444613	-0.379637
C	5.648195	6.678135	8.179240
H	6.295119	7.327864	7.589320
C	4.317608	6.480288	7.769185
C	3.509778	5.625167	8.537710
H	2.482348	5.445917	8.210254
C	4.427781	8.813825	6.311435
C	2.610883	7.394299	0.027545
C	3.410954	9.589848	2.237792
H	4.077680	9.383722	1.399803
C	2.354386	8.825931	-1.939552
H	2.044728	9.782852	-2.369882
C	3.820881	9.742957	7.176439
H	2.922356	9.439428	7.721494
C	1.627480	8.900248	3.704113
H	0.897545	8.148550	4.011554
C	2.436069	8.639585	2.588329

C	3.558220	10.767778	2.970137
H	4.344205	11.478243	2.703481
C	5.570908	9.218319	5.605221
H	6.060715	8.513548	4.937021
C	5.462796	11.427609	6.612249
H	5.857176	12.441661	6.716536
C	3.686689	6.109255	2.452788
C	4.435961	6.235273	4.891635
C	1.781980	10.073762	4.448338
H	1.174173	10.233485	5.341151
C	2.219112	8.611326	-0.566111
H	1.806299	9.402490	0.062950
C	2.889310	7.827979	-2.762292
H	3.003511	7.996503	-3.835999
B	5.641750	4.176388	2.361604
H	6.200093	3.391843	1.636272
C	5.325533	5.212259	10.085838
H	5.718992	4.718213	10.977793
C	6.146375	6.050562	9.321908
H	7.187050	6.210723	9.616689
B	6.404191	5.690579	3.032615
H	7.507001	6.035022	2.688784
B	6.126825	4.224667	4.065215
H	6.995093	3.470481	4.424583
C	4.001792	4.999246	9.684993
H	3.353113	4.337884	10.266003
C	3.280080	6.612192	-2.187152
H	3.709464	5.825305	-2.812732
C	2.744626	11.014220	4.080939
H	2.898112	11.909217	4.686001
B	4.941020	6.794487	3.389845
H	5.123572	7.967863	3.251461
B	4.766959	4.625436	5.102295
H	4.567002	4.144943	6.183222
C	6.073602	10.516279	5.747555
H	6.955288	10.813755	5.174309
B	6.020174	5.829153	4.758224
H	6.816868	6.256587	5.551045
B	3.938957	4.516317	2.143306
H	3.254333	3.968270	1.317079
B	5.156951	5.769693	1.790375
H	5.414209	6.217846	0.706422
C	4.333842	11.029222	7.339657
H	3.843043	11.730870	8.019748
B	4.441681	3.709754	3.633364
H	4.084054	2.569458	3.788670
B	3.428641	5.273763	3.881880
H	2.282399	5.162543	4.235641

Dianionic *nido*-ligand (***nido***-$\mathbf{L}^{2-}$)

P	12.767632	8.993113	21.032991
P	9.283148	7.258670	24.682926
C	9.385112	7.505835	22.879073
B	9.993972	10.002890	21.606907
C	13.411655	7.263132	20.996019
C	14.803199	7.078520	21.091924
H	15.448013	7.958213	21.174361
C	15.367163	5.802186	21.076116
H	16.451947	5.684155	21.144226
C	14.541808	4.674936	20.982304
H	14.976618	3.672235	20.975980
C	13.156087	4.845308	20.909958
H	12.498287	3.975433	20.848028
C	12.592458	6.124997	20.918083
H	11.509352	6.252254	20.834791
C	13.249175	9.513451	19.325112

C	13.596745	8.637610	18.284022
H	13.575611	7.562662	18.463182
C	13.949322	9.127167	17.023772
H	14.205796	8.426417	16.224864
C	13.949757	10.502881	16.773599
H	14.218141	10.883903	15.785089
C	13.592054	11.386230	17.798017
H	13.573316	12.463051	17.611826
C	13.251978	10.894246	19.058875
H	12.965720	11.582086	19.857719
C	10.640150	6.081787	25.068976
C	11.520003	5.613195	24.082156
H	11.336353	5.894767	23.046469
C	12.621157	4.822562	24.417999
H	13.301491	4.497420	23.628222
C	12.850861	4.460920	25.749038
H	13.712799	3.842657	26.012024
C	11.977969	4.915602	26.745622
H	12.153496	4.649618	27.791763
C	10.896936	5.732009	26.408985
H	10.241840	6.119891	27.193916
C	7.791752	6.213498	24.968819
C	7.780544	4.958736	25.599164
H	8.725556	4.485290	25.869907
C	6.578477	4.293368	25.863488
H	6.601337	3.313117	26.348276
C	5.357687	4.862526	25.493713
H	4.418899	4.339287	25.691182
C	5.355834	6.106727	24.848278
H	4.412916	6.555822	24.527010
C	6.551742	6.773230	24.593851
H	6.541786	7.732812	24.073101
B	10.464582	8.562324	22.550155
B	8.632712	9.012829	22.385971
B	8.507004	6.823179	21.847438
H	7.730008	5.960075	22.192813
B	7.704087	8.218120	20.845866
B	8.460132	9.790958	20.787596
H	7.755724	10.765920	20.740399
B	10.016854	9.641761	19.893148
H	10.504440	10.462924	19.166883
B	8.660612	8.618764	19.427437
B	8.758443	7.031433	20.134759
H	8.291855	6.111441	19.495716
B	10.245989	7.855251	19.786089
H	10.983375	7.488207	18.899088
C	10.961652	8.757285	20.979427
H	7.990544	9.532959	23.263080
H	8.181464	8.809203	18.336295
H	6.498803	8.164520	20.904149
H	10.445317	11.051945	21.981633
H	11.199492	8.934331	23.438572

1,5-Cyclooctadiene

C	-0.41185212371428	3.41590588214800	10.31328503005713
H	-0.44136709306268	2.33414663681654	10.47962611323184
C	-1.39608204280898	4.13019745659533	10.87830844435137
H	-2.15020447798168	3.56072998925915	11.43240906101921
C	-1.64539244085067	5.61402026003244	10.87918515304142
H	-1.98000271498881	5.89392818306824	11.89348479818368
H	-2.51115693392225	5.83047534803359	10.22533583318824
C	-0.47638422186483	6.53824937958188	10.48044803200364
H	-0.20871935036117	6.37652281925826	9.42964577987667
H	-0.84011057324584	7.57577430564365	10.53800811817250
C	0.72502592392791	6.40267634731401	11.38360769428802
H	0.76830652815249	7.12630871605275	12.20409951787104

C	1.71582044873241	5.50038728670505	11.33567902015101
H	2.48765385793220	5.58821061462692	12.10807748072953
C	1.95224064928247	4.36339303363498	10.37905677353430
H	2.30556438514229	3.50027526950277	10.97017175693717
H	2.80230440076682	4.62276433336367	9.72026836618447
C	0.76687236327611	3.90230481398781	9.50623678118875
H	0.47594259093813	4.69954435897611	8.81218153347965
H	1.12280082465037	3.07366496539885	8.87478471251035

[(^{Ph}BIAN)Co(η^4-cod)]$^-$ (phenyl substituted **1**)

Co	0.176648	4.284464	12.571629
N	0.370934	5.004246	14.367305
N	0.038557	2.582977	13.505580
C	0.341899	4.037148	15.326803
C	0.113474	2.720427	14.858617
C	0.089903	1.806819	16.003703
C	-0.024527	0.436191	16.212321
H	-0.148265	-0.256419	15.380156
C	0.014046	-0.067349	17.543247
H	-0.078729	-1.146562	17.688390
C	0.156273	0.750595	18.653271
H	0.171835	0.323289	19.658638
C	0.288363	2.163747	18.477181
C	0.441250	3.143723	19.507577
H	0.461410	2.833975	20.555055
C	0.557137	4.482390	19.167054
H	0.665753	5.224044	19.962377
C	0.548470	4.940773	17.819364
H	0.653122	6.006017	17.614797
C	0.413005	4.014627	16.789991
C	0.265192	2.636552	17.160500
C	-0.397320	1.368541	12.958797
C	0.328511	0.775072	11.909390
C	-0.116351	-0.401027	11.308634
H	0.466097	-0.844394	10.497804
C	-1.299709	-1.015107	11.736160
C	-2.034649	-0.427413	12.772247
H	-2.967999	-0.885858	13.107263
C	-1.591860	0.748548	13.376996
C	0.809019	6.292868	14.701021
C	2.020096	6.515388	15.386601
C	2.461922	7.811335	15.651293
H	3.407982	7.959772	16.177143
C	1.710022	8.917594	15.239594
C	0.510350	8.705593	14.549546
H	-0.085501	9.558439	14.216562
C	0.066356	7.412149	14.281586
C	-0.879665	3.745299	10.948157
H	-1.436468	2.831964	11.174892
C	-1.375612	4.955488	11.522885
H	-2.276148	4.874479	12.144786
C	-1.147973	6.326335	10.910866
H	-1.530042	7.083201	11.613767
H	-1.730077	6.458859	9.974540
C	0.357334	6.576867	10.668503
H	0.621146	6.349536	9.621416
H	0.588597	7.643812	10.814253
C	1.195643	5.735314	11.624071
H	1.768299	6.308940	12.357897
C	1.694896	4.437551	11.295503
H	2.611154	4.116695	11.807056
C	1.439742	3.758209	9.961763
H	1.836101	2.732264	10.017052
H	1.994222	4.254153	9.137313
C	-0.073701	3.699874	9.655063
H	-0.363185	4.532368	8.991242

H	-0.309617	2.776172	9.103566
H	-2.168122	1.216056	14.176315
H	-0.859154	7.230919	13.735311
H	1.242146	1.270161	11.580933
H	2.609644	5.651338	15.695406
H	-1.650300	-1.932901	11.260828
H	2.059435	9.931084	15.444463

[(^{Ph}BIAN)Co(η^4-cod)] (phenyl-substituted **Int-A**)

Co	0.18285955827941	4.31353830856844	12.48400949294306
N	0.64304127283696	4.97528732521083	14.26705170195598
N	-0.21345791092416	2.65684841178506	13.45135985702927
C	0.47246677938101	4.04978981907910	15.21454756227334
C	-0.02036228046401	2.77715135960982	14.76713293123919
C	-0.16222723348218	1.89576063937059	15.92509587762773
C	-0.56473406915622	0.58724907112282	16.15082049836386
H	-0.88938040025102	-0.05821320823595	15.33528690402214
C	-0.54960583513698	0.09115116973782	17.48282266149153
H	-0.86809171284365	-0.93838436534259	17.65441356267927
C	-0.15000947745287	0.86008286309496	18.56624503599226
H	-0.15742197912351	0.43583597452148	19.57191670531862
C	0.27280639187216	2.20801170447731	18.36928257169851
C	0.71393642622374	3.13015871030810	19.36405230547119
H	0.75069209854887	2.82187492207879	20.41049001287893
C	1.09504045342654	4.41419808308601	19.00233534586036
H	1.42883239251808	5.10467654129941	19.77862179472549
C	1.07226679794204	4.87350862439494	17.65726306622047
H	1.38506528643674	5.89129503294531	17.42604623814524
C	0.64959579406278	4.00068244944625	16.66502346763956
C	0.25351498142721	2.67968371228733	17.04831389160800
C	-0.72910670971158	1.42236607450045	12.97702368425796
C	0.13889928101701	0.44115792572239	12.47831883016970
C	-0.36751047028289	-0.77893329416623	12.02766644742722
H	0.31601563039786	-1.54016296711673	11.64875400145441
C	-1.74266414388429	-1.02763267013066	12.06286455071641
C	-2.61035581931896	-0.04842133847022	12.55456184338694
H	-3.68455274370907	-0.23632773145751	12.58744677257603
C	-2.10828217272429	1.17224674434333	13.00877666942359
C	1.15820794853336	6.23533831127372	14.66962707321876
C	2.54075986472687	6.42376000648573	14.80466809570596
C	3.04300233844939	7.65970792888806	15.21578713827699
H	4.12005604044563	7.79610756104926	15.32340723695535
C	2.17163280154443	8.71701231294791	15.49200655754089
C	0.79285172405264	8.53221839249395	15.35398173509995
H	0.10681974966379	9.35222293564822	15.57113302665510
C	0.28637780816273	7.29886138468740	14.94104103460431
C	0.07780265336987	3.39344656269370	10.65150233178091
H	0.22995487746577	2.32921120050151	10.84391146677669
C	-1.16777162767248	3.93215476782562	11.02767220009760
H	-1.89189122677556	3.23696270802969	11.46419951274763
C	-1.76625105027712	5.21238184788388	10.49313033707520
H	-2.61167775669957	5.48725636392438	11.14199088310176
H	-2.19051560855283	5.06033166188026	9.48205980686384
C	-0.73357775900261	6.35847553575714	10.49434694395549
H	-0.19314446694396	6.39651280660899	9.53767579985075
H	-1.25024744873941	7.32452963630956	10.59130591271625
C	0.23961119873092	6.18511032604204	11.64560550136428
H	0.11038927701512	6.88837091325286	12.47137058131714
C	1.49029217102554	5.54428266706735	11.55230012923716
H	2.23714752278466	5.81624643426717	12.30483878354901
C	2.05500436842108	4.89829695394555	10.30891705997910
H	2.91685453066401	4.28315444549957	10.60912310229711
H	2.44876461568135	5.66103784642882	9.60990322113183
C	1.00787215130517	4.00076269164751	9.61817999756741
H	0.43370551061841	4.57326570740982	8.87580397749187
H	1.51385369021823	3.19875285313607	9.06107107265581

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H    -2.77236015145866       1.93885991418967      13.41001670064790
H    -0.78702520023346       7.13559452705273      14.83784870461569
H    1.21000434274223       0.64639717573102      12.46641661869242
H    3.20807483222581       5.58532194600151      14.60127451364636
H    -2.13643863412404      -1.98102178824957      11.70915286917690
H    2.56560072672795       9.68180556961827      15.81322578901032
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Int-B (with phenyl groups)

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Co       8.271950     5.415248   22.056285
P       11.837756     6.613412   21.091105
P        8.346178     6.746012   25.104822
N        9.228333     3.760836   21.590980
N        7.065914     4.085439   23.066844
C        8.656477     2.644929   22.098302
C        7.544556     2.828038   22.969825
C        7.092792     1.513545   23.431272
C        6.075995     1.016476   24.242473
H        5.386215     1.684968   24.756914
C        5.948711    -0.391132   24.405146
H        5.147907    -0.763871   25.049719
C        6.792784    -1.302645   23.786996
H        6.659219    -2.376524   23.941132
C        7.839400    -0.829088   22.934225
C        8.773308    -1.625974   22.199371
H        8.736603    -2.715890   22.274720
C        9.712156    -1.006850   21.387109
H       10.417150    -1.625646   20.825390
C        9.801058     0.406127   21.242464
H       10.554075     0.834367   20.581579
C        8.911703     1.211521   21.948719
C        7.948911     0.558381   22.787539
C        6.102451     4.365613   24.045904
C        4.897403     4.993963   23.685488
C        3.956259     5.330629   24.658508
H        3.036040     5.838239   24.361654
C        4.196087     5.051959   26.007475
C        5.389914     4.421222   26.374181
H        5.599354     4.219397   27.426912
C        6.336189     4.086629   25.407748
C       10.247833     3.528315   20.635491
C       11.578903     3.358310   21.045697
C       12.570423     3.050220   20.113536
H       13.603757     2.932458   20.445762
C       12.253976     2.926677   18.757481
C       10.933617     3.119720   18.342295
H       10.680426     3.053717   17.282265
C        9.936492     3.418202   19.271459
C        8.335110     7.097007   23.317033
B        9.824273     8.860642   21.632255
C       12.430775     6.419530   19.355110
C       11.653425     6.437861   18.188463
H       10.591662     6.660421   18.255675
C       12.226245     6.153545   16.944928
H       11.594786     6.166798   16.053456
C       13.584333     5.851334   16.834880
H       14.025626     5.627133   15.860947
C       14.372956     5.830044   17.991741
H       15.436823     5.588181   17.927928
C       13.797899     6.098139   19.231261
H       14.414577     6.058904   20.133072
C       12.823091     8.118230   21.529977
C       13.179284     9.111125   20.602877
H       12.882607     8.996953   19.559830
C       13.879213    10.247234   21.010119
H       14.136769    11.016131   20.277529
C       14.225157    10.417624   22.355265
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H	14.757921	11.316007	22.676097
C	13.876239	9.436072	23.286672
H	14.121493	9.563690	24.342867
C	13.193976	8.290196	22.873039
H	12.910209	7.532862	23.605081
C	6.947846	7.622134	25.931516
C	6.048529	8.519522	25.336728
H	6.164957	8.782251	24.288147
C	4.998876	9.069152	26.078615
H	4.304674	9.757488	25.590952
C	4.832944	8.746715	27.427787
H	4.006834	9.174413	28.000813
C	5.730343	7.861750	28.035001
H	5.609006	7.590845	29.086718
C	6.764751	7.299951	27.288563
H	7.445526	6.582357	27.753998
C	9.726596	7.797739	25.758491
C	9.664453	9.196206	25.854302
H	8.745662	9.709842	25.570566
C	10.775271	9.930218	26.272399
H	10.718541	11.020263	26.315082
C	11.964425	9.278434	26.615822
H	12.835133	9.856235	26.933834
C	12.033132	7.884519	26.542215
H	12.959220	7.366117	26.801428
C	10.920331	7.153293	26.119506
H	10.974568	6.065715	26.034808
B	9.732955	7.433810	22.715780
B	8.233126	8.718170	22.580122
B	7.006330	7.173845	22.484686
H	5.974276	7.085318	23.077642
B	6.916470	8.437586	21.235739
B	8.345441	9.355056	20.867113
H	8.227108	10.533897	20.668742
B	9.519376	8.345533	19.990694
H	10.233063	8.719783	19.104142
B	7.796196	8.061141	19.763429
B	7.140813	6.748301	20.742740
H	6.218346	6.143763	20.252196
B	8.844475	6.638970	20.169710
H	9.148829	5.884848	19.293245
C	10.103186	7.270833	21.110797
H	10.678503	7.435036	23.449303
H	8.062899	9.562677	23.413473
H	7.337564	8.295132	18.676225
H	5.859714	9.014097	21.227658
H	13.037215	2.725113	18.025453
H	3.474800	5.351012	26.769898
H	8.902022	3.568245	18.965097
H	4.732946	5.219190	22.632888
H	7.284125	3.627365	25.686500
H	11.813493	3.471200	22.103199
H	10.716375	9.609347	21.888431

Int-C (with phenyl groups)

Co	8.529797	5.480325	22.136027
P	11.922576	6.386787	21.207813
P	8.455798	6.922082	25.275686
N	9.285363	3.852807	21.438623
N	7.499853	4.272710	23.206958
C	8.707186	2.748011	21.936575
C	7.705819	2.981590	22.906552
C	7.111074	1.701096	23.300884
C	6.103712	1.269817	24.151085
H	5.523425	1.972174	24.748413
C	5.833307	-0.124658	24.237562

H	5.038156	-0.454050	24.909507
C	6.534030	-1.073338	23.508762
H	6.291542	-2.133633	23.607343
C	7.572794	-0.663339	22.620060
C	8.376130	-1.500963	21.789439
H	8.226686	-2.582737	21.803808
C	9.338530	-0.938518	20.965077
H	9.944181	-1.592802	20.334696
C	9.574570	0.463287	20.898174
H	10.342161	0.850586	20.229102
C	8.811882	1.305188	21.694112
C	7.823376	0.714006	22.545592
C	6.484304	4.498324	24.181309
C	5.189071	4.861489	23.794374
C	4.199194	5.040227	24.761519
H	3.196800	5.342626	24.455106
C	4.491053	4.847473	26.114688
C	5.776125	4.456748	26.496885
H	6.011618	4.303974	27.550723
C	6.773728	4.285677	25.535457
C	10.277841	3.571112	20.451361
C	11.594985	3.318785	20.851107
C	12.548015	2.930228	19.906479
H	13.575950	2.748539	20.222429
C	12.192712	2.791104	18.563803
C	10.874339	3.033170	18.168075
H	10.590318	2.931627	17.119740
C	9.917886	3.420717	19.106358
C	8.437110	7.096493	23.454179
B	9.807955	8.564645	21.882640
C	12.478521	6.259944	19.452989
C	11.709296	6.289358	18.283073
H	10.641989	6.479441	18.340157
C	12.300892	6.062075	17.036231
H	11.677037	6.086209	16.140512
C	13.667278	5.804702	16.929810
H	14.122900	5.627747	15.953711
C	14.447551	5.770223	18.091044
H	15.518480	5.566303	18.028974
C	13.856269	5.985488	19.333046
H	14.470000	5.943142	20.236755
C	12.810962	7.944798	21.651188
C	13.065697	8.971925	20.728933
H	12.745206	8.854082	19.694017
C	13.700483	10.145601	21.134126
H	13.879060	10.941957	20.408864
C	14.087467	10.312189	22.467894
H	14.571894	11.237077	22.786801
C	13.848459	9.291237	23.390299
H	14.136923	9.415450	24.434788
C	13.224162	8.111794	22.981224
H	13.024773	7.321145	23.705486
C	6.955971	7.681739	26.027832
C	5.943782	8.402828	25.378230
H	6.019693	8.609522	24.314360
C	4.829153	8.857880	26.088980
H	4.048286	9.408221	25.560441
C	4.711767	8.618780	27.459445
H	3.838032	8.975039	28.008554
C	5.723297	7.916445	28.122288
H	5.645542	7.720427	29.193689
C	6.823651	7.445365	27.408730
H	7.599307	6.871360	27.922560
C	9.707529	8.196571	25.759541
C	9.442602	9.573161	25.792761
H	8.447907	9.934115	25.533015
C	10.444401	10.479912	26.143303
H	10.227581	11.549840	26.146861
C	11.721959	10.023744	26.479809
H	12.504565	10.735341	26.749392

C	11.990863	8.652852	26.471688
H	12.983377	8.285899	26.740970
C	10.989016	7.748138	26.116439
H	11.195651	6.676329	26.103430
B	9.861413	6.929201	22.908089
B	8.095636	8.625603	22.651379
B	7.114402	7.069979	22.556034
H	6.111031	6.921931	23.175552
B	6.940742	8.272569	21.288594
B	8.445474	9.155414	21.006198
H	8.422467	10.334734	20.799360
B	9.622989	8.098440	20.199830
H	10.390886	8.426107	19.348568
B	7.899666	7.891156	19.868867
B	7.219391	6.567374	20.834461
H	6.334354	5.909185	20.355341
B	8.880486	6.454547	20.246711
H	9.198760	5.725098	19.366378
C	10.129116	6.967779	21.313116
H	10.816359	6.741919	23.603218
H	7.860923	9.485061	23.447529
H	7.514431	8.124817	18.758436
H	5.873455	8.811605	21.196079
H	12.944799	2.515029	17.824192
H	3.722177	5.013120	26.870294
H	8.883199	3.598301	18.817620
H	4.979513	5.002181	22.735151
H	7.782235	3.988093	25.815495
H	11.852304	3.421212	21.903283
H	10.687600	9.231799	22.322982

2 (isolated product, phenyl groups)

Co	8.46119589552652	6.51288929634681	22.64612951951804
P	11.68172684778420	9.86536941398784	21.81008856361535
P	9.62624701327115	7.50954746765845	25.62987656509710
N	9.57663035402917	4.94355042262857	22.70479901498552
N	7.17567467808002	5.34866401233725	23.48237330344316
C	8.97170185465215	3.88413186888978	23.25431103751334
C	7.63911339715784	4.11369704097667	23.69504677038575
C	7.12685515957183	2.89030993496038	24.31824206184539
C	5.94992737840818	2.48678562171859	24.93021365911822
H	5.10754838640964	3.16857268480313	25.04487769381391
C	5.85874622875903	1.15295078348454	25.41685501314555
H	4.92935989118421	0.84193401149513	25.89829057287804
C	6.89659081855407	0.23940812906813	25.30610904716688
H	6.78084659591039	-0.77431099828163	25.69571650422868
C	8.12207239517547	0.62349514828185	24.68368768889464
C	9.28400016824333	-0.18272098572330	24.49210812208554
H	9.28930226167054	-1.21806176428840	24.83967259978656
C	10.40181007153299	0.35047528162902	23.86753358129354
H	11.28208103588895	-0.28075885061724	23.72966211684260
C	10.45727795220694	1.69222578561349	23.39769222720893
H	11.36315827380147	2.06407917680258	22.91948908857892
C	9.34461553033313	2.50244840997865	23.56847278655664
C	8.19360937981659	1.94178127131310	24.21037694703269
C	5.92536574476201	5.65042505944599	24.09325946641508
C	4.73312139603695	5.58513290438317	23.36726120827191
C	3.51987742050511	5.85491124571354	24.00501513433504
H	2.59041554383656	5.80476150549948	23.43519488312220
C	3.49353804799465	6.20151515208396	25.35910651043601
C	4.68988955153655	6.27357976456609	26.08022708611487
H	4.68771265708612	6.56208428658258	27.13253161783165
C	5.90108992113057	5.99449342437132	25.45039645086107
C	10.96500260515224	4.78343785963663	22.44334748525456
C	11.86256336879691	4.82113159622652	23.51782381347581
C	13.22102143879918	4.59286207455724	23.30094122137074

H	13.91534708555460	4.62123134781744	24.14277532369106
C	13.68947155996465	4.32766005531142	22.01126297466294
C	12.79432974300027	4.30747375857350	20.93889827536734
H	13.15841758868669	4.12320505119122	19.92764065493672
C	11.43458999230314	4.53869180934685	21.14901884996088
C	9.04090288882167	7.93251715978453	23.95525155748876
C	10.01169321848482	9.06564390123286	21.65694201698312
C	12.79850279651695	8.66503138972535	20.96165684438403
C	13.86865269160615	8.15087718572521	21.70527068849804
H	13.95017766396069	8.41615408801336	22.76074436403041
C	14.81716971704957	7.31875296710468	21.10535382035674
H	15.64587868752652	6.92494725468403	21.69615645209779
C	14.69520406973219	6.98288910583222	19.75675127382754
H	15.43285907715998	6.33030283290019	19.28551178996649
C	13.61470897147316	7.47052820354970	19.01322226198674
H	13.50766538912888	7.19833256518398	17.96129660378267
C	12.67443075595934	8.30937529268002	19.61024764558463
H	11.83701709779279	8.69383770115909	19.02732920114804
C	11.80945531308009	11.23624594949493	20.57217621761392
C	12.88448666499712	12.11078422306602	20.81420649690446
H	13.51358997695336	11.94361685358720	21.69254797106967
C	13.15458310179623	13.17778137455628	19.95645818826181
H	13.99992568440306	13.83821047887351	20.16038971623705
C	12.33282879005237	13.40784739197486	18.84922960629994
H	12.53146889087580	14.24832415619614	18.18143949203820
C	11.24894296778495	12.55890043670355	18.61099680181428
H	10.59567543984531	12.73394644529144	17.75368438607550
C	10.99023005107867	11.48040573707198	19.46052621085970
H	10.14537509070371	10.82680894833392	19.25752160843987
C	8.42629970191180	8.30812474231134	26.77749782533106
C	7.74505172707529	9.50951635375401	26.51901851495994
H	7.92549402802394	10.04664933255403	25.58825443400893
C	6.81510008513111	10.00826549323170	27.43152156150542
H	6.28602901576027	10.93633884252397	27.20805009182637
C	6.54845222221781	9.31664789134061	28.61754757329831
H	5.81167548681688	9.70422423968161	29.32368397625974
C	7.22100876481343	8.12297489502416	28.88905784629801
H	7.01440423221817	7.57233821216483	29.80882191312221
C	8.14933527318535	7.62386066856106	27.97142585772194
H	8.66050839090181	6.67841325365249	28.16882367424201
C	11.10581124526334	8.60776209176947	25.79987952196089
C	11.05338846294090	9.96047784583433	26.16529509993736
H	10.09788292086854	10.41396687077675	26.42790038105986
C	12.21278874648545	10.73810010939282	26.18718557630257
H	12.14858229822267	11.79443139055620	26.45507626705727
C	13.44631737688236	10.17470235456399	25.85234643008309
H	14.34992581166594	10.78671563239105	25.85962051575518
C	13.51483368365495	8.82258760889851	25.50845272828305
H	14.47433308193343	8.36864026735830	25.25289345543625
C	12.35524973392751	8.04701242791311	25.48686122936373
H	12.41222596779995	6.99621559356910	25.20180332649902
B	10.11778624464870	7.83403097062410	22.85316363928589
H	11.25180260477478	7.57030094231107	23.13200905131359
B	8.97683872202614	9.47792134640698	23.16027072267393
B	7.55362779368944	8.24499957936339	23.60055543167434
H	6.75851554094457	8.25123721567326	24.49080276000148
B	7.30344495892929	9.55427933399473	22.42970378415554
B	8.67326638337771	10.05278406224548	21.47341935965521
H	8.88506196576570	11.20533694531105	21.24936808283584
B	9.06480373017470	8.76279369649725	20.28390546466881
H	9.51329615567817	9.00486226607746	19.20401679355892
B	7.39077656710727	9.05379300878055	20.74642697746996
B	6.91619345035390	7.87665641061845	21.96241546251299
H	5.77686870851001	7.50927141509630	22.00217358104795
B	8.02553404626636	7.36685027399384	20.69886772744063
H	7.69448657175108	6.62587751119808	19.81165115529177
B	9.70614140632453	7.41813490434217	21.17770960347779
H	10.63585634070439	6.86359078688499	20.67912369343134
H	9.45013674732668	10.34093434892348	23.83894935662612
H	6.61722584557451	9.49849755379928	19.94683625789483

H	6.50808836262548	10.38007013323554	22.78107838189348
H	14.75231867857076	4.15430552734939	21.83852552266736
H	2.54384770900754	6.42446389771188	25.84841831965016
H	10.72220668082793	4.52431655023180	20.32553286617642
H	4.77403900021851	5.32687627622496	22.31013261820588
H	6.84296902795680	6.05342596870893	25.99472565296800
H	11.46702026926670	5.01444325547677	24.51619027621696

2 (isolated product, xylyl groups)

Co	8.55402005041267	6.50379886662418	22.93752156382546
P	11.71468501726361	9.87963003565017	21.95005077633607
P	9.74928698259570	7.88415686442691	25.91723311061255
N	9.64993658002357	4.90550197424760	22.89418636372034
N	7.23284856762310	5.28962959104242	23.65170643942589
C	9.00558265100712	3.81648483520941	23.32374334470085
C	7.66753901790400	4.03317884387735	23.75382228965612
C	7.09853739474372	2.75952527702883	24.20081871844968
C	5.88781642879089	2.32237342167190	24.71652757443925
H	5.05812041847286	3.01090590952521	24.87693714361505
C	5.74376050301381	0.94268251680965	25.03320920050695
H	4.78848090737625	0.60388809001126	25.43915358328038
C	6.76054210631011	0.01754897973531	24.84674259090685
H	6.60218909941494	-1.03209490084857	25.10349747841046
C	8.01816719097182	0.43507464691736	24.31647654646765
C	9.16260864511553	-0.37809974544420	24.05870208363809
H	9.12748579641760	-1.44803065617903	24.27484149835506
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H	10.53350606621564	4.07256034078786	19.12804960122819
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2’ (phenyl groups)

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  H   10.13272208593571    11.74208841344876    22.45234482098884
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H	6.30299856918055	11.02654510094670	25.03956611526838

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