Supporting Information

A Monoanionic Pentadentate Ligand Platform for Scandium-Pnictogen Multiple Bonds

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Experimental Details

General Considerations

Manipulation and storage of all air/moisture sensitive materials was performed under an argon atmosphere in an MBRAUN glove box. Reactions were performed on a double manifold high vacuum line fitted with an OxisorBW scrubber (Matheson Gas products) argon purification cartridge, using standard techniques. Glassware was stored at 135 °C in an oven overnight prior to immediate transfer to the glovebox antechamber or assembly on the vacuum line and evacuated while hot.

Toluene, THF and *n*-pentane were dried and purified using a Grubbs/Down purification system,[1] and stored in evacuated thick-walled vessels over sodium/benzophenone ketal. Benzene, benzene-d_6, toluene-d_8, and THF-d_8 were dried and stored over sodium/benzophenone ketyl. 1,2-dichlorobenzene, 1,2-dichlorobenzene-d_4, dichloromethane, and CD_2Cl_2 were dried over CaH_2. All dried solvents were degassed and vacuum transferred prior to use into thick-walled glass vessels for storage.

4-(trimethylsilyl)toluene,[2] 2,2'-[1-(6-Bromopyridin-2-yl)ethane-1,1-diyl]dipyridine,[3] lithium pyrazolate,[4] $Sc(CH_2SiMe_2Ph)_3(thf)_2$,[5] 2,6-diisopropylaniline-^{15}N,[6] and 2,6-diisopropylphosphine[7] were prepared according to literature procedures. Pyrazole was sublimed, and 2,6-diisopropylaniline was dried over CaH_2 and distilled under reduced pressure prior to use. All other chemicals were obtained from commercial suppliers and used without further purification. CO_2 (Coleman Instrument grade, 99.99%) was purchased from Air Liquide and used as received. $^{13}CO_2$ (99%) was purchased from Sigma-Aldrich and used as received.

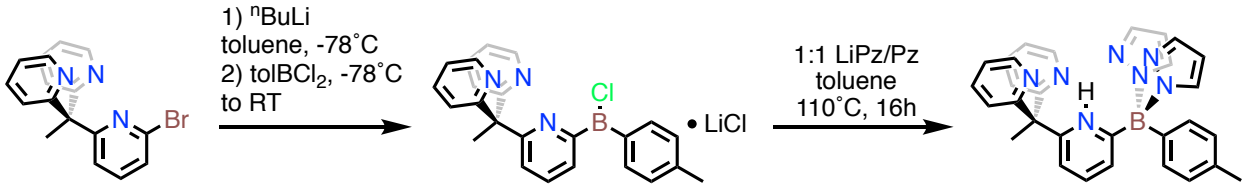
Nuclear magnetic resonance spectroscopy experiments were performed on either an Ascend-500 or Avance-600 Bruker spectrometer. All ^1H and $^{13}C\{^1H\}$ NMR spectra were internally referenced relative to Si(CH3)4 using residual solvent protons and naturally abundant ^{13}C resonances for all deuterated solvents[8], except for 1,2-dichlorobenzene-d_4 which was referenced relative to HMDSO using residual solvent

protons and naturally abundant ^{13}C resonances. ^{15}N NMR was externally referenced to 90% nitromethane in $CDCl_3$. NMR spectra were processed and analyzed with MestReNova (v. 9.0.1- 13254).

X-ray crystallographic analyses were performed by Dr. Benjamin Gelfand, and structural solutions generated by both Dr. Gelfand and Evan Patrick. Single crystals of each complex were grown as described in the experimental procedure section. Crystals were coated in Fomblin Y HVAC 140/13 oil, and a suitable crystal was selected and mounted on a glass loop. Diffraction experiments were performed on a Bruker Smart diffractometer using either a Incoatec Microfocus (Cu Kα, λ = 1.54178 Å) or Siemens Fine Focus Ceramic Tube (graphite monochromated Mo Kα, λ = 0.71069 Å), and an APEX II CCD detector. The crystal was kept at 173 K during data collection. Diffraction spots were integrated and scaled with SAINT[9] and the space group was determined with XPREP.[10] Using Olex2,[11] the structure was solved with the ShelXT[12] structure solution program using Intrinsic Phasing and refined with the ShelXL[13] refinement package using Least Squares minimization. In order to improve the completeness of the reflections collected for ***4***, the crystal was remounted to a new position, missing reflections collected, and the resulting datasets were merged isotropically with XPREP.[10] Electron density contributions from non-coordinating solvent molecules in ***2-N*** were modelled using the SQUEEZE routine in PLATON.[14] More details on individual structures can be found in Table S2.

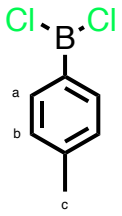
Elemental analyses were performed by Johnson Li using a Elementar UNICUBE analyzer at the Instrumentation Facility of the Department of Chemistry, University of Calgary. Infrared spectra were also collected by Mr. Li on a Nicolet Avater FT-IR spectrometer with samples prepared as KBr pellets. Solution high-resolution mass spectrometry (ESI-MS) was performed by Wade White using a Kratos MS-80 spectrometer on samples prepared in a glovebox and transported/injected via gas-tight syringe. Absorption spectra were measured using a Varian Cary-50 single beam spectrophotometer.

Experimental Procedure



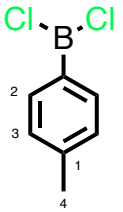
Scheme S1 – Overview of BPz_2Py_3H ligand synthesis

Dichlorotolylborane:



This is a modification of a published procedure for a similar dichloroarylborane.[15] A 50ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar was cooled to -78˚C and charged with BCl_3 (1M in DCM, 27ml, 26.78mmol) via syringe under gentle flow of argon. A solution of 4-(trimethylsilyl)toluene (3.78g, 24.34mmol) in DCM (~3-5ml) was then added dropwise via syringe. The vessel was then sealed, slowly warmed to 0˚C, and stirred for 1 hour. The reaction mixture was then allowed to warm to room temperature and stirred overnight. The vessel was then cooled to 0˚C, and the volatiles were carefully removed *in vacuo* (since the product is also volatile). To isolate > 95% pure material, vacuum was applied at 0˚C for 3-4 hours, checking progress by NMR. Product was obtained as a yellowish oil that solidifies upon cooling (3.64g, 92%) and stored at -30˚C. Though dichlorotolylborane is known in the literature, no NMR data could be found.

^{1}H NMR (500 MHz, Benzene-d_6) δ 7.96 (d, J = 7.8 Hz, 2H_a), 6.85 (d, J = 7.7 Hz, 2H_b), 1.93 (s, 3H_c).

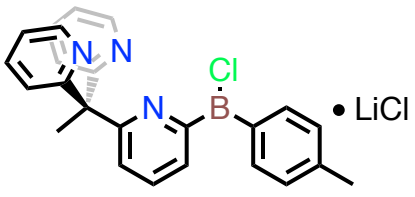


^{11}B{^{1}H} NMR (161 MHz, C_6D6) δ 55.54.

^{13}C{^{1}H} NMR (126 MHz, Benzene-d_6) δ 146.46 (C_1), 137.47(C_2), 129.17(C_3), 21.71 (C_4), B-**C_{ipso}** was not observed.

BPz_2Py_3H:

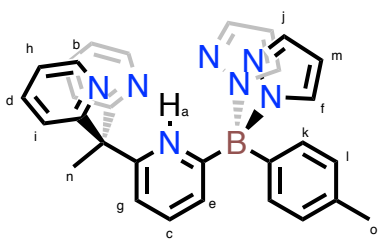
Part A:



A 2-neck 500ml RBF was charged with a stirbar, 2,2'-[1-(6-Bromopyridin-2-yl)ethane-1,1-diyl]dipyridine (5.480g, 16.1mmol), and toluene (150ml), and cooled to

-78˚C. ^{n}BuLi (1.6M in hexanes, 10.1ml, 16.2mmol) was added dropwise via syringe turning the orange solution deep red, and stirred for 1h. Separately, a 2-neck 500ml RBF was charged with a stirbar, dichlorotolylborane (3.059g, 17.7mmol), and attached to the long end of a large diameter swivel frit. Toluene (100ml) was then added via vacuum transfer, and the solution cooled to -78˚C. With both sides at -78˚C, and while swabbing the needle with LN_2, the lithiate solution was then cannula transferred onto the borane solution dropwise, turning cloudy beige/orange. Once complete, the mixture was stirred at -78˚C for 1h, slowly warmed to RT, and stirred for an additional 1h. The precipitate was then collected on the frit, washed with pentane (3x100ml), and dried *in vacuo*. The resulting crude beige solid was then used in the next step without further purification.

Part B:



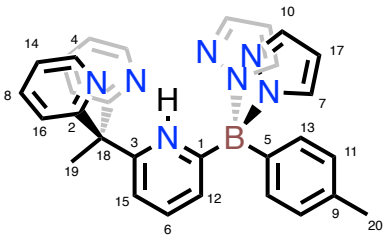
In a 500ml RBF, product from Part A (5.738g, 13.0mmol), pyrazole (0.888g, 13.0mmol), lithium pyrazolate (0.965g, 13.0mmol), and a stirbar were combined and attached to the long end of a swivel frit. Toluene (150ml) was then vacuum transferred in, and the solution heated to 105˚C for 12 hours. The red solution was then filtered, concentrated under vacuum (~40ml), and set to crystallize at -30˚C. After four days, the first crop of faint pink crystals was collected, washed with pentane, and dried *in vacuo*. A second crop of crystals was obtained by concentrating the toluene filtrate further (~20ml) and cooling again to -30˚C (total isolated material 4.567g, 57% over both steps). Single crystals suitable for x-ray diffraction were grown from a concentrated toluene solution at -30˚C. Elemental Analysis: Calcd. (%) for $C_{30}H_{28}BN_7$: C, 72.44; H, 5.67; N, 19.71. Found: C, 72.09; H, 5.43; N, 19.25.

^{1}H NMR (500 MHz, CD_2Cl_2) δ 17.02 (s, 1H, H_a), 8.50 (ddd, J = 4.8, 1.9, 0.9 Hz, 2H, H_b), 7.94 (t, J = 7.9 Hz, 1H, H_c), 7.71 (td, J = 7.8, 1.9 Hz, 2H, H_d), 7.59 (dd, J = 7.9, 1.2 Hz, 1H, H_e), 7.41 (d, J = 1.6 Hz, 2H, H_f), 7.29 (dd, J = 8.1, 1.3 Hz, 1H, H_g), 7.25 (ddd, J = 7.6, 4.8, 1.0 Hz, 2H, H_h), 7.22 (dt, J = 8.0, 1.1 Hz, 2H, H_i), 7.07 (d, J = 2.2 Hz, 2H, H_j), 7.01

(d, J = 7.6 Hz, 2H, H_k), 6.80 (d, J = 7.6 Hz, 2H, H_l), 6.17 (t, J = 1.9 Hz, 2H, H_m), 2.39 (s, 3H, H_n), 2.30 (s, 3H, H_o).

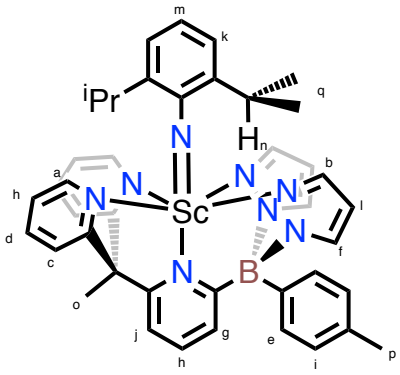
$^{11}B\{^1H\}$ NMR (161 MHz, CD_2Cl_2) δ -1.23.

$^{13}C\{^1H\}$ NMR (126 MHz, CD_2Cl_2) δ 174.39 (br, C_1), 162.71(C_2), 157.70(C_3), 149.62(C_4), 145.62(br, C_5), 141.22(C_6), 139.61(C_7), 137.27(C_8), 136.04(C_9), 134.56(C_{10}), 133.11(C_{11}), 129.92(C_{12}), 128.36(C_{13}), 123.30(C_{14}), 122.86(C_{15}), 122.79(C_{16}), 103.88(C_{17}), 58.43(C_{18}), 27.07(C_{19}), 21.28(C_{20}).



***2-N**:*

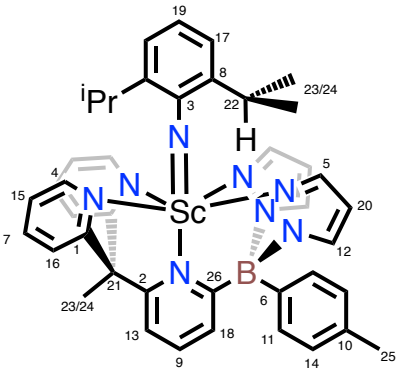
A 50ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar was charged with BPz_2Py_3H (214mg, 0.43mmol), $Sc(CH_2SiMe_2Ph)_3(thf)_2$ (274mg, 0.43mmol), and toluene (10 ml), and stirred until all material dissolved, turning the solution orange. A solution of 2,6-diisopropylaniline (76mg, 0.43mmol) in toluene (5 ml) was then added, and the mixture stirred for 5 days. The dark mixture was then filtered through a fine porosity frit, washed with toluene (2ml) and pentane (3x10ml). The resulting purple solid (175mg, 57%) was stored at -30˚C. Similarly, the ^{15}N labelled material (**2-^{15}N**) was synthesized using 2,6-diisopropylaniline-^{15}N. Since this material was found to be extremely sensitive to air, moisture, as well as dichloromethane, it could only be handled in a *rigorously* maintained glovebox atmosphere. It was also found to be thermally sensitive as an isolated solid, and degrades over time at room temperature or upon drying completely under high vacuum. Single crystals suitable for x-ray diffraction were obtained by layering toluene onto a concentrated solution of ***2-N*** in THF. Elemental Analysis: Calcd. (%) for **2-N•toluene (**$C_{49}H_{52}BN_8Sc$**):** C, 72.77; H, 6.48; N, 13.85. Found: C, 72.45; H, 6.59; N, 13.60.



^{1}H NMR (500 MHz, THF-d_8) δ 9.88 (dd, J = 5.2, 1.8 Hz, 2H, H_a), 8.30 (d, J = 2.0 Hz, 2H, H_b), 7.97 (d, J = 8.3 Hz, 2H, H_c), 7.91 (td, J = 8.3, 1.7 Hz, 2H, H_d), 7.71 (d, J = 7.9 Hz, 2H, H_e), 7.61 (d, J = 2.3 Hz, 2H, H_f), 7.58 (dd, J = 8.3, 1.1 Hz, 1H, H_g), 7.48 – 7.39 (m, 3H, H_h), 7.25 (d, J = 7.9 Hz, 2H, H_i), 7.18 – 7.16 (m, 1H, H_j), 6.41 (d, J = 7.3 Hz, 2H, H_k), 6.12 (t, J = 2.1 Hz, 2H, H_l), 5.83 (t, J = 7.3 Hz, 1H, H_m), 3.76 (hept, J = 6.8 Hz, 2H, H_n), 2.74 (s, 3H, H_o), 2.41 (s, 3H, H_p), 0.62 (d, J = 6.9 Hz, 12H, H_q).

^{11}B{^{1}H} NMR (161 MHz, THF-d_8) δ -0.46.

^{13}C{^{1}H} NMR (126 MHz, THF-d_8) δ 175.52 (observed in HMBC but not in ^{13}C{^{1}H}, C_{26}), 159.73 (C_1), 158.65(C_2), 156.63 (C_3), 152.60 (C_4), 143.83 (C_5), 143.14 (br, C_6), 139.89 (C_7), 139.30 (C_8), 136.74 (C_9), 136.55 (C_{10}), 136.33 (C_{11}), 135.77 (C_{12}), 129.88 (C_{13}), 128.84 (C_{14}), 122.94 (C_{15}), 122.33 (C_{16}), 121.19 (C_{17}), 118.84 (C_{18}), 108.20 (C_{19}), 104.05 (C_{20}), 53.96 (C_{21}), 26.36 (C_{22}), Overlapping with THF signal at 25.14 (C_{23}/C_{24}), 21.17 (C_{25}).

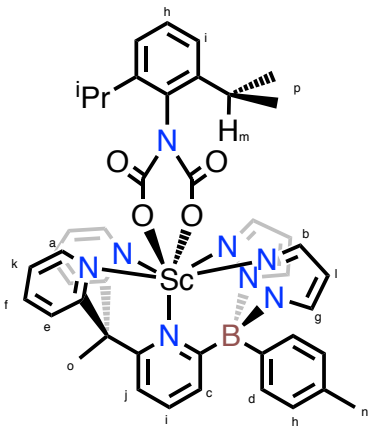


^{15}N NMR (^{15}N enriched sample, 61 MHz, *o*-$C_6Cl_2D_4$) δ 291.80 (s).

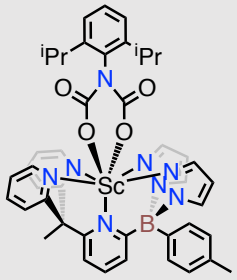
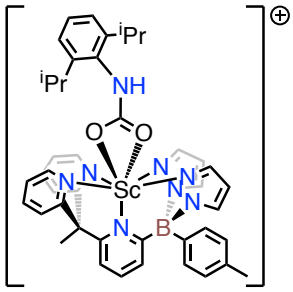
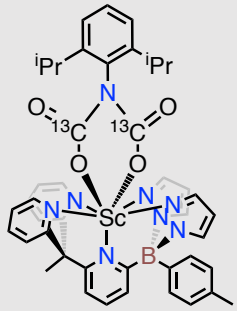
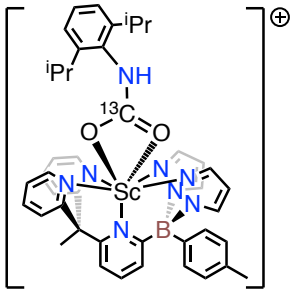
FT-IR $\nu_{Sc\text{-}N}$: 920 cm^{-1}

***3-N**:*

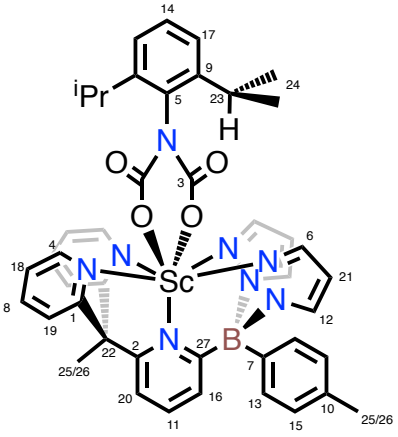
A 50ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar was charged with **2-N** (48mg, 0.07mmol) and THF (5 ml). After three freeze-pump-thaw cycles, the flask was placed under 1atm of CO_2, immediately turning the deep purple solution very faint yellow/colorless. After stirring 30 minutes, a white precipitate formed, which was collected on a fine porosity frit and washed with THF (5ml), pentane (3x5ml), and dried *in vacuo*. (29mg, 54%). Similarly, the ^{13}C/^{15}N labelled materials were synthesized using $^{13}CO_2$ and/or **2-^{15}N**. Elemental Analysis: Calcd. (%) for **(**$C_{44}H_{44}BN_8O_4Sc$**):** C, 65.68; H, 5.51; N, 13.93. Found:



C, 62.33; H, 5.40; N, 12.96. Results for EA are consistently low in carbon and nitrogen, presumably due to incomplete combustion.

HRMS (ESI)	*Ion observed (loss of $^{n}CO_2$, gain of H^+)*	*m/z* calcd	*m/z* found
 $C_{44}H_{44}BN_8O_4Sc$		761.3318	761.3313
 $C_{42}{}^{13}C_2H_{44}BN_8O_4Sc$		762.3346	762.3310

^{1}H NMR (500 MHz, *o*-$Cl_2C_6D_4$) δ 10.34 (d, *J* = 5.5 Hz, 2H, H_a), 8.92 (d, 2H, H_b), 7.60 (d, *J* = 7.0 Hz, 1H, H_c), 7.46 (d, *J* = 7.0 Hz, 2H, H_d), 7.30 (d, *J* = 8.3 Hz, 2H, H_e), 7.22 (t, *J* = 7.8 Hz, 2H, H_f), 7.17 (d, 2H, H_g), 7.13 – 7.10 (m, 3H, H_h), 7.07 – 7.03 (m, 3H, H_i), 6.93 (d, *J* = 7.7 Hz, 1H, H_j), 6.76 (t, *J* = 6.0 Hz, 2H, H_k), 5.88 (d, *J* = 2.4 Hz, 2H, H_l), 3.13 (hept, *J* = 6.3 Hz, 2H, H_m), 2.27 (s, 3H, H_n), 2.23 (s, 3H, H_o), 1.04 (d, *J* = 6.2 Hz, 12H, H_p).



^{11}B{^{1}H} NMR (161 MHz, *o*-$Cl_2C_6D_4$): peak too broad to observe.

^{13}C{^{1}H} NMR (126 MHz, *o*-$Cl_2C_6D_4$) δ 174.66 (observed in HMBC but not in ^{13}C{^{1}H}, C_{27}), 157.19 (C_1), 156.59 (C_2), 153.99 (C_3), 151.45 (C_4), 144.42 (C_5), 142.81 (C_6), 138.37 (C_7), 137.51 (C_8), 136.02 (C_9), 134.72 (C_{10}), 134.53 (C_{11}),

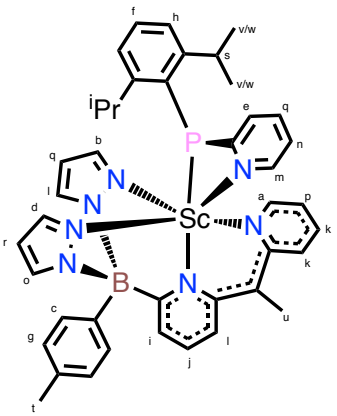
134.32 (C_{12}), 133.62 (C_{13}), 127.27 (C_{14}), 126.87 (C_{15}), 126.77 (C_{16}), 121.13 (C_{17}), 120.88 (C_{18}), 119.12 (C_{19}), 116.68 (C_{20}), 102.14 (C_{21}), 50.77 (C_{22}), 26.84 (C_{23}), 22.07 (C_{24}), 19.37 ($C_{25/26}$).

$^{13}C\{^{1}H\}$ NMR ($^{13}C/^{15}N$ enriched sample, 151 MHz, *o*-$C_6Cl_2D_4$) δ 153.98 (d, $^{1}J_{CN}$ = 17.4 Hz).

^{15}N NMR ($^{13}C/^{15}N$ enriched sample, 61 MHz, *o*-$C_6Cl_2D_4$) δ 136.85 (t, $^{1}J_{NC}$ = 17.3 Hz).

FT-IR: $\nu_{C=O}$: 1632 cm^{-1}, 1685 cm^{-1}

4:



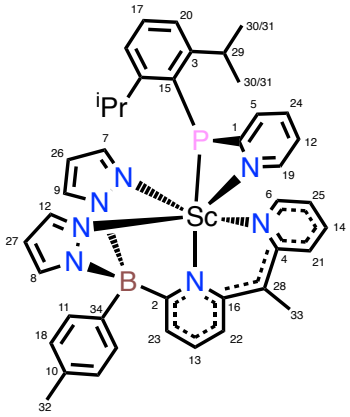
A 50ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar was charged with BPz_2Py_3H (90mg, 0.18mmol), $Sc(CH_2SiMe_2Ph)_3(thf)_2$ (115mg, 0.18mmol), and benzene (5 ml), and stirred until all material dissolved, turning the solution orange. A solution of 2,6-diisopropylphosphine (35mg, 0.18mmol) in benzene (5 ml) was then added, and the mixture stirred for 5 days resulting in a blood-red solution. The solvent was then removed *in vacuo*, and the oily solid lyophilized from benzene. The dark red powder was then extracted with pentane (4ml), filtered through a fine porosity frit, and the solution cooled to -50˚C for 3 days yielding x-ray quality red crystals that were isolated (85mg, 58%) and stored at -50˚C. This product is thermally sensitive as a solid, and could only be isolated pure as single crystals with 1 equivalent of pentane present. Elemental Analysis: Calcd. (%) for ***4•pentane*** **(**$C_{47}H_{56}BN_7PSc$**):** C, 70.06; H, 7.01; N, 12.17. Found: C, 69.91; H, 6.70; N, 12.27.

^{1}H NMR (500 MHz, C_6D_6) δ 8.54 (d, *J* = 5.2 Hz, 1H, H_a), 8.04 (d, *J* = 1.8 Hz, 1H, H_b), 8.01 (d, *J* = 7.7 Hz, 2H, H_c), 7.93 (d, *J* = 2.1 Hz, 1H, H_d), 7.40 (d, *J* = 5.4 Hz, 1H, H_e), 7.31 (t, *J* = 7.6 Hz, 1H, H_f), 7.27 (d, *J* = 7.7 Hz, 2H, H_g), 7.21 (d, *J* = 7.6 Hz, 2H, H_h), 7.04 (d, *J* = 6.9 Hz, 1H, H_i), 6.93 (dd, *J* = 8.7, 6.9 Hz, 1H, H_j), 6.90 – 6.87 (m, 2H, H_k), 6.87 – 6.81 (m, 2H, H_l), 6.62 (d, *J* = 8.3 Hz, 1H, H_m), 6.30 (t, *J* = 7.5 Hz, 1H, H_n), 6.27 (d, *J* = 2.0 Hz, 1H, H_o), 6.23 (td, *J* = 5.7, 2.6 Hz, 1H, H_p), 5.75 – 5.69 (m, 2H, H_q), 5.62

(t, J = 2.2 Hz, 1H, H_r), 4.16 (s, 2H, H_s), 2.35 (s, 3H, H_t), 2.18 (s, 3H, H_u), 1.15 (s, 6H, $H_{v/w}$), 0.92 (s, 6H, $H_{v/w}$).

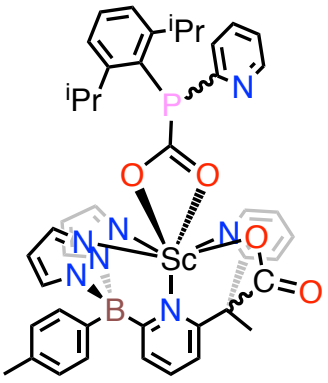
$^{11}B\{^1H\}$ NMR (161 MHz, C_6D_6) δ 0.57.

^{31}P NMR (203 MHz, C_6D_6) δ -40.49.



$^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6) δ 186.20 (d, J = 36.7 Hz, C_1), 168.10 (br, C_2), 155.73 (br, C_3), 151.70 (d, J = 3.2 Hz, C_4), 145.94 (d, J = 6.6 Hz, C_5), 144.98 (d, J = 10.7 Hz, C_6), 140.50 (d, J = 5.1 Hz, C_7), 140.42 (br, C_{34}) 140.02 (C_8), 137.62 (C_9), 136.95 (C_{10}), 136.22 (C_{11}), 135.58 (C_{12}), 135.55 (C_{13}), 135.13 (C_{14}), 134.18 (d, J = 27.2 Hz, C_{15}), 133.66 (C_{16}), 129.44 (C_{17}), 129.07 (C_{18}), 124.81 (C_{19}), 123.71 (d, J = 3.1 Hz, C_{20}), 119.69 (C_{21}), 117.27 (C_{22}), 116.93 (C_{23}), 111.93 (d, J = 5.4 Hz, C_{24}), 109.02 (C_{25}), 104.22 (C_{26}), 104.08 (C_{27}), 79.99 (C_{28}), 34.19 (d, J = 11.7 Hz, C_{29}), 25.33 (C_{30}), 24.52 (C_{31}), 21.46 (C_{32}), 18.06 (C_{33}).

***5**:*



Method A: A 25ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar was charged with ***4•pentane*** (35mg, 0.04mmol) and benzene (10 ml), producing a blood red solution. The vessel was then evacuated of gas via three freeze-pump-thaw cycles, then placed under 1 atm of CO_2, immediately turning the solution a very light pink color. The solution was stirred for 15min, then allowed to stand at RT overnight, after which the white precipitate that was produced was collected on a fine porosity frit, washed with pentane (3x2ml) and dried *in vacuo* (21mg, 59%). Similarly, ^{13}C labelled material was generated using $^{13}CO_2$.

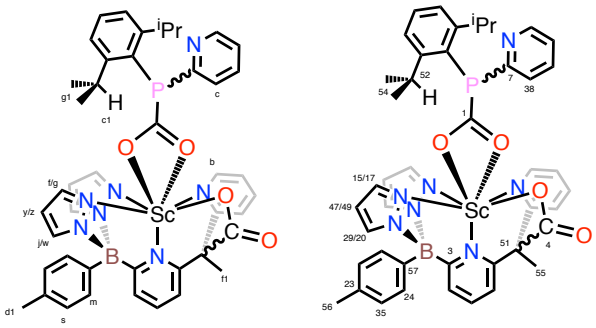
Method B: A 50ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar was charged with BPz_2Py_3H (84mg, 0.17mmol), $Sc(CH_2SiMe_2Ph)_3(thf)_2$ (108mg, 0.17mmol), and benzene (5 ml), and stirred until all material dissolved, turning the solution

orange. A solution of 2,6-diisopropylphosphine (33mg, 0.17mmol) in benzene (5 ml) was then added, and the mixture stirred for 5 days resulting in a blood-red solution. The solution was then filtered through a fine porosity frit, and quantitatively transferred into another 50ml thick-walled glass vessel equipped with a Kontes PTFE tap and stirbar with additional benzene (3x2ml). The vessel was then evacuated of gas via three freeze-pump-thaw cycles, then placed under 1 atm of CO_2, gradually turning the solution an orange/pink color over 5 min. The solution was stirred overnight, after which it was concentrated to ~10ml *in vacuo* and cooled to 5˚C for 2h. The white precipitate that was produced was collected on a fine porosity frit, washed with pentane (3x5ml) and dried *in vacuo* (45mg, 32%).

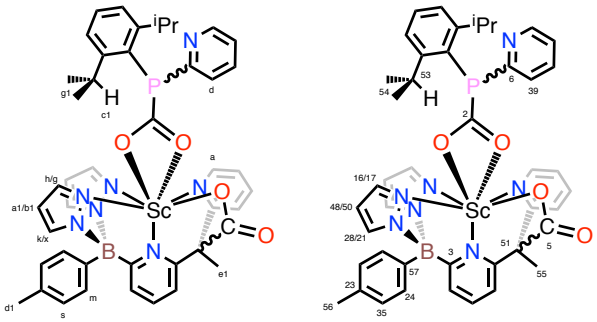
Elemental Analysis: Calcd. (%) for **(**$C_{44}H_{44}BN_7O_4PSc$**):** C, 64.32; H, 5.40; N, 11.93. Found: C, 64.41; H, 5.64; N, 11.97.

Due to the presence of both diastereomers (3:1 ratio) the 1H and $^{13}C\{^1H\}$ NMR spectra of ***5*** are quite complex and contain many overlapping signals, making deconvolution of peaks difficult. As a result, these could only partially be assigned:

"Major"



"Minor"



^{1}H NMR (600 MHz, THF-d_8) δ 9.43 (d, J = 5.0 Hz, 1H, H_a), 9.19 (dd, J = 5.5, 1.8 Hz, 3H, H_b), 8.56 (d, J = 8.5 Hz, 3H, H_c), 8.46 (d, J = 8.0 Hz, 1H, H_d), 8.38 (d, J = 4.3 Hz, 4H, H_e), 8.22 (d, J = 2.0 Hz, 3H, H_f), 8.21 – 8.18 (m, 4H, H_g), 8.10 (d, J = 2.1 Hz, 1H, H_h), 7.96 – 7.92 (m, 1H, H_i), 7.89 (d, J = 2.3 Hz, 3H, H_j), 7.87 – 7.83 (m, 4H, H_k), 7.81 (d, J = 8.2 Hz, 1H, H_l), 7.77 – 7.74 (m, 13H, H_m), 7.66 – 7.63 (m, 5H, H_n), 7.59 – 7.54 (m, 5H, H_o), 7.53 – 7.51 (m, 4H, H_p), 7.48 – 7.44 (m, 1H, H_q), 7.38 – 7.34 (m, 1H, H_r), 7.32 – 7.28 (m, 14H, H_s), 7.15 (dd, J = 7.9, 3.0 Hz, 3H, H_t), 7.11 – 7.07 (m, 7H, H_u), 7.07 – 7.03 (m, 2H, H_v), 6.95 (d, J = 2.3 Hz, 3H, H_w), 6.92 (d, J = 2.3 Hz, 1H, H_x), 6.13 (t, J = 2.2 Hz, 3H, H_y), 6.09 (t, J = 2.2 Hz, 3H, H_z), 6.07 (t, J = 2.0 Hz, 1H, H_{a1}), 6.03 (t, J = 2.4 Hz, 1H, H_{b1}), 3.79 – 3.59 (m, 8H, H_{c1}), 2.42 (s, 12H, H_{d1}), 2.20 (s, 3H, H_{e1}), 2.18 (s, 9H, H_{f1}), 0.86 – 0.83 (m, 48H, H_{g1}).

^{11}B{^{1}H} NMR (161 MHz, THF-d_8) δ -0.87.

^{31}P{^{1}H} NMR (203 MHz, THF-d_8) δ -31.59, -32.15.

^{13}C{^{1}H} NMR (151 MHz, THF-d_8) δ 198.57 (d, $^{1}J_{CP}$ = 15.0 Hz, C_1), 198.05 (d, $^{1}J_{CP}$ = 16.1 Hz, C_2), 174.30 (br, C_3), 169.54 (C_4), 169.43 (C_5), 163.51 (d, J = 9.2 Hz, C_6), 162.81 (d, J = 9.3 Hz, C_7), 161.28 (C_8), 160.95 (C_9), 160.20 (C_{10}), 160.11 (C_{11}), 156.45 (C_{12}), 149.95 (C_{13}), 142.62 (C_{14}), 142.54 (C_{15}), 142.13 (C_{16}), 141.85 (C_{17}), 141.02 (br, C_{57}), 140.66 (C_{18}), 140.46 (C_{19}), 138.31 (C_{20}), 138.03 (C_{21}), 137.65 (C_{22}), 137.27 (C_{23}), 136.25 (C_{24}), 135.96 (C_{25}), 135.72 (d, J = 3.1 Hz, C_{26}), 135.56 (C_{27}), 135.42 (C_{28}), 135.20 (C_{29}), 131.43 (C_{30}), 131.31 (C_{31}), 129.57 (C_{32}), 129.51 (C_{33}), 129.29 (C_{34}), 129.17 (C_{35}), 129.05 (C_{36}), 128.73 (C_{37}), 127.55 (d, J = 20.3 Hz, C_{38}), 127.17 (d, J = 18.0 Hz, C_{39}), 123.92 (C_{40}), 123.12 (C_{41}), 122.35 (C_{42}), 122.04 (C_{43}), 121.87 (C_{44}), 119.58 (C_{45}), 119.53 (C_{46}), 104.69 (C_{47}), 104.66 (C_{48}), 104.48 (C_{49}), 104.42 (C_{50}), 60.21 (C_{51}), 34.28 (d, C_{52}), 34.12 (d, C_{53}), 23.69 (C_{54}), 22.57 (C_{55}), 21.15 (C_{56}).

^{31}P{^{1}H} NMR (^{13}C enriched sample**,** 203 MHz, C_6D_6) δ -30.66 (d, $^{1}J_{PC}$ = 15.5 Hz, major product), -31.07 (d, $^{1}J_{PC}$ = 16.9 Hz, minor product).

^{13}C{^{1}H} NMR (^{13}C enriched sample, 126 MHz, C_6D_6) δ 199.09 (d, $^{1}J_{CP}$ = 15.6 Hz, major), 198.64 (d, $^{1}J_{CP}$ = 16.8 Hz, minor), 169.88 (s, major), 169.82 (s, minor).

Supporting Figures

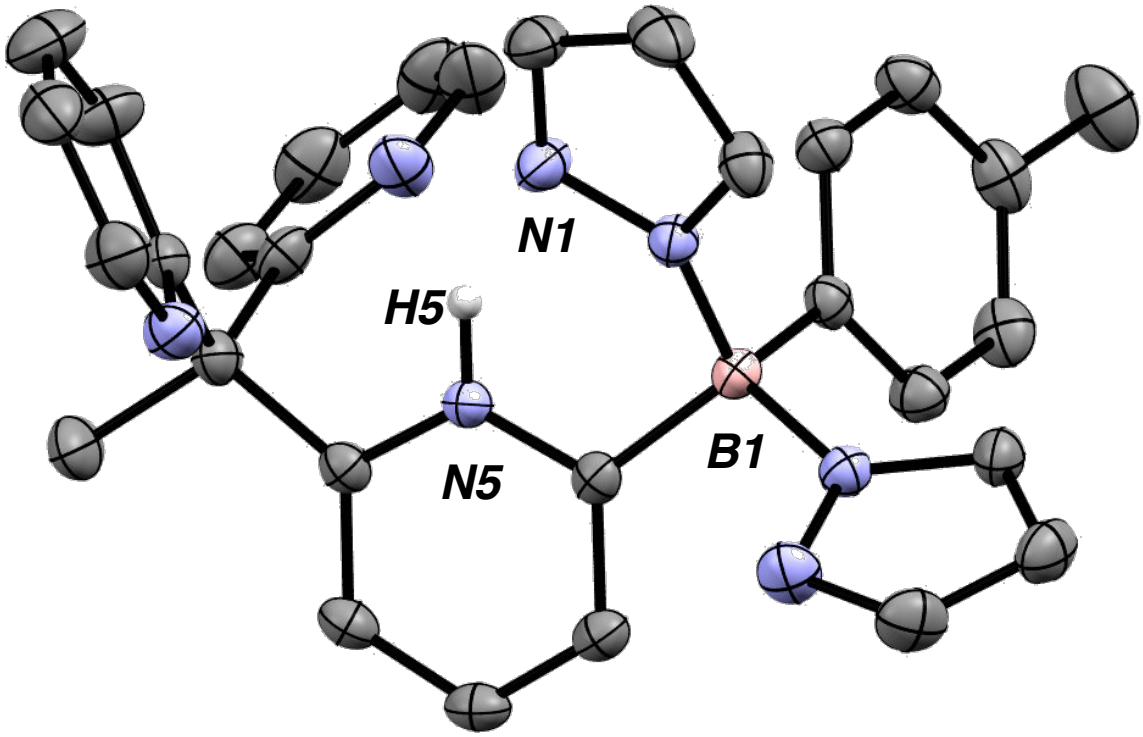


Figure S1 - Molecular structure of BPz_2Py_3H. Most hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level. Selected bond length (Å) for BPz_2Py_3H: N1–H5, 1.86(2)

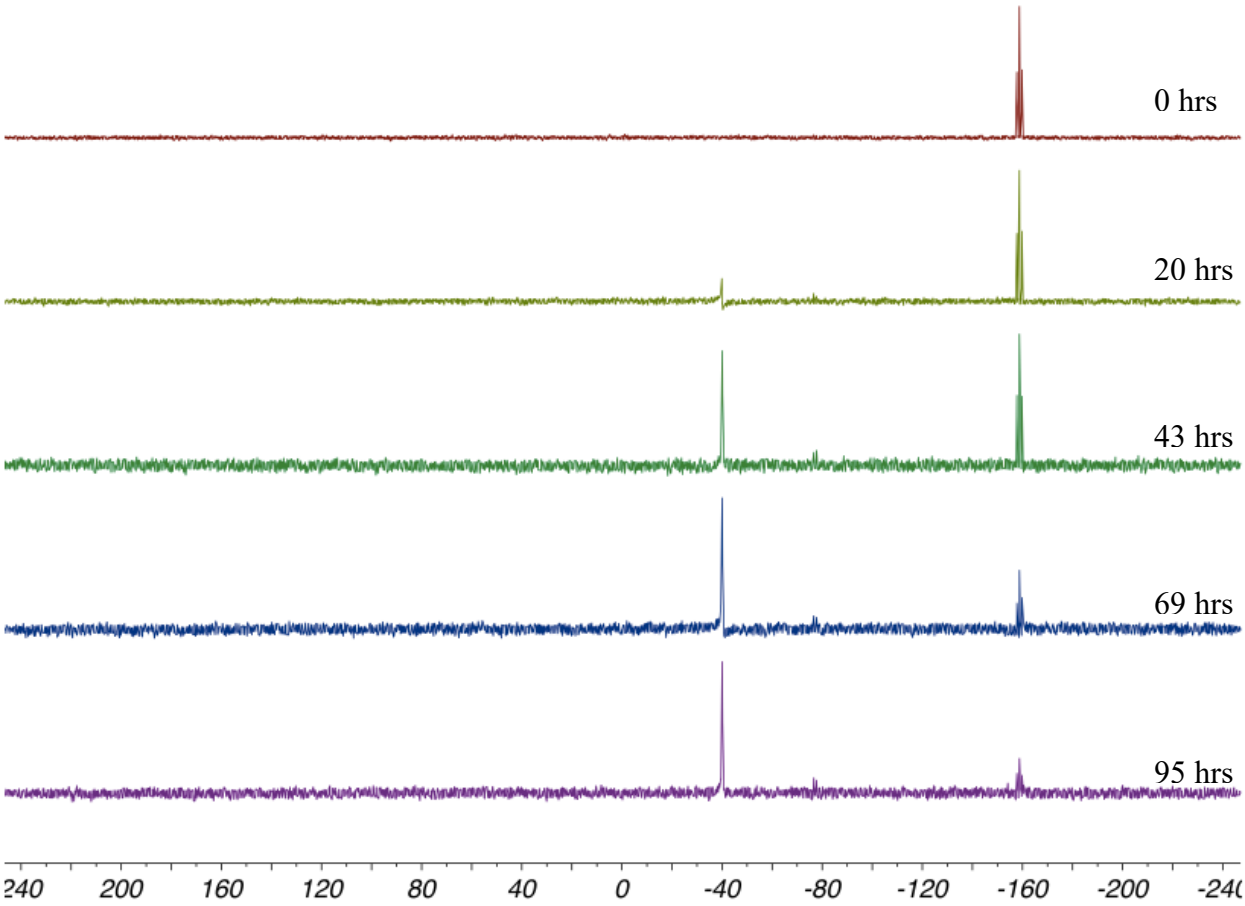


Figure S2 - Monitoring reaction progress of 1 + 2,6-diisopropylphosphine by ^{31}P NMR in toluene-d_8. Loss of 2,6-diisopropylphosphine starting material at -158.8ppm (t, $^{1}J_{PH}$ = 203.6 Hz) produces an intermediate doublet at -77.2ppm (d, $^{1}J_{PH}$ = 221.0 Hz), which is quickly consumed to yield the product 4 at -40.5ppm.

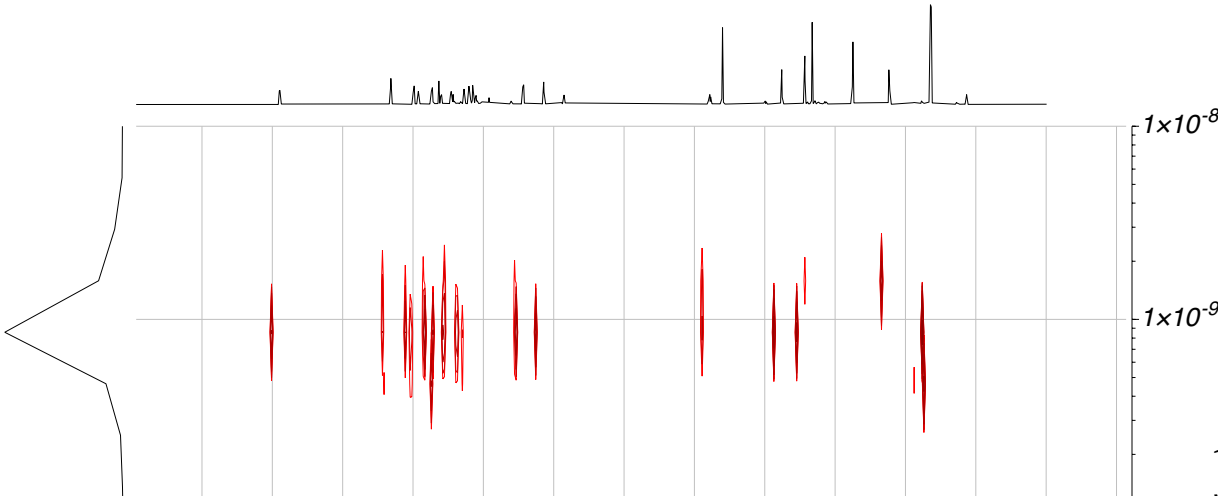


Figure S3 - 2D DOSY spectrum of 2-N at approx. 0.02M in thf-d_8 at 298K. The gradient amplitude was varied from 2% to 95% with an optimized δ (gradient pulse length) of 2000μs and a Δ(diffusion time) of 75ms. Diffusion coefficient was measured as 8.5 × 10^{-10} m^2s^{-1} (units of vertical axis are m^2s^{-1}).

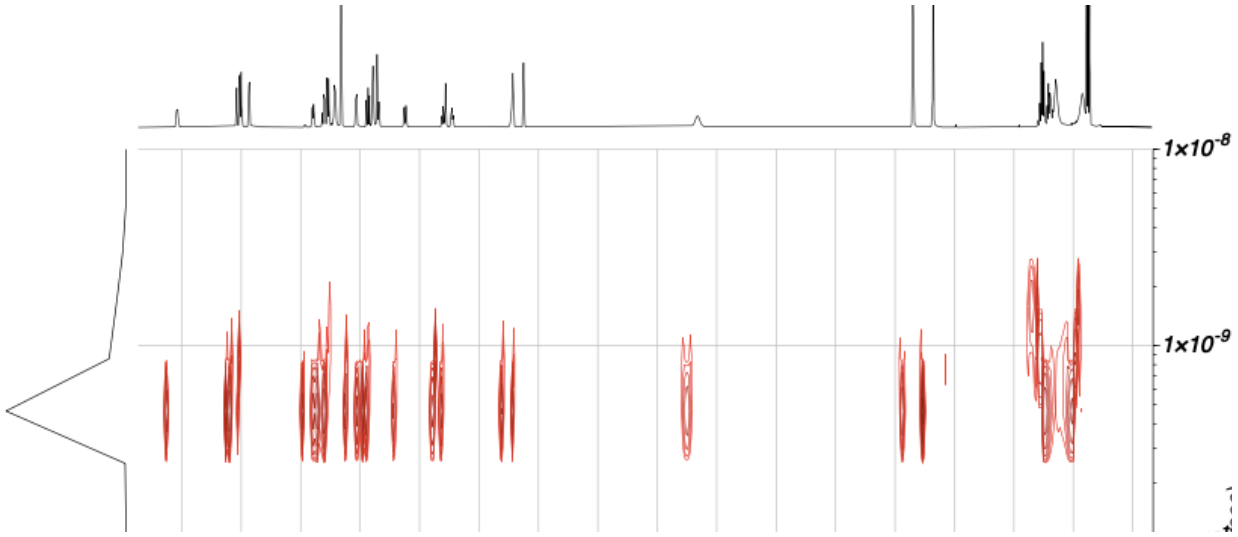


Figure S4 - 2D DOSY spectrum of 4 at approx. 0.02M in C_6D_6 at 298K. The gradient amplitude was varied from 2% to 95% with an optimized δ (gradient pulse length) of 2500μs and a Δ(diffusion time) of 75ms. Diffusion coefficient was measured as 6.7 × 10^{-10} m^2s^{-1} (units of vertical axis are m^2s^{-1}).

Compound	D ($\times 10^{-10}$ m^2s^{-1})	r (Å)
2-N	8.5±0.5	5.3±0.7
4	6.7±0.4	5.1±0.5
2_{Sc}-H*	4.8±0.5	7.1±0.7
2_{Sc}-Me*	6.9±0.5	5.0±0.7
3_{Sc}*	4.8±0.5	7.1±0.7

Table S1 - Diffusion coefficients determined from 2D DOSY NMR, and the respective hydrodynamic radii calculated using the Stokes-Einstein equation. Estimated standard error was obtained from the width of a Gaussian lineshape in the diffusion domain.[16] All samples were measured in C_6D_6, with the exception of 2-N which was measured in thf-d_8. Viscosity of C_6D_6 (0.6392 mPa•s)[17] and THF (0.4766 mPa•s)[18] solvent at 298K were used. Values for other dimeric (2_{Sc}-H, 3_{Sc}) and monomeric (2_{Sc}-Me) Sc complexes of the related [B_2Pz_4Py] ligand are included for comparison.[19]

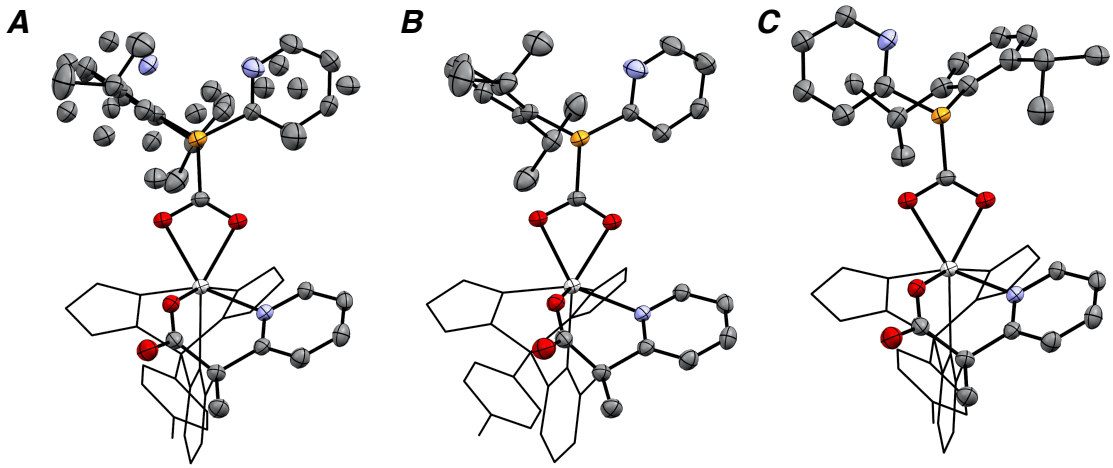


Figure S5 – Molecular structure of 5 (A, complete disordered structure) and the major (B, 92%) and minor (C, 8%) components that were modeled. Hydrogen atoms omitted and borate fragment of ligand depicted as wire-frame for clarity. Thermal ellipsoids are shown at the 50% probability level.

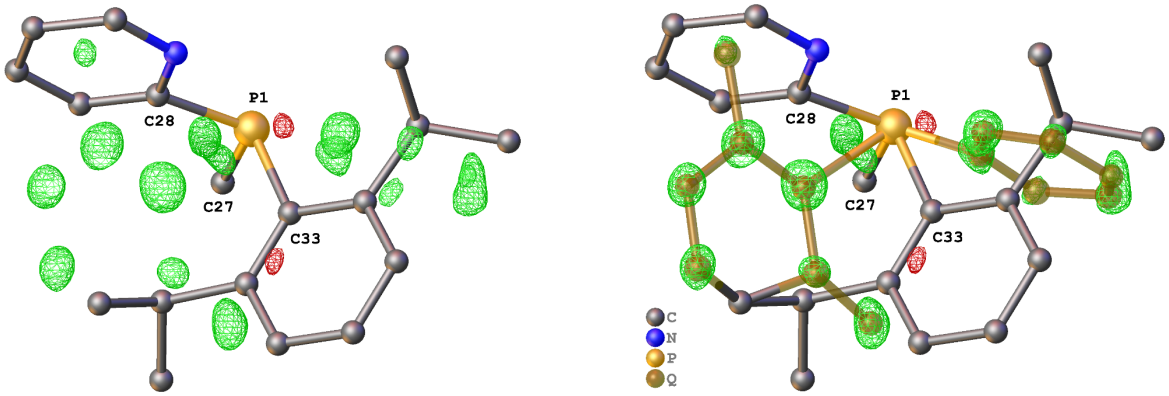


Figure S6 - Left: Residual electron density around the phosphine in 5 (prior to assignment of the disorder). Right: residual electron density around the phosphine in 5, and the corresponding Q-peaks, which highlights the presence of the opposite diastereomer. The remainder of 5 and hydrogen atoms have been omitted for clarity.

Characterization Data

NMR Data

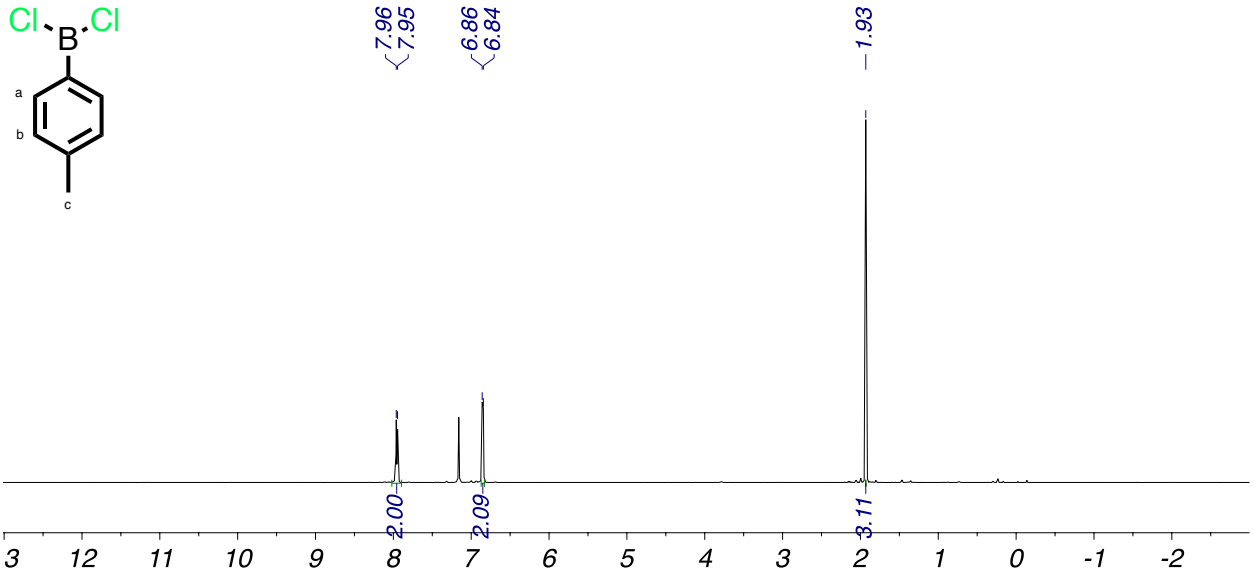


Figure S7 ^{1}H NMR of dichlorotolylborane in C_6D_6

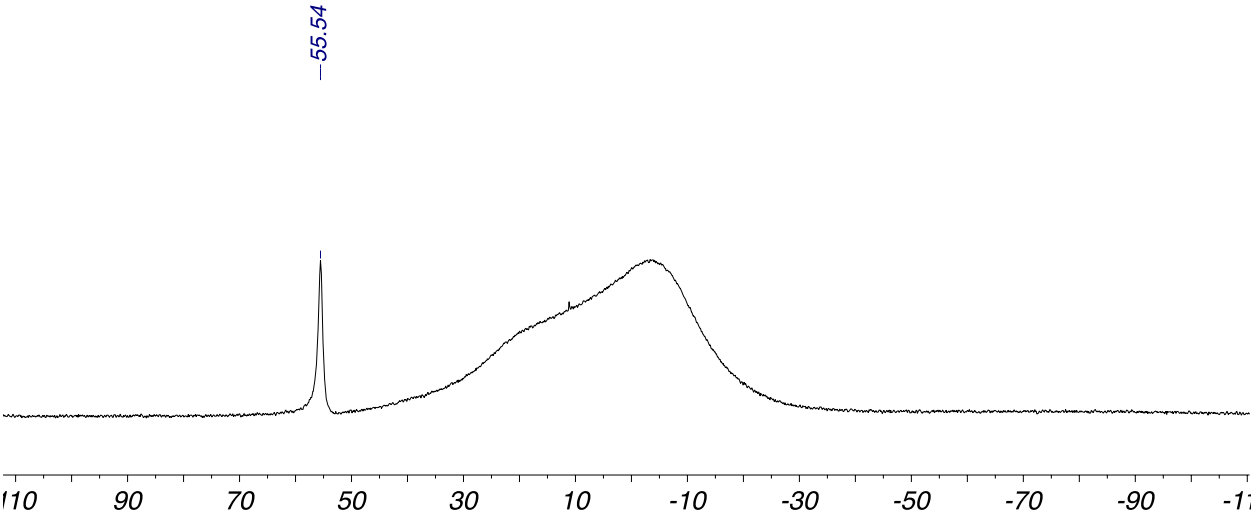


Figure S8 ^{11}B NMR of dichlorotolylborane in C_6D_6.

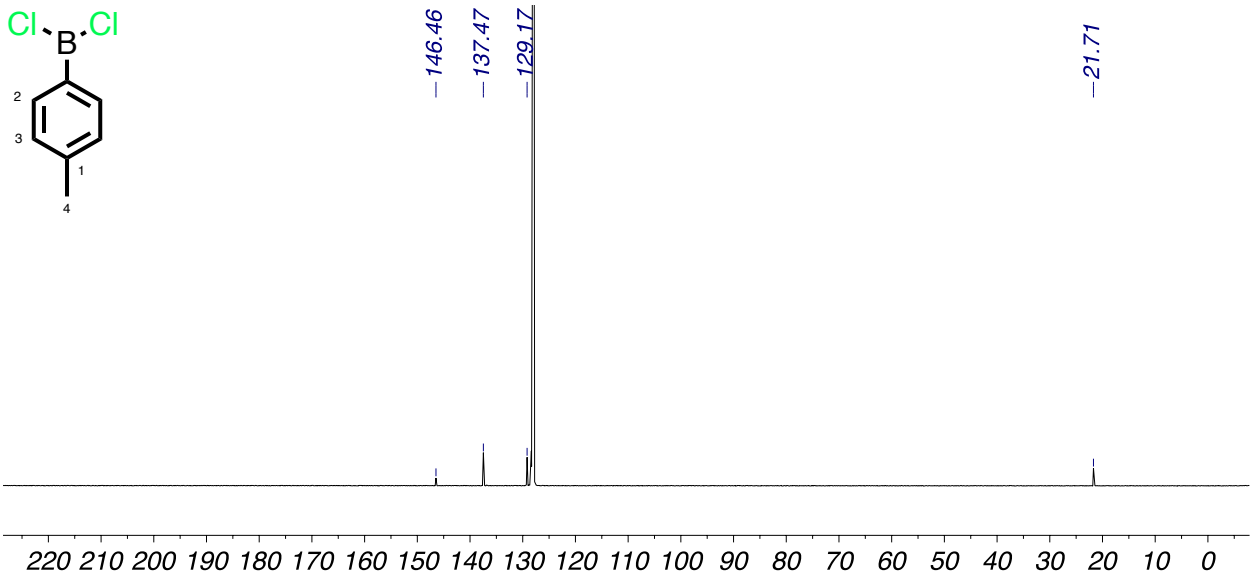


Figure S9 $^{13}C\{^{1}H\}$ NMR of dichlorotolylborane in C_6D_6.

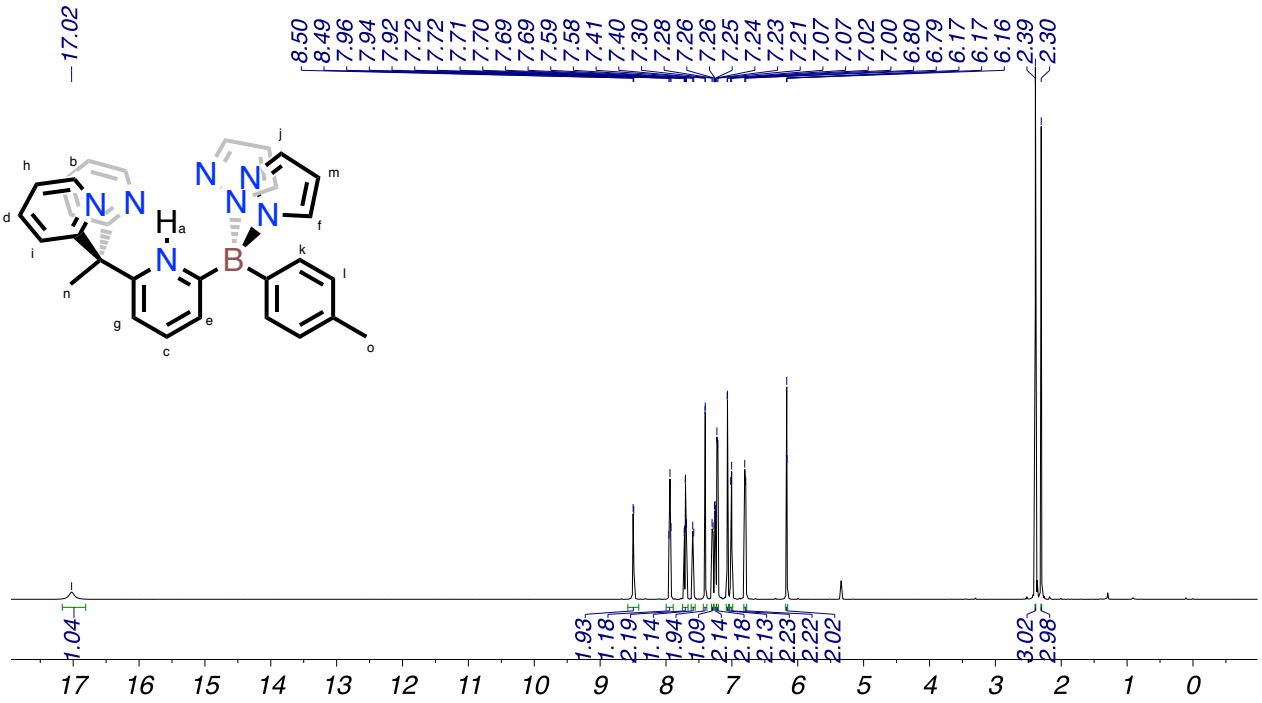


Figure S10 ^{1}H NMR of BPz_2Py_3H in CD_2Cl_2

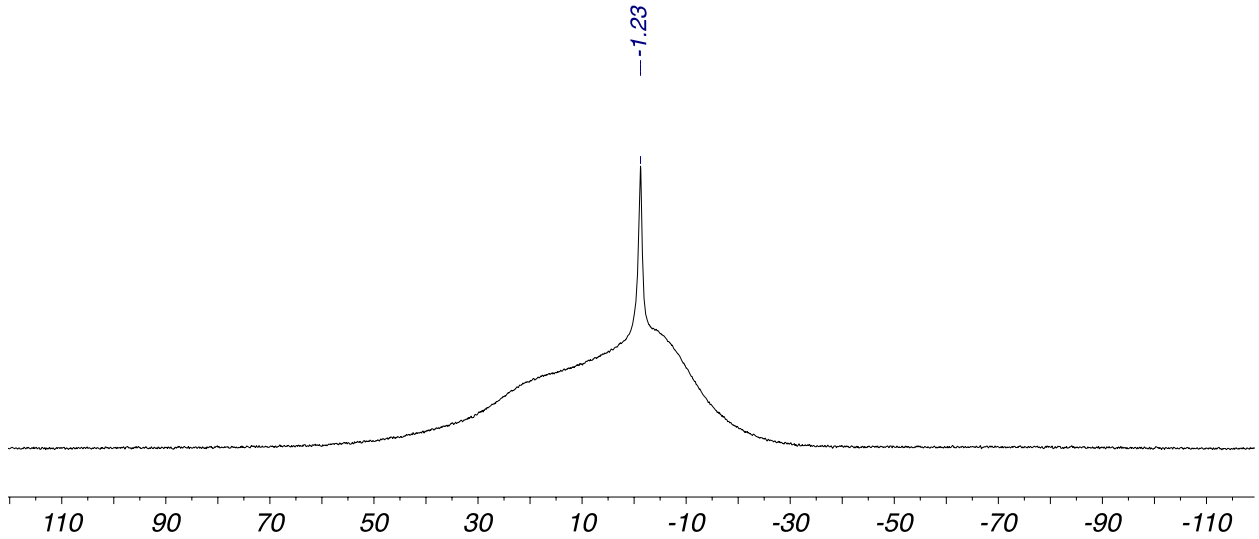


Figure S11 ^{11}B NMR of BPz_2Py_3H in CD_2Cl_2

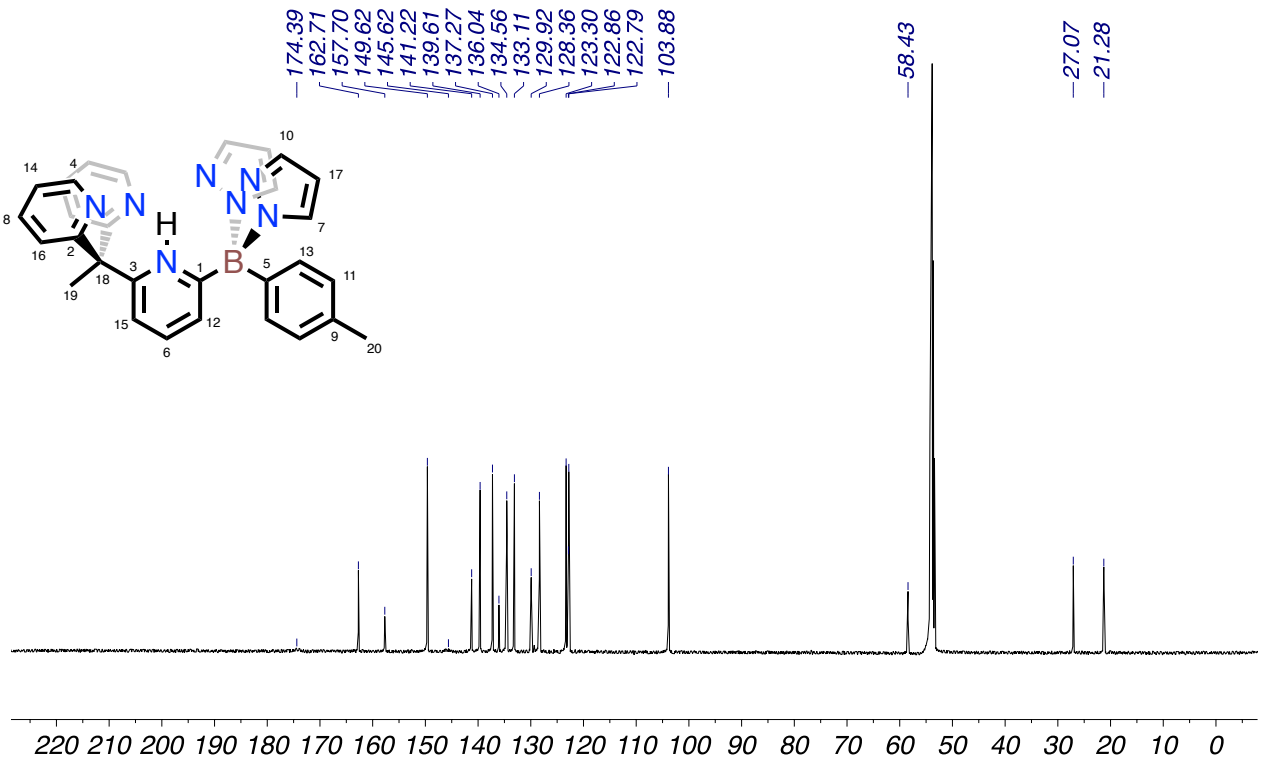


Figure S12 $^{13}C\{^{1}H\}$ NMR of BPz_2Py_3H in CD_2Cl_2

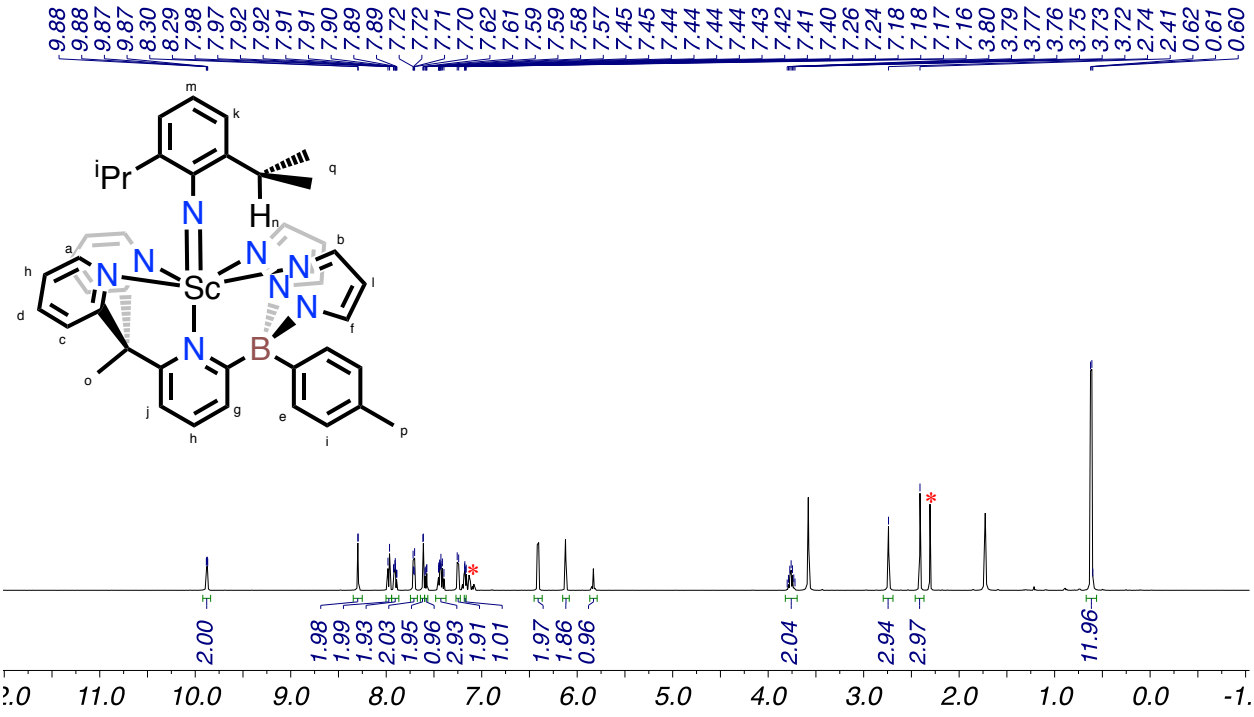


Figure S13 ^{1}H NMR of 2-N in THF-d_8. Residual toluene denoted with *.

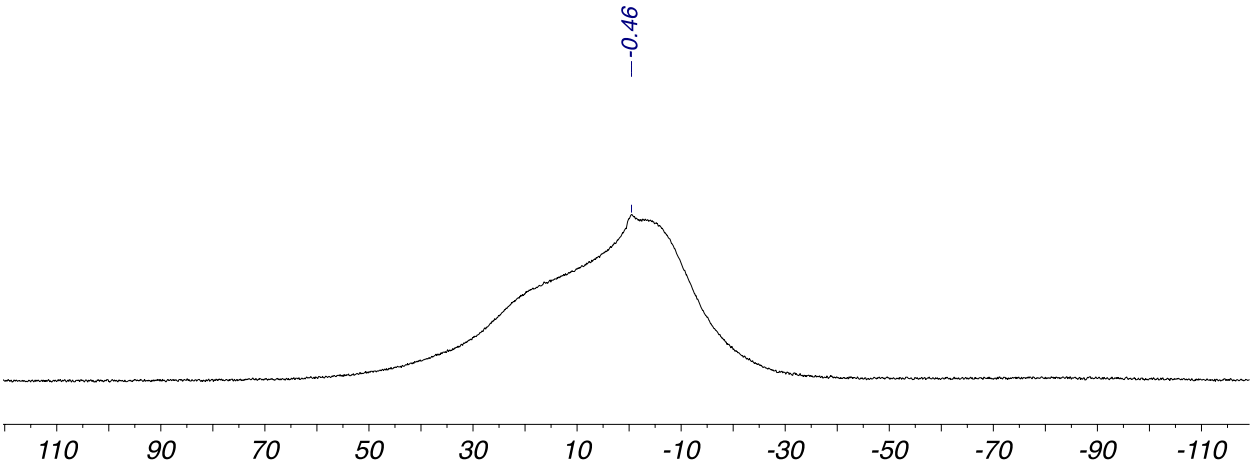


Figure S14 ^{11}B NMR of 2-N in THF-d_8

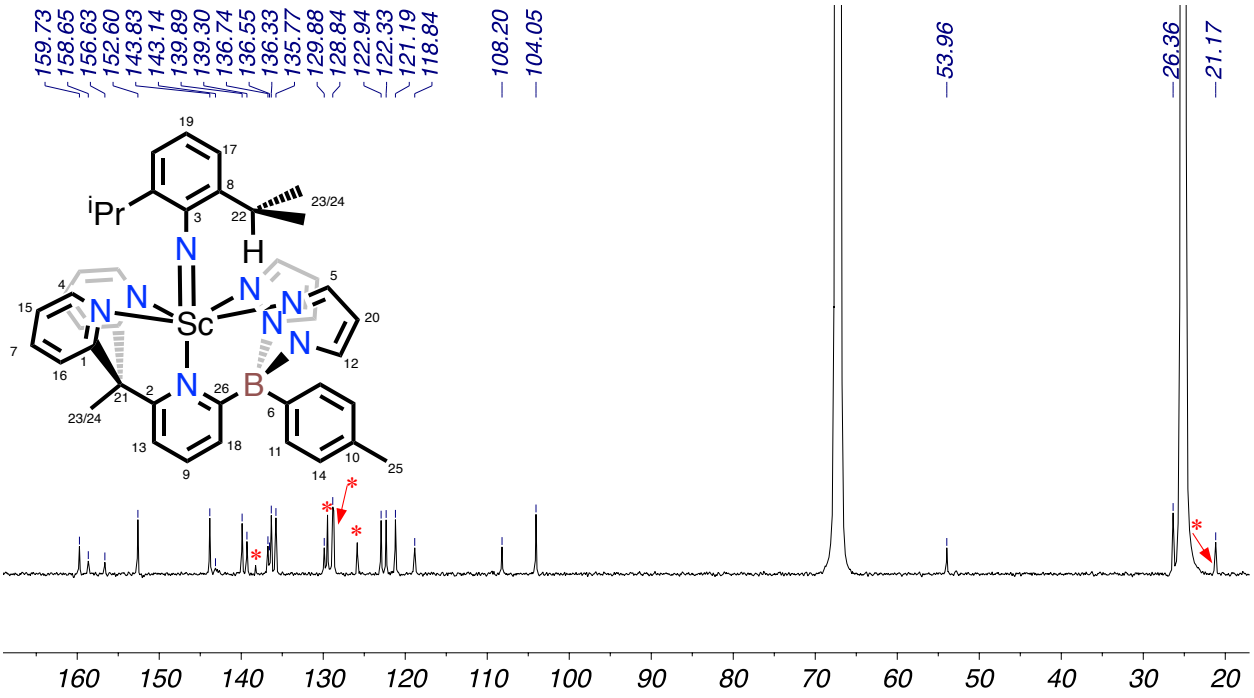


Figure S15 $^{13}C\{^{1}H\}$ NMR of 2-N in THF-d_8. Residual toluene denoted with *.

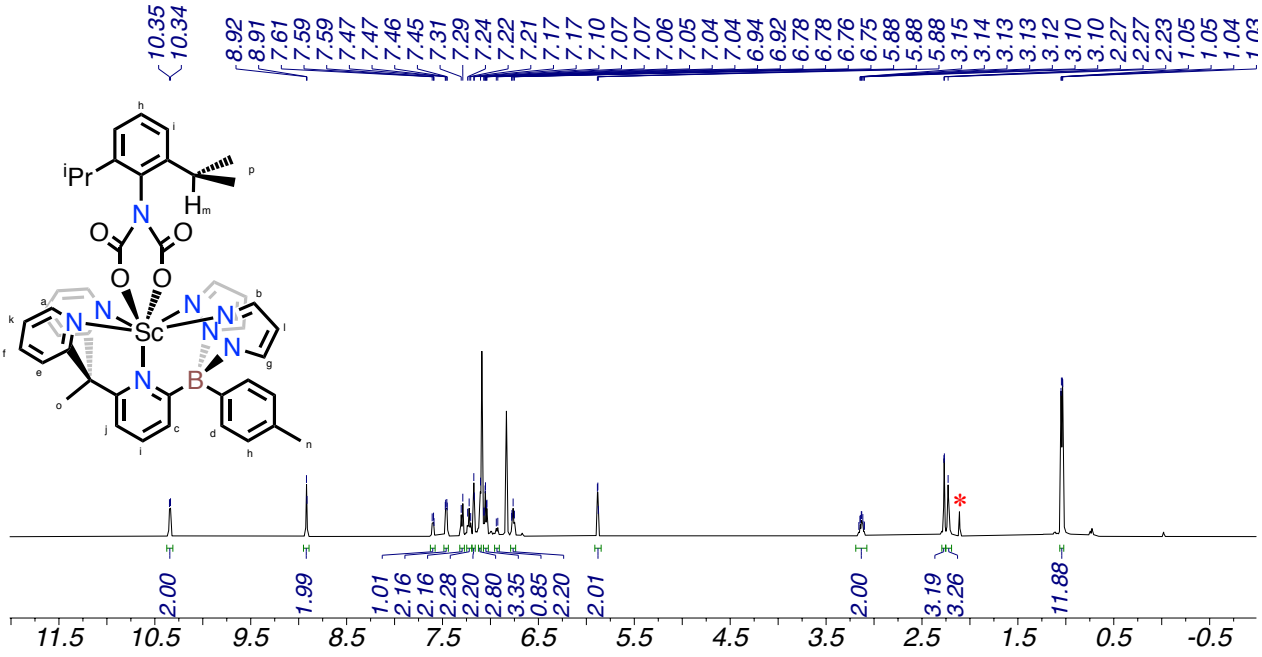


Figure S16 ^{1}H NMR of 3-N in o-$Cl_2C_6D_4$. Residual toluene denoted with *.

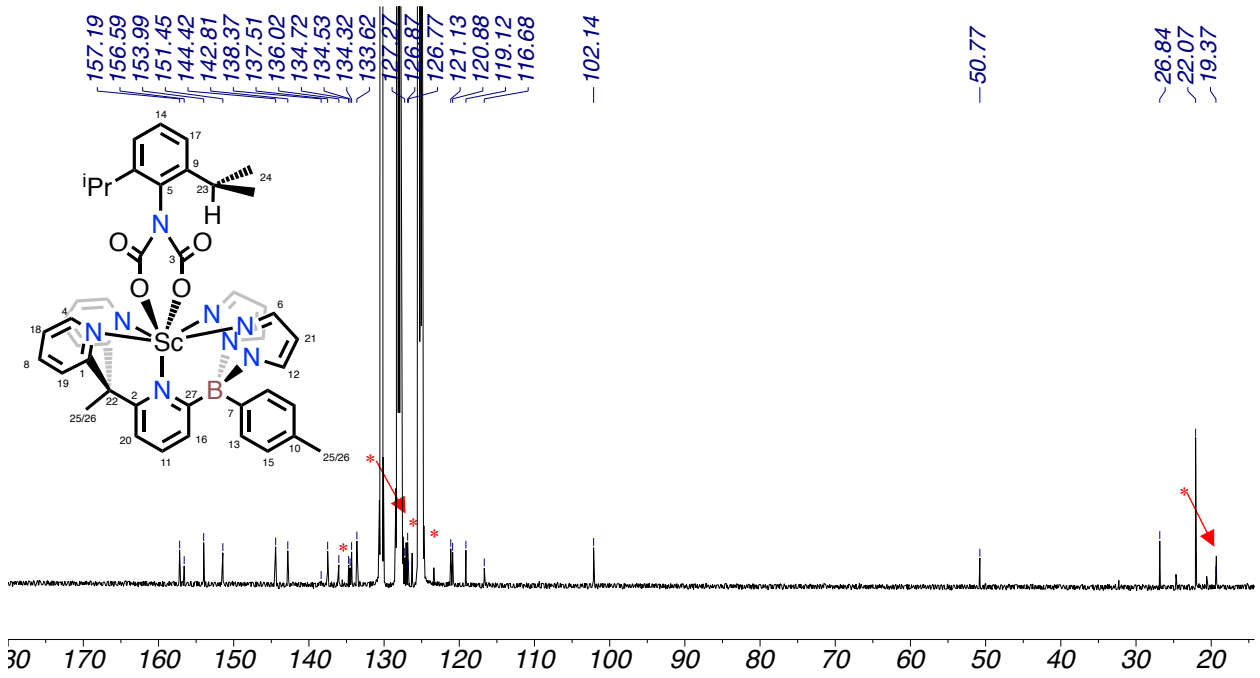


Figure S17 $^{13}C\{^{1}H\}$ NMR of 3-N in o-$Cl_2C_6D_4$. Residual toluene denoted with *.

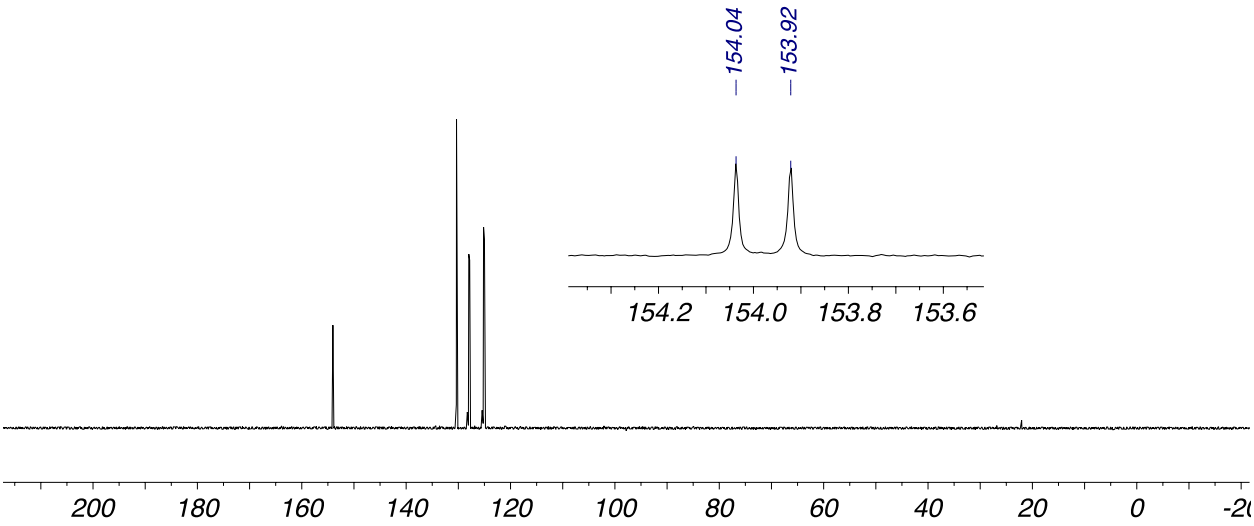


Figure S18 $^{13}C\{^{1}H\}$ NMR of 2-^{15}N + $^{13}CO_2$ in o-$C_6Cl_2D_4$.

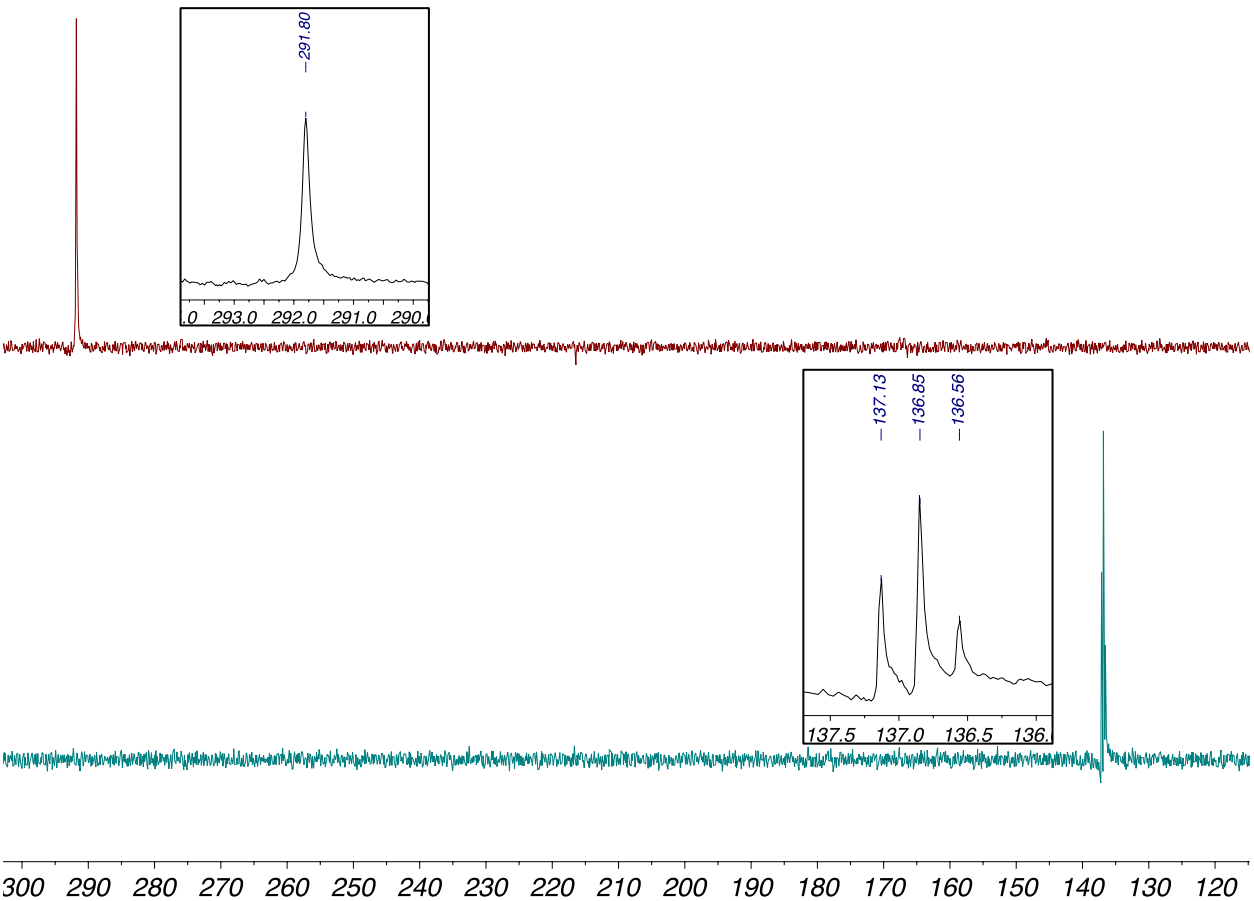


Figure S19 ^{15}N NMR of 2-^{15}N (top), and after addition of $^{13}CO_2$ (bottom) in o-$C_6Cl_2D_4$.

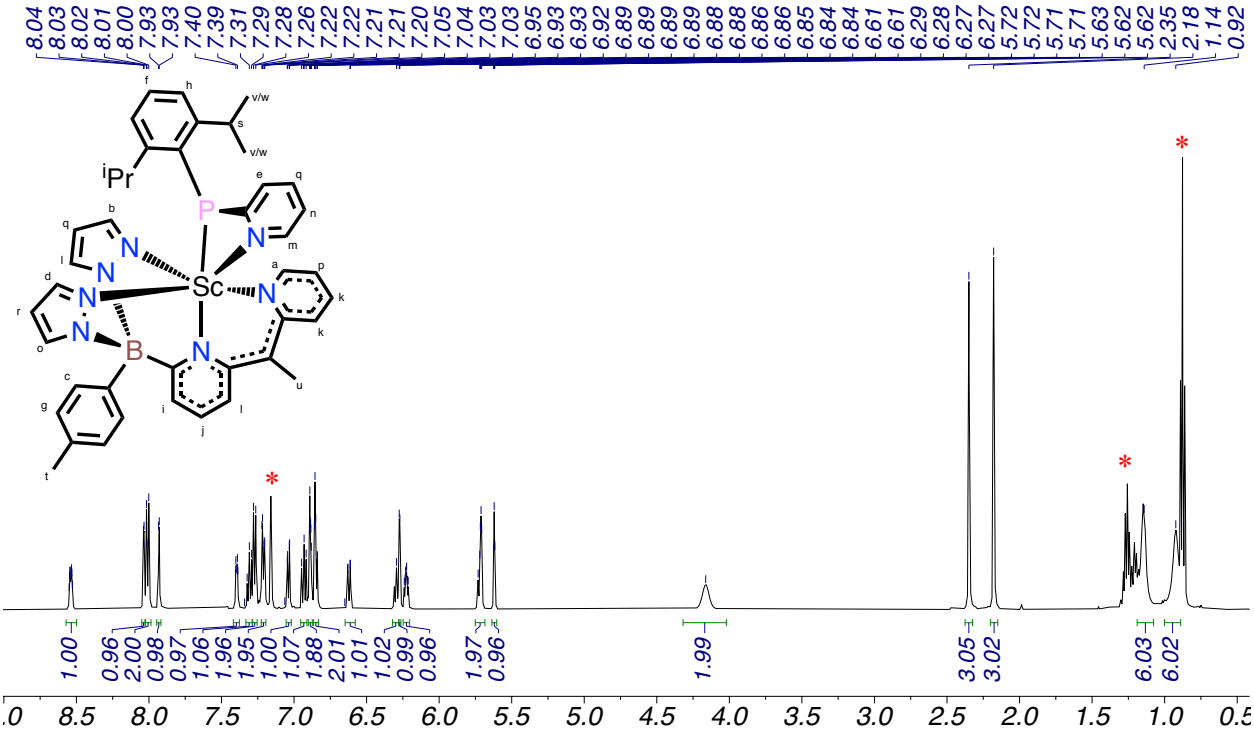


Figure S20 ^{1}H NMR of 4. Residual pentane and benzene solvent signals denoted with *.

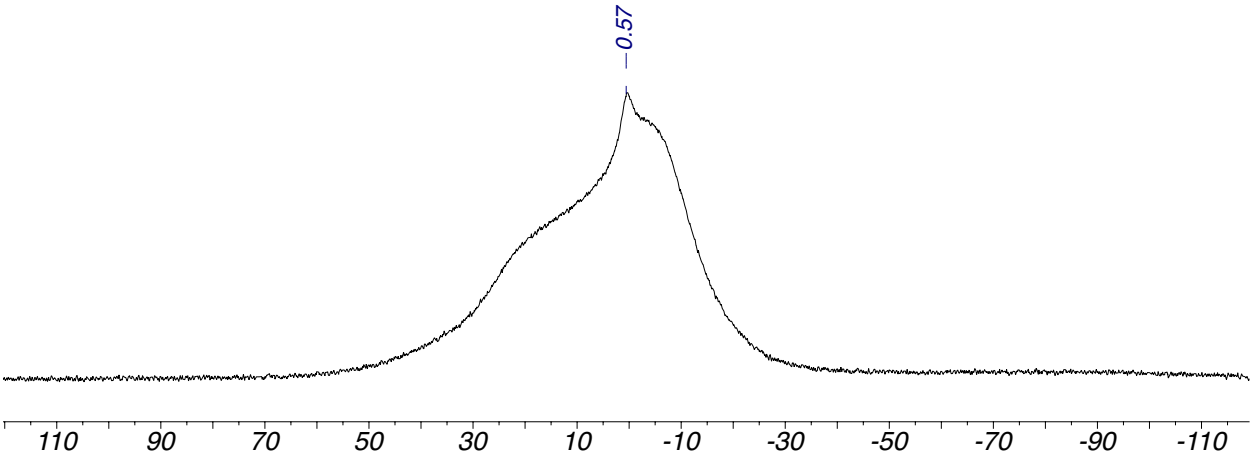


Figure S21 ^{11}B{^{1}H} NMR of 4.

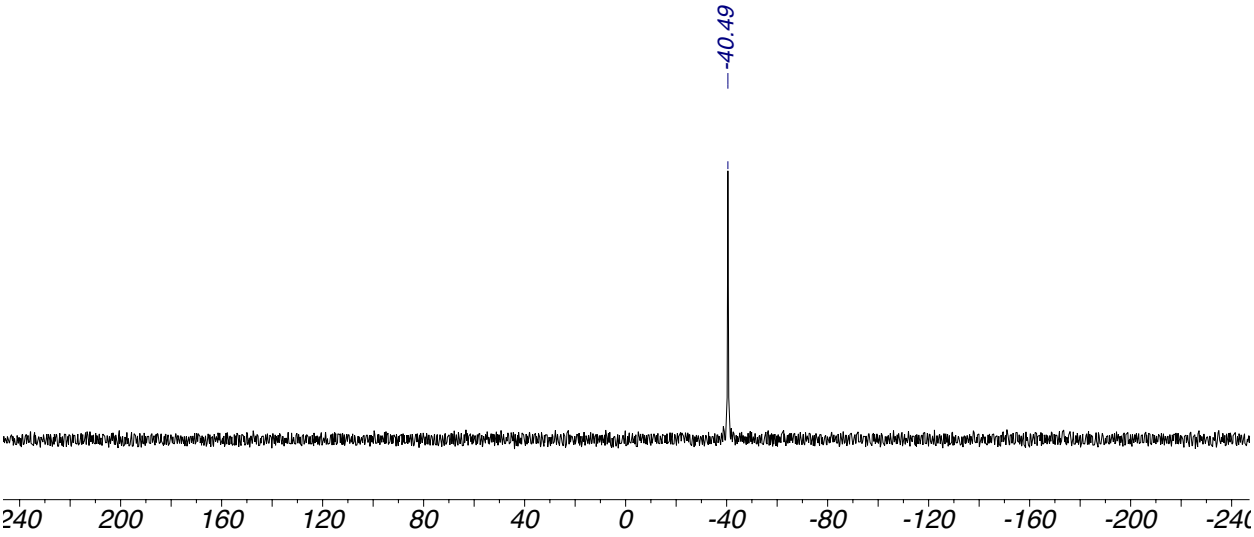


Figure S22 ^{31}P NMR of 4.

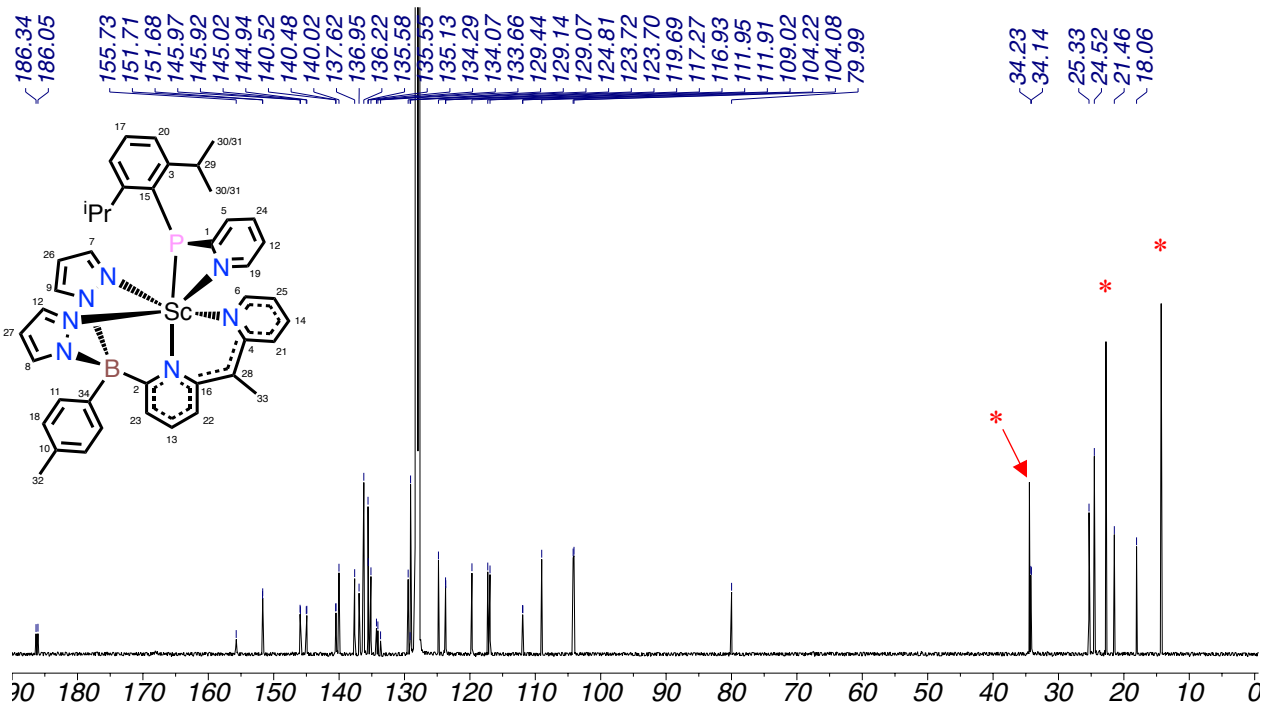


Figure S23 ^{13}C{^{1}H} NMR of 4. Residual pentane denoted with *.

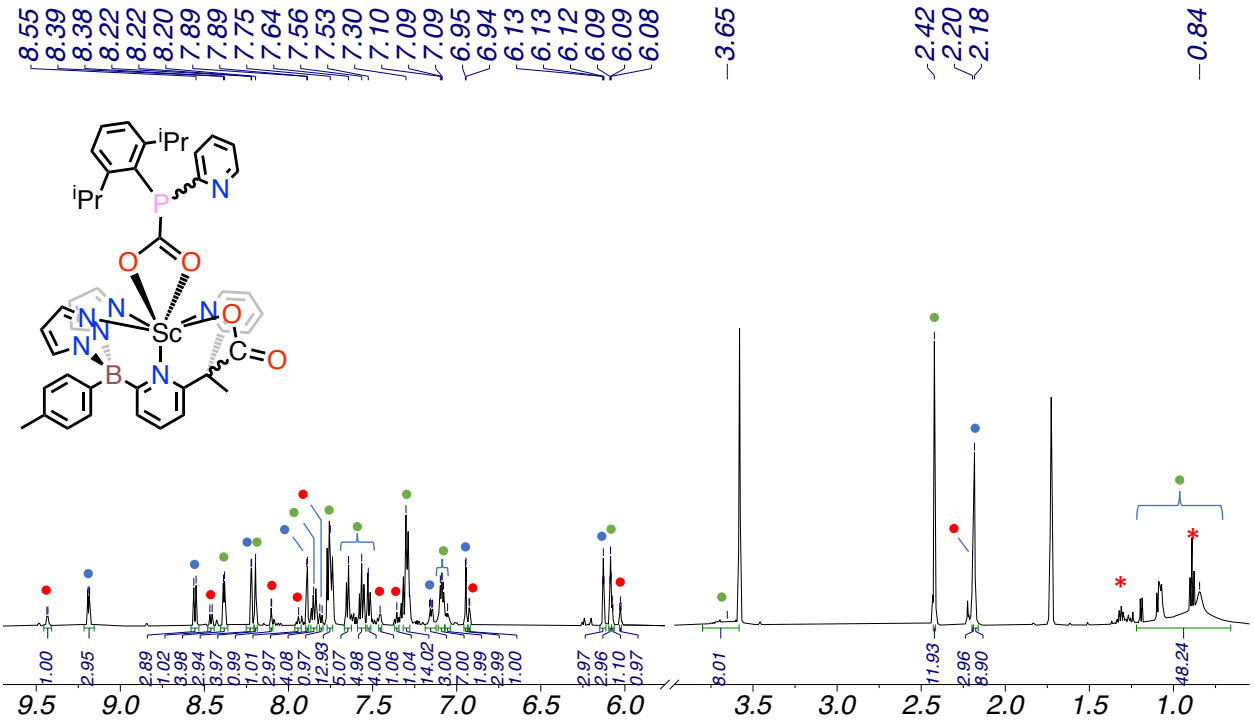


Figure S24 - ^{1}H NMR of 5 in THF-d_8. Blue and red markers denote signal from major or minor diastereomer, respectively. Green markers denote overlapping signals. Residual pentane denoted with *.

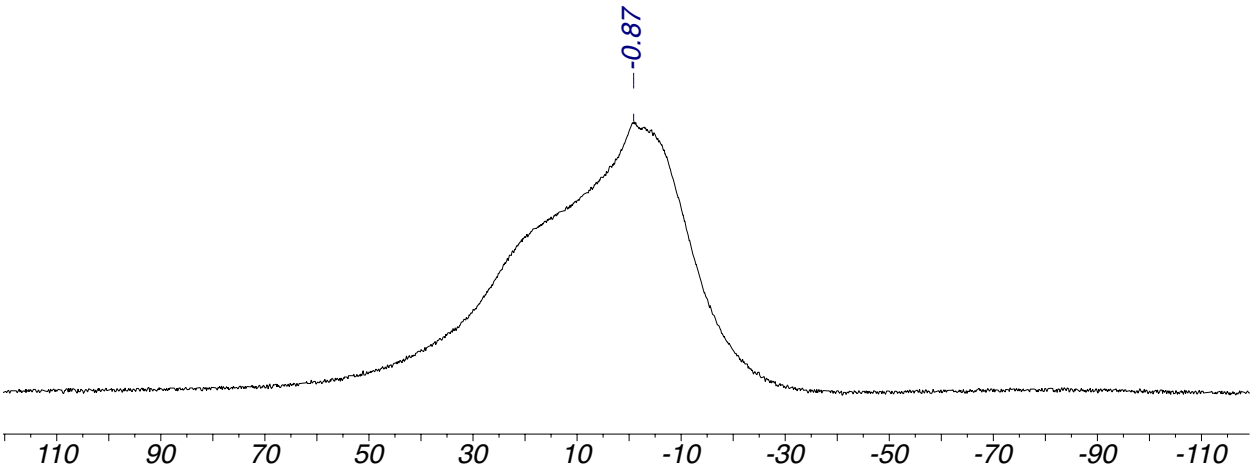


Figure S25 - ^{11}B{^{1}H} NMR of 5 in THF-d_8.

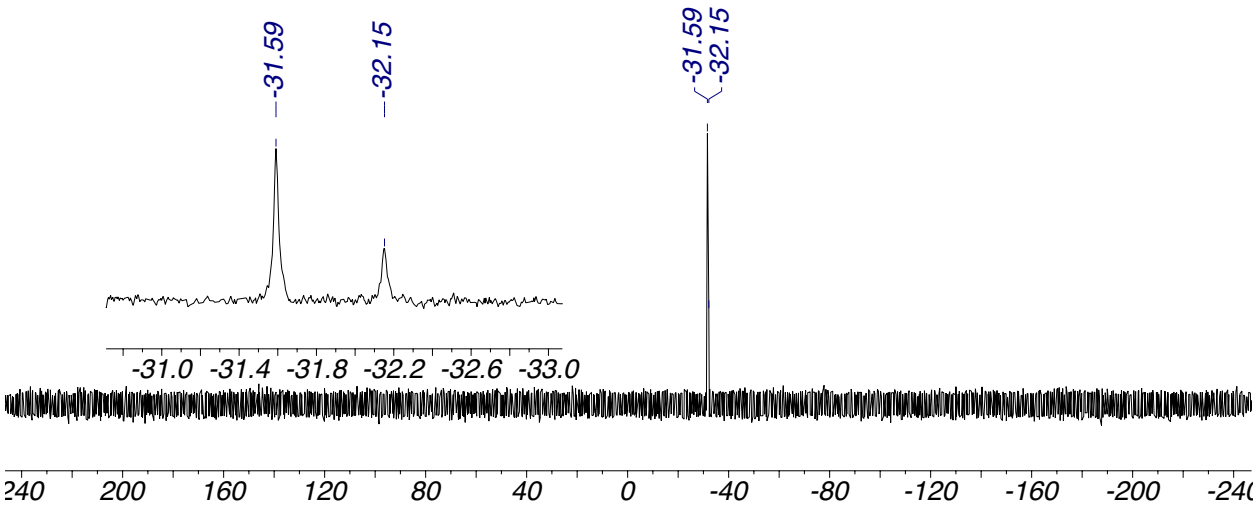


Figure S26 - $^{31}P\{^{1}H\}$ NMR of 5 in THF-d_8.

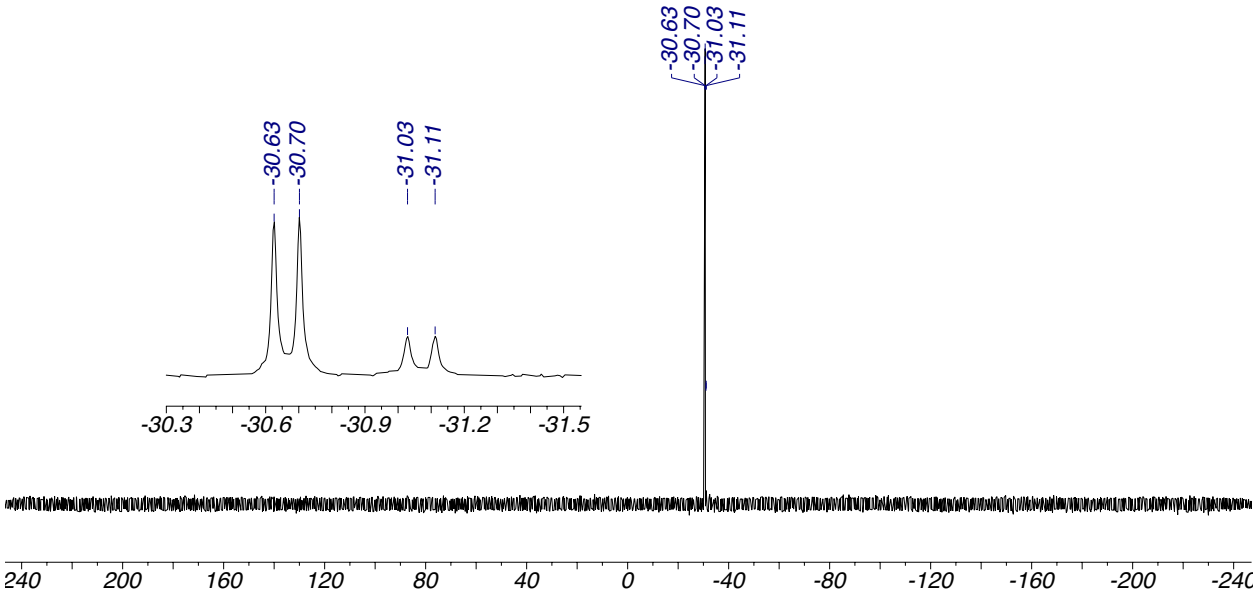


Figure S27 – $^{31}P\{^{1}H\}$ NMR of 4 + $^{13}CO_2$ in C_6D_6.

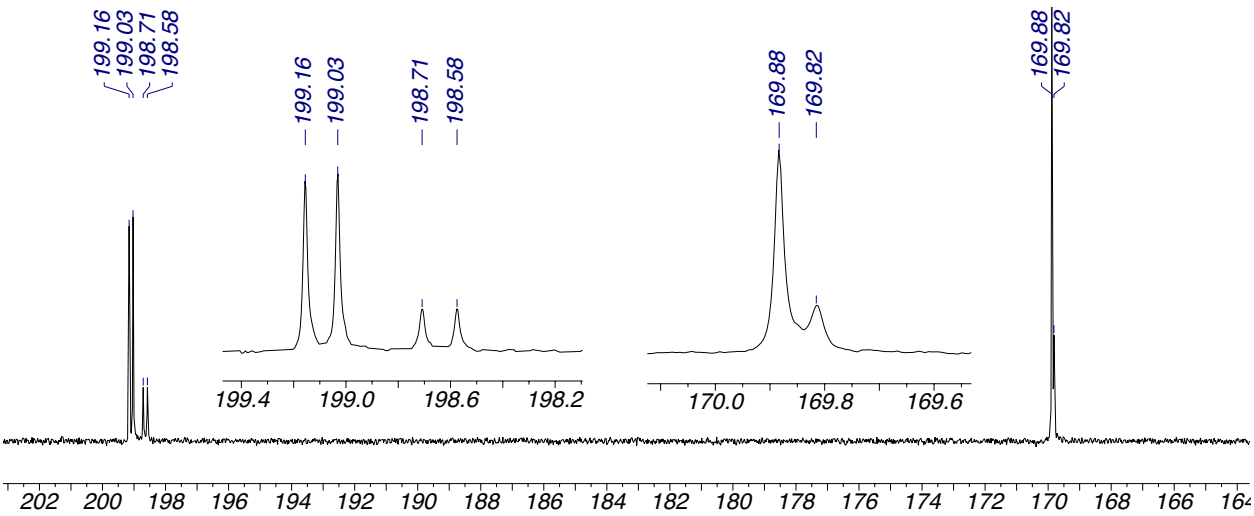


Figure S28 – $^{13}C\{^{1}H\}$ NMR of 4 + $^{13}CO_2$ in C_6D_6.

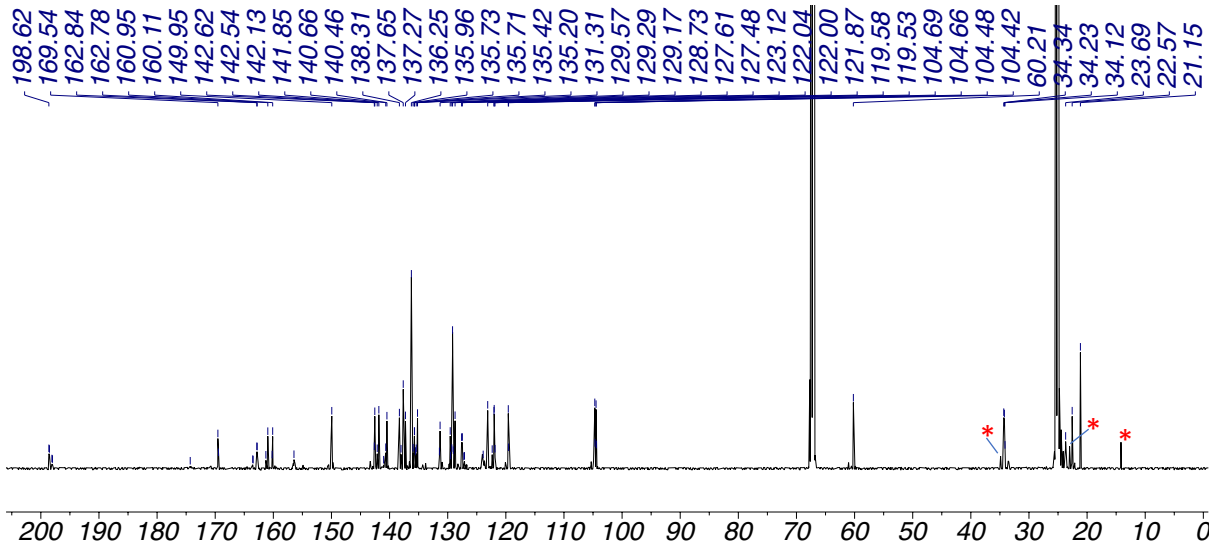


Figure S29 - $^{13}C\{^{1}H\}$ NMR of 5 in THF-d_8. Residual pentane denoted with *.

IR Spectroscopy Data

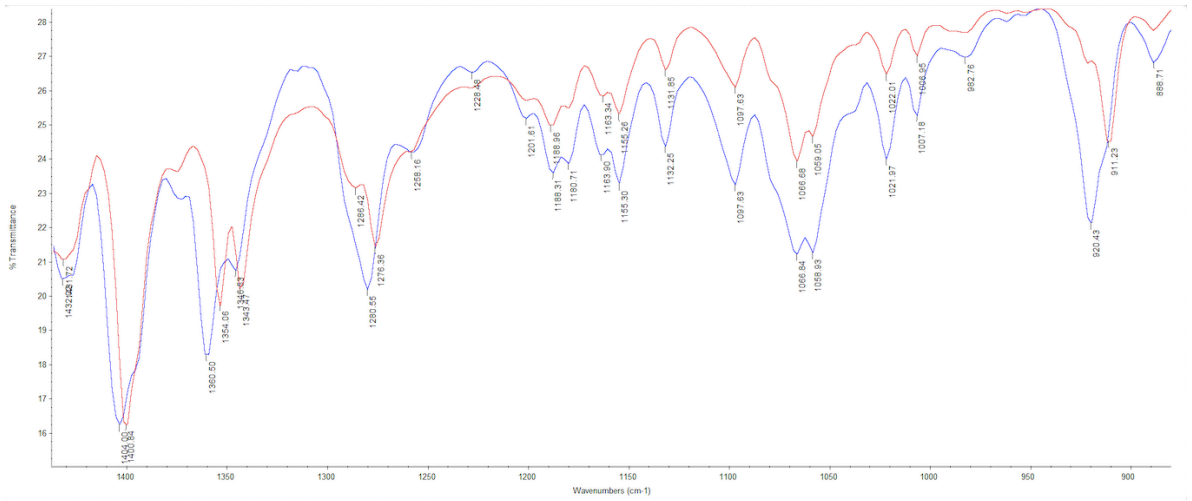


Figure S30 - Overlapping FT-IR spectrum (KBr pellet) of 2-N (blue trace) and 2-^{15}N (red trace).

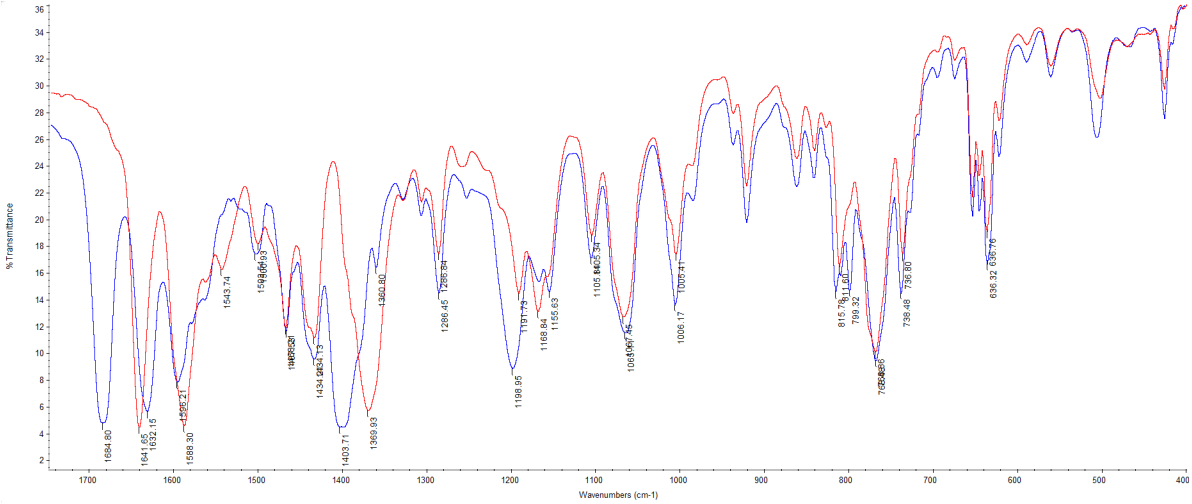


Figure S31 - Overlapping FT-IR spectrum (KBr pellet) of 2-N + CO_2 (blue trace) and 2-N + $^{13}CO_2$ (red trace).

UV-Vis Spectroscopy Data

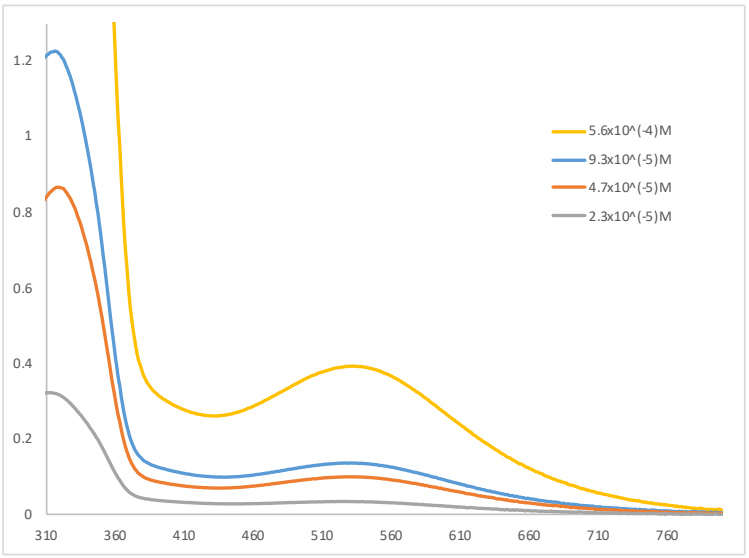


Figure S32 - UV-Vis spectra of 2-N at different concentrations in THF. Epsilon at λ_{318} (14,000 $M^{-1}cm^{-1}$) was calculated without using the yellow trace. Epsilon at λ_{532} (1,200 $M^{-1}cm^{-1}$) was calculated using all four traces.

Crystallographic Data

Table S2 - Single crystal x-ray diffraction details for complexes BPz2Py3H, 2-N, 4, and 5.

Identification code	***BPz_2Py_3H***	***2-N***	***4***
Empirical formula	$C_{30}H_{28}BN_7$	$C_{42}H_{44}BN_8Sc$	$C_{47}H_{56}BN_7PSc$
Formula weight	497.40	716.62	805.72
***T* (K)**	173.0	173	173.0
Crystal system	triclinic	monoclinic	triclinic
Space group	P-1	C2/c	P-1
***a* (deg)**	9.2828(10)	17.9420(13)	8.3970(18)
***b* (deg)**	12.5090(14)	20.4968(17)	10.808(2)
***c* (deg)**	12.9773(14)	26.1685(19)	24.445(5)
α (deg)	118.2260(10)	90	93.476(6)
β (deg)	96.3920(10)	93.504(5)	95.859(7)
γ (deg)	94.6160(10)	90	91.758(6)
***V* (Å^3)**	1304.1(2)	9605.6(13)	2201.4(8)
Z	2	8	2
ρ_{calc} (g/cm^3)	1.267	0.991	1.216
μ (mm^{-1})	0.078	1.560	2.080
F(000)	524.0	3024.0	856.0
Crystal size (mm^3)	0.282 × 0.259 × 0.202	0.076 × 0.054 × 0.039	0.424 × 0.182 × 0.056
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)
2θ range for data collection (deg)	3.614 to 56.638	6.554 to 130.398	3.64 to 133.19
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17	-21 ≤ h ≤ 21, -21 ≤ k ≤ 24, -30 ≤ l ≤ 22	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -28 ≤ l ≤ 29
Reflections collected	46401	32708	29561
Independent reflections	6500 [R_{int} = 0.0413, R_{sigma} = 0.0257]	7921 [R_{int} = 0.0594, R_{sigma} = 0.0577]	7754 [R_{int} = 0.0294, R_{sigma} = 0.0246]
Data/restraints/parameters	6500/0/349	7921/0/475	7754/1123/698
Goodness-of-fit on F^2	1.019	1.058	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0439 wR_2 = 0.1032	R_1 = 0.0638 wR_2 = 0.1817	R_1 = 0.0359 wR_2 = 0.0949
Final R indexes [all data]	R_1 = 0.0602 wR_2 = 0.1146	R_1 = 0.0883 wR_2 = 0.1955	R_1 = 0.0375 wR_2 = 0.0962
Largest diff. peak/hole / e Å^{-3}	0.44/-0.26	0.57/-0.49	0.36/-0.30

Table S2 continued

Identification code	***5***
Empirical formula	$C_{50}H_{50}BN_7O_4PSc$
Formula weight	899.71
***T* (K)**	173.0
Crystal system	triclinic
Space group	P-1
***a* (deg)**	8.7025(3)
***b* (deg)**	12.7011(4)
***c* (deg)**	21.2188(10)
α (deg)	90.965(3)
β (deg)	91.117(3)
γ (deg)	101.418(2)
***V* (Å^3)**	2297.98(15)
Z	2
ρ_{calc} (g/cm^3)	1.300
μ (mm^{-1})	2.122
F(000)	944.0
Crystal size (mm^3)	0.221 × 0.065 × 0.059
Radiation	CuKα (λ = 1.54178)
2θ range for data collection (deg)	4.166 to 133.188
Index ranges	$-10 \le h \le 10$, $-15 \le k \le 13$, $-23 \le l \le 25$
Reflections collected	26336
Independent reflections	7812 [R_{int} = 0.0621, R_{sigma} = 0.0718]
Data/restraints/parameters	7812/1276/726
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0528 wR_2 = 0.1284
Final R indexes [all data]	R_1 = 0.0652 wR_2 = 0.1355
Largest diff. peak/hole / e Å^{-3}	0.54/-0.36

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Computational Details

Calculations were carried out with Gaussian09[i] at the DFT level, with the hybrid functional B3PW91.[ii] Scandium and phosphorus atoms were treated with small-core pseudopotentials from the Stuttgart group, with additional polarization orbitals.[iii] The other atoms that were part of the systems (boron, nitrogen, carbon, and hydrogen) were treated with the extended all electron Gaussian-Type 6-31G** Pople basis set.[iv] No symmetry constraints were considered for the geometry optimizations that took as starting point the experimentally obtained geometries of both reagents and products. Analytical calculations of the vibrational frequencies confirmed that the structures obtained were the critical points involved in the reactive process, and also obtained the thermal corrections over the energies. Transition states obtained where connected with its respective intermediates with Intrinsic Reaction Coordinate (IRC) calculations. Bonding was studied doing Natural Bond Orbital analysis over the optimized structures, with NBO software.[v]

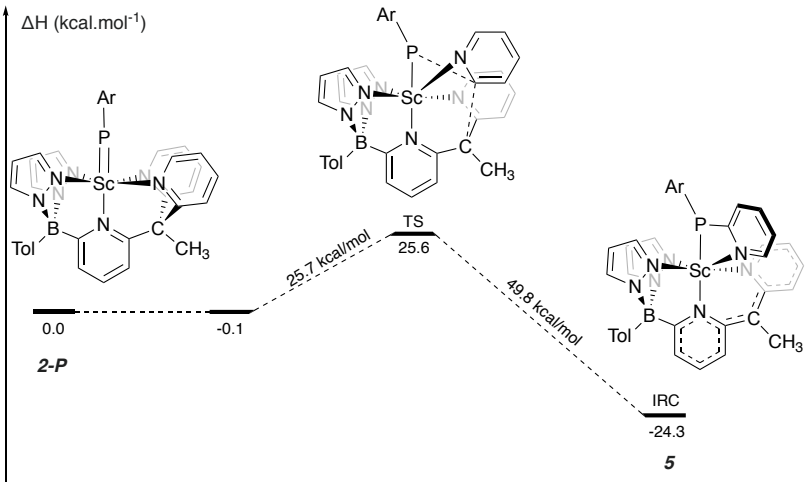

Figure S33 - Computed enthalpy profile at room temperature for the formation of 5 from the putative 2-P

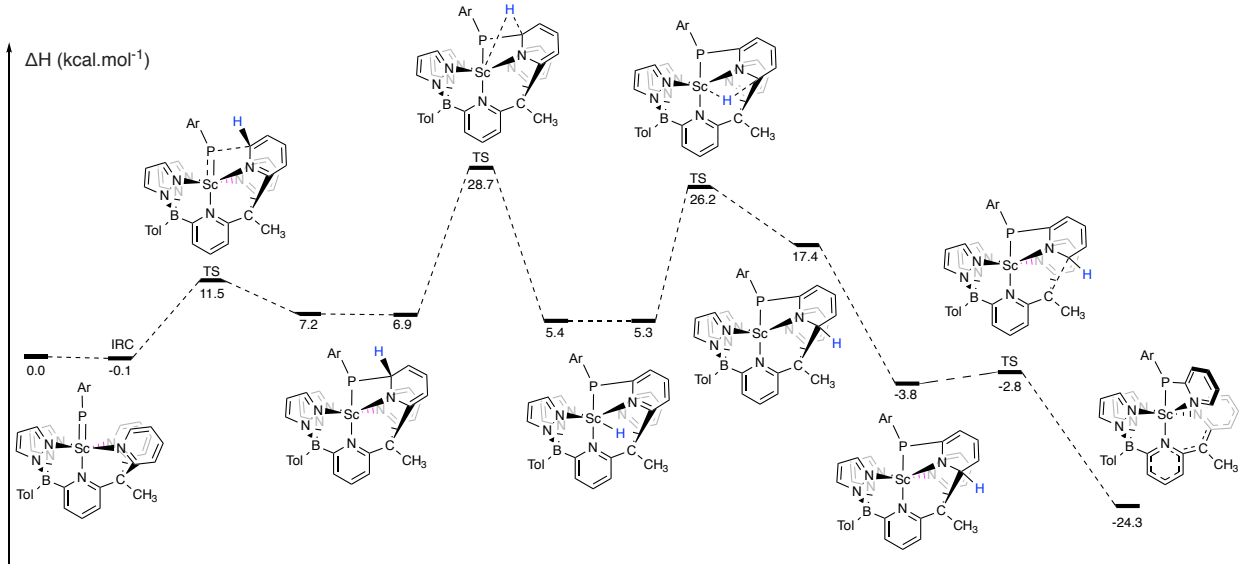

Figure S34 - Computed enthalpy profile at room temperature of an alternative pathway for the formation of 5 from the putative 2-P

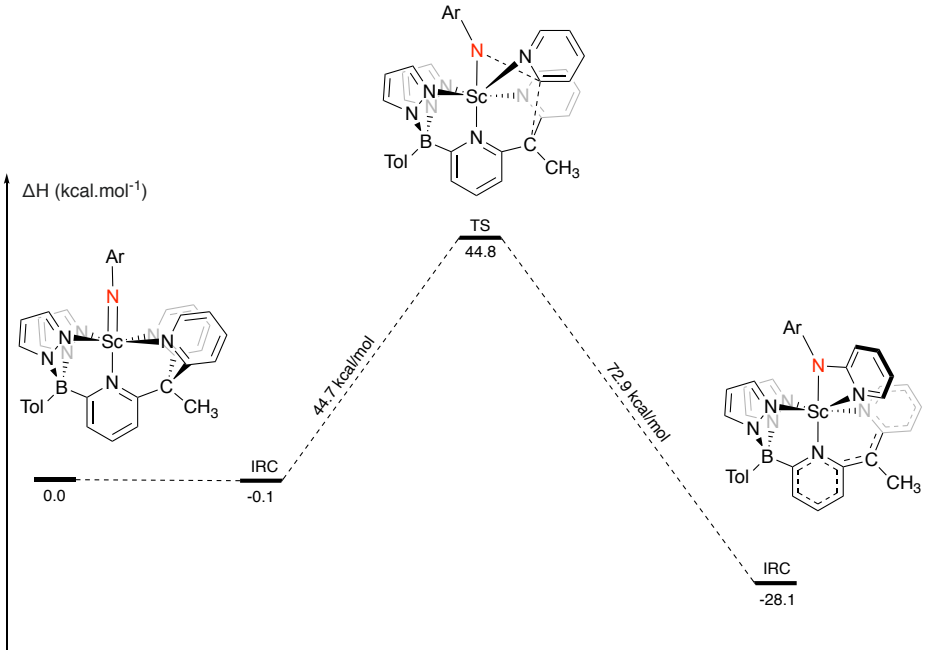

Figure S35 - Computed enthalpy profile at room temperature for the formation of putative 5-N from the putative 2-N

Computational references

(i) *Gaussian 09, Revision A.02*, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone,V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov,V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V.; Voth,G.G.A.; Salvador, P.; Dannenberg, J. J.; Dapprich,S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

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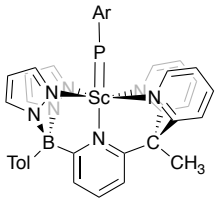
(v) *NBO Version 3.1*, Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F.

Cartesian Coordinates of Optimized Structures



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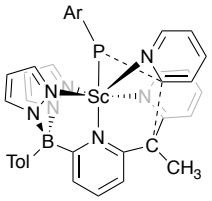

TS

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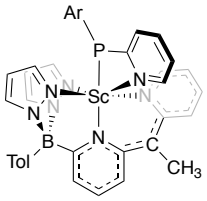

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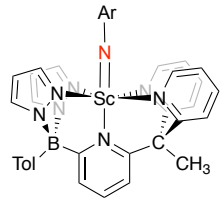

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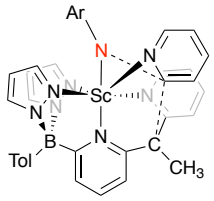

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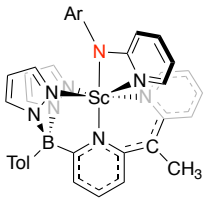

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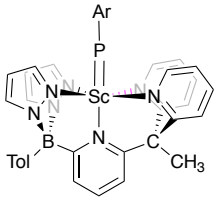

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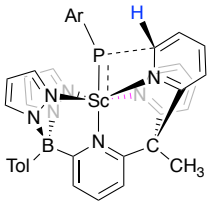

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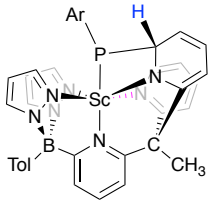

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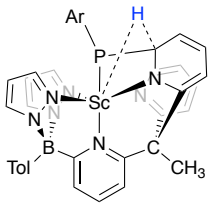

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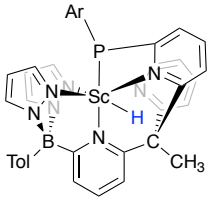

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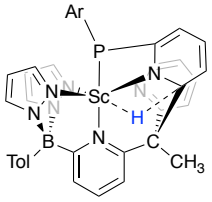

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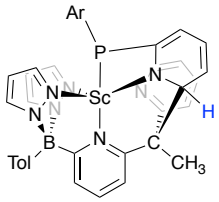

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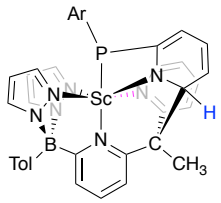

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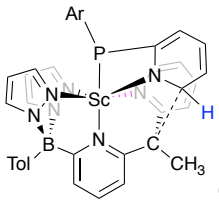

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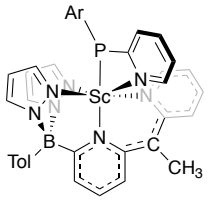

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C	1.17658800	-3.16132800	2.04744100
C	0.50798800	-2.36204100	2.96368500
C	0.19266600	2.59238300	1.27369600
C	-0.16147400	3.22045200	2.46574100
C	-0.71495600	2.20415700	3.23534400
C	-1.28342100	-0.66277200	4.48467500
C	-2.03448000	-1.73292300	5.01001200
C	-2.00098200	-2.08095800	6.35787400
C	-1.19690100	-1.38399400	7.26604400
C	-0.40270100	-0.35451300	6.75596000
C	-0.44041700	-0.01399800	5.40349600
C	-1.19030200	-1.72954800	8.73115800
C	-2.66451200	-0.48549400	2.06691000

C	-3.87520200	-0.68543700	2.71276900
C	-5.03774800	-0.90701000	1.96158600
C	-4.97511900	-0.89025500	0.59054900
C	-3.75886800	-0.55306600	-0.06517900
C	-3.77557500	-0.36080400	-1.49573600
C	-4.87816100	-1.05762600	-2.26591700
C	-1.48947400	2.43730500	-2.08535800
C	-1.96325900	3.02501800	-3.23180400
C	-2.98213300	2.34004700	-3.93233700
C	-3.51419300	1.18827500	-3.41785700
C	-3.07385200	0.67444400	-2.14983100
C	-0.95587900	-2.23647100	-2.81144700
C	-0.50089700	-2.81369100	-3.98391600
C	0.73945200	-2.38218000	-4.48574600
C	1.46437700	-1.41544600	-3.81761600
C	0.95523100	-0.86344900	-2.61799300
B	-1.24393700	-0.38340900	2.88467000
H	1.05876800	-2.98517000	-0.19075100
H	1.85191500	-3.97708900	2.25700300
H	0.51117500	-2.38177800	4.04194800
H	0.67469700	2.99339100	0.39277900
H	-0.03028900	4.25635700	2.73963000
H	-1.13770600	2.23249700	4.22766700
H	-2.64503800	-2.33492900	4.34265300
H	-2.60325200	-2.91695400	6.70890000
H	0.26775500	0.18416000	7.42304300
H	0.23859300	0.76164100	5.06126000
H	-1.34206900	-2.80154400	8.89159800
H	-0.24670000	-1.44507100	9.20641800
H	-1.99395800	-1.20581000	9.26385600
H	-3.91341500	-0.69635000	3.79414700
H	-5.98692300	-1.08719700	2.46099500
H	-5.87193000	-1.04090500	0.00270800
H	-5.80657600	-0.47230100	-2.35879100
H	-5.14093000	-2.00985100	-1.79648300
H	-4.55258500	-1.29931600	-3.28310200
H	-0.65595800	2.87337600	-1.54280100
H	-1.53977600	3.95412500	-3.59394300
H	-3.35976900	2.73590300	-4.87183300
H	-4.32482100	0.69374300	-3.93747700
H	-1.91343000	-2.51075400	-2.37526700
H	-1.08996200	-3.57013100	-4.48964200
H	1.13196100	-2.81260900	-5.40416000
H	2.42509800	-1.07346300	-4.18761700
Sc	-0.74516500	-0.02250000	-0.36953500
P	1.67523200	0.34222900	-1.51917100

C	3.24232600	0.92008400	-2.30698600
C	4.47803700	0.40246800	-1.83489100
C	3.23900100	1.89392300	-3.33991800
C	5.66950900	0.84930300	-2.41682900
C	4.45776300	2.30202900	-3.89300200
C	5.66563600	1.78661400	-3.44109600
H	6.61660200	0.45218600	-2.05985000
H	4.45839200	3.04278000	-4.68908800
H	6.60174700	2.11864100	-3.88305800
C	4.57349700	-0.62596400	-0.71717500
H	3.54740300	-0.84695600	-0.39978500
C	1.96791100	2.54072700	-3.86819500
H	1.12611200	2.09083400	-3.33073100
C	1.95381800	4.04696300	-3.57284300
H	2.06030600	4.24221900	-2.50063800
H	2.77077600	4.56796100	-4.08473900
H	1.01365400	4.49637600	-3.91155400
C	1.75639400	2.27203600	-5.36395900
H	1.73610500	1.19875300	-5.57455600
H	0.80222200	2.69656900	-5.69461200
H	2.54859000	2.72039500	-5.97461400
C	5.20084100	-1.93846600	-1.20507900
H	4.63901400	-2.35670400	-2.04635400
H	6.23708400	-1.79739700	-1.53320600
H	5.20806500	-2.68123300	-0.39950200
C	5.32177900	-0.06929700	0.50110200
H	4.84542700	0.84298700	0.87373400
H	5.32736500	-0.80392800	1.31397200
H	6.36481500	0.17131700	0.26444000