Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Scandium Alkyl and Hydride Complexes Supported by a Pentadentate Diborate Ligand: Reactions with CO_2 and N_2O

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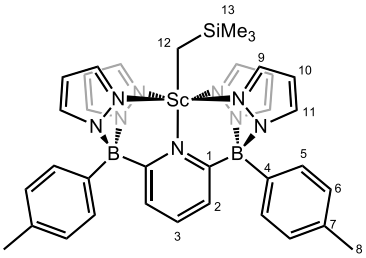
Experimental Details

General Considerations

Manipulation and storage of all oxygen and moisture sensitive materials was performed under an argon atmosphere in a 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 in a 135 °C oven prior to immediate transfer to the glovebox antechamber or assembly on the vacuum line and evacuated while hot. Tetrahydrofuran, toluene and pentane were dried and purified using a Grubbs/Down purification system,[1] and stored in evacuated 500 mL thick-walled vessels over sodium/benzophenone ketal. 1,4-Dioxane and C_6D_6 were dried over sodium/benzophenone ketal, and HMDSO was dried over calcium hydride. All dried solvents were degassed, vacuum transferred prior to use into thick-walled glass vessels for storage over activated molecular sieves (4 Å). Li[tol-Pz_4B_2PyH],[2] $ScCl_3(THF)_3$,[3] $LiCH_2SiMe_3$,[4] $LiCH_2SiMe_2Ph$,[5] Li^{n}Pr[6] and $LiDBEt_3$[7] were prepared according to literature procedures. Li^{i}Bu was synthesized using the same procedure for $LiCH_2SiMe_3$. MeLi (1.6 M in Et_2O), $NaBHEt_3$ (1.0 M in toluene), LiHMDS, LiD, BEt_3, HCOONa and NaOAc were purchased from Sigma-Aldrich and used as received. Solutions of MeLi, $NaHBEt_3$ and $LiDBEt_3$ were evaporated *in vacuo* and stored in a glove box freezer at -35 ^oC. LiHMDS and $B(C_6F_5)_3$ were sublimed prior to use. CO_2 (Coleman Instrument grade, 99.99%) was purchased from Air Liquide and used as received. Nuclear magnetic resonance spectroscopy experiments including ^1H, ^2H, $^{11}B\{^1H\}$, $^{13}C\{^1H\}$, $^{19}F\{^1H\}$, ^1H-^{13}C HMBC, ^1H-^{13}C HSQC and DOSY were performed on Bruker-400, Ascend-500 or Avance-600 spectrometers. For DOSY experiments, the gradient amplitude was varied from 2% to 95% with an optimized δ (gradient pulse length) of 2600 μs and a Δ (diffusion time) of 0.075 s. All ^1H and $^{13}C\{^1H\}$ NMR spectra were internally referenced relative to $Si(CH_3)_4$ using residual solvent protons and naturally abundant ^{13}C resonances for all deuterated solvents. NMR spectra were processed and analyzed with MestReNova (v. 9.0.1-13254). X-ray crystallographic analyses were performed by Chris Gendy, Dr. Benjamin Gelfand, and Dr. Jian-Bin Li on a Nonius Kappa CCD diffractometer using graphite-monochromated Mo Kα radiation. Crystals were coated in Fomblin Y HVAC 140/13 oil. Elemental analyses were performed by Johnson Li using a Perkin Elmer Model 2400 Series II analyser at the Instrumentation Facility of the Department of Chemistry, University of Calgary. Solution high-resolution mass spectrometry (APCI-MS) measurements were performed by Wade White on samples prepared in the glove box in a gas tight syringe. Infrared spectra were collected on a Nicolet Avatar FT-IR spectrometer, and samples were prepared either as a KBr pellet or thin film by evaporation of a benzene solution on AgCl plates.

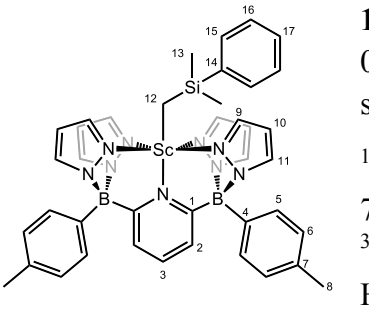
Synthesis of 2-CH_2SiMe_3



1 (115 mg, 0.183 mmol) was reacted with $LiCH_2SiMe_3$ (18 mg, 0.191 mmol, 1.05 equiv.) to yield **2-CH_2SiMe_3** as a pale yellow solid (68 mg, 0.100 mmol, 55%). Single crystals suitable for X-ray diffraction were obtained by layering HMDSO onto a concentrated solution of **2-CH_2SiMe_3** in benzene.

^{1}H NMR (500 MHz, C_6D_6): δ 8.10 (d, $^3J_{HH}$ = 2.2 Hz, 4H, H9), 7.78 (d, $^3J_{HH}$ = 7.8 Hz, 4H, H5), 7.45 (d, $^3J_{HH}$ = 2.2 Hz, 4H, H11), 7.39 (d, $^3J_{HH}$ = 7.8 Hz, 2H, H2), 7.20 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H6), 6.72 (t, $^3J_{HH}$ = 7.8 Hz, 1H, H3), 5.85 (t, $^3J_{HH}$ = 2.2 Hz, 4H, H10), 2.32 (s, 6H, H8), 0.71 (s, 2H, H12), 0.21 (s, 9H, H13). $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ 172.2 (C1), 141.0 (C9), 140.7 (C4), 136.9 (C7), 136.5 (C11), 136.2 (C5), 134.5 (C3), 129.0 (C6), 127.4 (C2), 104.6 (C10), 42.3 (C12), 21.4 (C8), 3.8 (C13). ^{11}B NMR (161 MHz, C_6D_6) δ -0.01. Elemental Analysis: Calcd. (%) for $C_{35}H_{40}B_2N_9ScSi$: C, 61.69; H, 5.92; N, 18.50. Found: C, 60.74; H, 5.86; N, 18.10.

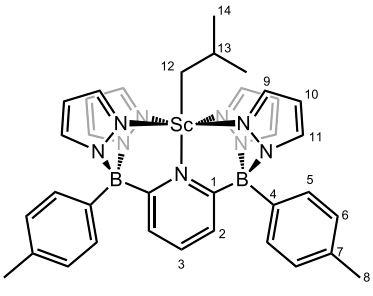
Synthesis of 2-CH_2SiMe_2Ph



1 (88 mg, 0.140 mmol) was reacted with $LiCH_2SiMe_2Ph$ (23 mg, 0.147 mmol, 1.05 equiv.) to yield **2-CH_2SiMe_2Ph** as a pale yellow solid (80 mg, 0.108 mmol, 77%).

^{1}H NMR (500 MHz, C_6D_6): δ 7.91 (d, $^3J_{HH}$ = 2.0 Hz, 4H, H9), 7.80 – 7.75 (m, 6H, H5 and H15), 7.44 (d, $^3J_{HH}$ = 2.2 Hz, 4H, H11), 7.38 (d, $^3J_{HH}$ = 7.8 Hz, 2H, H2), 7.34 (m, 2H, H16), 7.30 – 7.26 (m, 1H, H17), 7.20 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H6), 6.70 (t, $^3J_{HH}$ = 7.7 Hz, 1H, H3), 5.82 (t, $^3J_{HH}$ = 2.2 Hz, 4H, H10), 2.32 (s, 6H, H8), 0.87 (s, 2H, H12), 0.29 (s, 6H, H13).$^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ 172.2 (C1), 146.2 (C14), 141.1 (C9), 140.6 (C4), 136.9 (C7), 136.5 (C11), 136.2 (C5), 134.5 (C3), 134.2 (C15), 129.0 (C6), 128.2 (C17), 128.0 (C16), 127.3 (C2), 104.6 (C10), 38.3 (C12), 21.4 (C8), 2.3 (C13). ^{11}B NMR (161 MHz, C_6D_6) δ -0.05. Elemental Analysis: Calcd. (%) for $C_{40}H_{42}B_2N_9ScSi$: C, 64.62; H, 5.69; N, 16.96. Found: C, 64.16; H, 5.41; N, 16.31.

Synthesis of 2-^{i}Bu

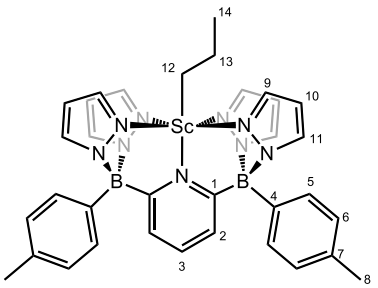


1 (62 mg, 0.098 mmol) was reacted with Li^{i}Bu (7 mg, 0.109 mmol, 1.11 equiv.) to yield **2-^{i}Bu** as a pale yellow solid (40 mg, 0.060 mmol, 61%).

^{1}H NMR (500 MHz, C_6D_6): δ 8.09 (d, $^3J_{HH}$ = 2.1 Hz, 4H, H9), 7.77 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H5), 7.45 (d, $^3J_{HH}$ = 2.3 Hz, 4H, H11), 7.39 (d, $^3J_{HH}$ = 7.7 Hz, 2H, H2), 7.20 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H6), 6.73 (t, $^3J_{HH}$ = 7.8 Hz, 1H, H3), 5.86 (t, $^3J_{HH}$ = 2.2 Hz, 4H, H10),

2.50 (sept, $^3J_{HH}$ = 6.5 Hz, 1H, H13), 2.32 (s, 6H, H8), 1.19 (d, $^3J_{HH}$ = 6.4 Hz, 6H, H14), 1.17 (d, $^3J_{HH}$ = 6.7 Hz, 2H, H12). $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ 172.3 (C1), 140.9 (C4), 140.7 (C9), 136.8 (C7), 136.5 (C11), 136.2 (C5), 134.4 (C3), 129.0 (C6), 127.3 (C2), 104.6 (C10), 64.6 (C12), 31.9 (C13), 29.6 (C14), 21.4 (C8). ^{11}B NMR (161 MHz, C_6D_6) δ 0.08. Elemental Analysis: Calcd. (%) for $C_{35}H_{38}B_2N_9Sc$: C, 64.54; H, 5.88; N, 19.35. Found: C, 57.13; H, 4.71; N, 17.58.

Synthesis of 2-^{n}Pr



1 (79 mg, 0.125 mmol) was reacted with Li^{n}Pr (7 mg, 0.140 mmol, 1.12 equiv.) to yield **2-^{n}Pr** as an off-white solid (66 mg, 0.101 mmol, 81%).

^1H NMR (500 MHz, C_6D_6): δ 8.05 (d, $^3J_{HH}$ = 2.1 Hz, 4H, H9), 7.78 (d, $^3J_{HH}$ = 7.9 Hz, 4H, H5), 7.45 (d, $^3J_{HH}$ = 2.3 Hz, 4H, H11), 7.39 (d, $^3J_{HH}$ = 7.8 Hz, 2H, H2), 7.20 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H6), 6.74 (t, $^3J_{HH}$ = 7.8 Hz, 1H, H3), 5.85 (t, $^3J_{HH}$ = 2.2 Hz, 4H, H10), 2.32 (s, 6H, H8), 2.06 (m, 2H, H13), 1.27 (t, $^3J_{HH}$ = 7.1 Hz, 3H, H14), 1.15 (m, 2H, H12). $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ 172.3 (C1), 140.8 (C4), 140.6 (C9), 136.8 (C7), 136.4 (C11), 136.2 (C5), 134.5 (C3), 129.0 (C6), 127.3 (C2), 104.7 (C10), 55.0 (C12), 25.4 (C13), 22.5 (C14), 21.4 (C8). ^{11}B NMR (161 MHz, C_6D_6) δ -0.01. Elemental Analysis: Calcd. (%) for $C_{34}H_{36}B_2N_9Sc$: C, 64.08; H, 5.69; N, 19.78. Found: C, 62.73; H, 5.64; N, 19.05.

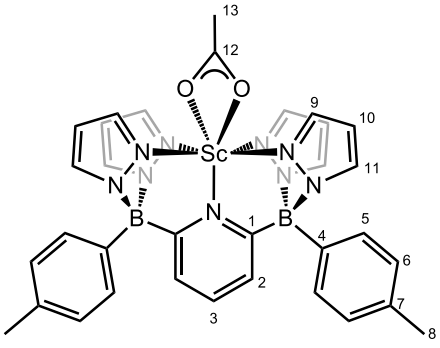
Synthesis of tol-Pz$_4$B$_2$PyScD (2-D)

Same synthetic procedure as **2-H** but used $LiDBEt_3$ instead of $NaHBEt_3$.

1 (104 mg, 0.165 mmol) was reacted with $LiDBEt_3$ (18 mg, 0.170 mmol, 1.03 equiv.) to yield **2-D** as a white solid (53 mg, 0.089 mmol, 54%).

^2H NMR (77 MHz, C_6H_6) δ 9.16.

Synthesis of tol-Pz$_4$B$_2$PyScOOCCH$_3$ (4-Me)



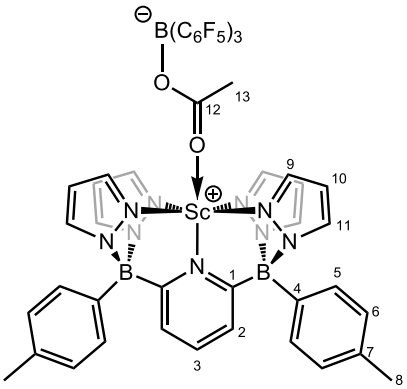
Method A: A J-Young NMR tube was charged with **2-Me** (10 mg, 0.017 mmol) and dissolved in C_6D_6. The colourless solution was degassed by freeze-pump-thaw at -78 °C and backfilled with 1 atm of CO_2. The solution was heated to 70 °C for 2 hours to ensure complete formation of **2-Me**. Quantitative conversion by NMR.

Method B: A 50 mL thick-walled glass vessel equipped with a Kontes PTFE valve plug was charged with both **1** (125 mg, 0.199 mmol) and NaOAc (17 mg, 0.207 mmol, 1.04 equiv.). The apparatus was connected to the vacuum line and 20 mL of THF was vacuum transferred to the solid mixture at -78 °C. The cloudy white mixture was heated to 60 °C for 24 hours after which the solvent was removed *in*

vacuo. The residue was extracted with 20 mL toluene and filtered through a 0.1 µm PTFE syringe filter to remove NaCl and excess NaOAc. The filtrate was transferred into a 50 mL thick-walled glass vessel and subsequently evaporated *in vacuo* to yield a colourless residue. The residue was triturated and sonicated with 20 mL of pentane. The white suspension was then filtered through a medium porosity frit and washed with 2x3 mL of pentane. The product was isolated as a white solid and dried *in vacuo* (98 mg, 0.150 mmol, 76%). Single crystals suitable for X-ray diffraction were obtained by slow vapour diffusion of pentane onto a concentrated solution of **4-Me** in benzene.

^{1}H NMR (500 MHz, C_6D_6): δ 8.47 (d, $^3J_{HH}$ = 2.1 Hz, 4H, H9), 7.85 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H5), 7.63 (d, $^3J_{HH}$ = 7.7 Hz, 2H, H2), 7.41 (d, $^3J_{HH}$ = 2.3 Hz, 4H, H11), 7.21 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H6), 6.81 (t, $^3J_{HH}$ = 7.7 Hz, 1H, H3), 5.86 (t, $^3J_{HH}$ = 2.2 Hz, 4H, H10), 2.33 (s, 6H, H8), 1.82 (s, 3H, H13). ^{13}C NMR (101 MHz, C_6D_6) δ 189.1 (C12), 173.4 (C1), 142.1 (C9), 141.0 (C4), 136.7 (C7), 136.4 (C11), 136.3 (C5), 134.3 (C3), 129.0 (C6), 127.3 (C2), 104.3 (C10), 22.4 (C13), 21.4 (C8). ^{11}B NMR (161 MHz, C_6D_6) δ -0.29. $\nu_{C\text{-}O}$: 1535 cm^{-1}. Elemental Analysis: Calcd. (%) for $C_{32}H_{30}B_2N_9O_2Sc$: C, 60.67; H, 4.94; N, 19.30. Found: C, 61.83; H, 5.36; N, 18.05.

Synthesis of [tol-Pz$_4$B$_2$PySc][MeCOOB(C$_6$F$_5$)$_3$] (5-Me)



A 50 mL thick-walled glass vessel equipped with a Kontes PTFE valve plug was charged with **4-Me** (49 mg, 0.075 mmol) and $B(C_6F_5)_3$ (40 mg, 0.078 mmol, 1.04 equiv.). 10 mL was added to dissolve the solids to give a colourless solution. The solution was stirred for 1 h after which the solvent was removed *in vacuo*. The resulting residue was triturated and sonicated with 20 mL of pentane. The white suspension was then filtered through a medium porosity frit and washed with 2x3 mL of pentane. The product was isolated as a white solid and dried *in vacuo* (83 mg, 0.071 mmol, 95%).

^{1}H NMR (500 MHz, C_6D_6) δ 7.65 (d, $^3J_{HH}$ = 8.0 Hz, 4H, H5), 7.59 (d, $^3J_{HH}$ = 2.2 Hz, 4H, H9), 7.36 (d, $^3J_{HH}$ = 2.3 Hz, 4H, H11), 7.28 (d, $^3J_{HH}$ = 7.8 Hz, 2H, H2), 7.20 (d, $^3J_{HH}$ = 7.7 Hz, 4H, H6), 6.64 (t, $^3J_{HH}$ = 7.8 Hz, 1H, H3), 5.73 (t, $^3J_{HH}$ = 2.3 Hz, 4H, H10), 2.32 (s, 6H, H8), 1.59 (s, 3H, H13). ^{13}C{^{1}H} NMR (126 MHz, C_6D_6) δ 183.1 (C12), 171.3 (C1), 148.6 (dm, $^1J_{CF}$ = 240 Hz, [MeCO$_2$B(*C*$_6$F$_5$)$_3$]$^-$), 140.2 (dm, $^1J_{CF}$ = 251 Hz, [MeCO$_2$B(*C*$_6$F$_5$)$_3$]$^-$), 139.9 (C9), 138.7 (C4), 137.5 (dm, $^1J_{CF}$ = 262 Hz, [MeCO$_2$B(*C*$_6$F$_5$)$_3$]$^-$), 137.6 (C7), 137.5 (C11), 136.0 (C3), 135.7 (C5), 129.4 (C6), 128.2 (C2), 119.5 ([MeCO$_2$B(*C*$_6$F$_5$)$_3$]$^-$), 105.4 (C10), 24,3 (C13), 21.3 (C8). ^{11}B NMR (161 MHz, C_6D_6) δ -0.20. ^{19}F NMR (471 MHz, C_6D_6) δ -135.45 (d, $^3J_{FF}$ = 22.2 Hz, *o*-F), -158.54 (t, $^3J_{FF}$ = 20.9 Hz, *p*-F), -165.24 (t, $^3J_{FF}$ = 20.9 Hz, *m*-F). $\nu_{C\text{-}O}$: 1571 cm^{-1}. Elemental Analysis: Calcd. (%) for $C_{51}H_{32}B_3F_{15}N_9O_2Sc$: C, 52.57; H, 2.77; N, 10.82. Found: C, 5.25; H, 3.05; N, 10.51.

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Computational Details

All DFT calculations were carried out with the Gaussian 09 suite of programs.[i] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional. [ii] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Scandium atoms were treated with Stuttgart effective core potential and their associated basis set. [iii] For the other elements (H, C, O, N and B), Pople's double-ζ basis set 6 31G(d,p) was used. [iv]

Computational References

[i] Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheesman, 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., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; A., R.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; 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. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian Inc., 2009, Wallingford CT
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[iv] (a) Hariharan, P. C.; Pople, J. A. The Influence of Polarization Functions on Molecular Orbital Hydrogenation Energies. *Theor. Chem. Acc.* **1973**, *28*, 213 – 222. (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972**, *56*, 2257 – 2261.

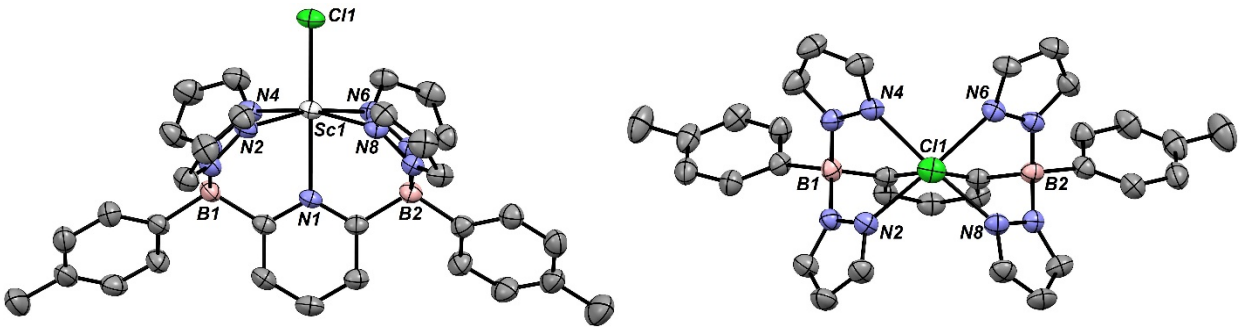

Figure S1. Molecular structure of **1**, front view (left) and top view (right). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level. Selected bond lengths (Å) and angles (°): Sc1–N1, 2.306(3); Sc1–N2, 2.224(4); Sc1–N4, 2.183(3); Sc1–N6, 2.197(4); Sc1–N8, 2.213(3); Sc1–Cl1, 2.396(1); N2–Sc1–N8, 98.60(14); N2–Sc1–N4, 83.78(14); N4–Sc1–N6, 91.55(13); N6–Sc1–N8, 82.93(13).

NMR Spectra

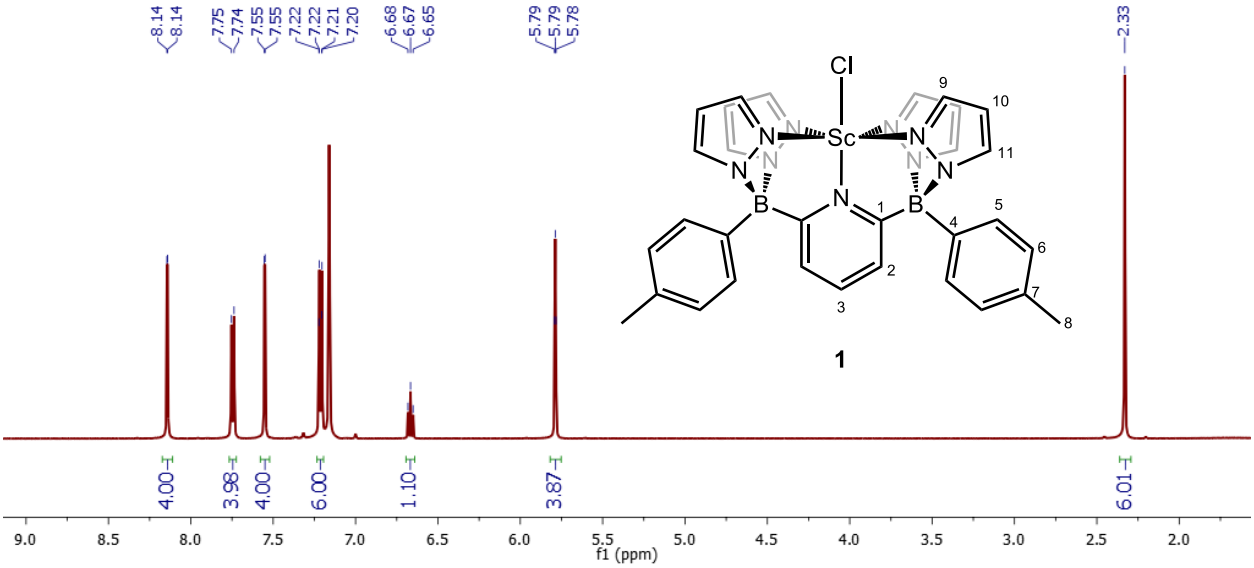

Figure S2. ^{1}H NMR spectrum of **1** in C_6D_6.

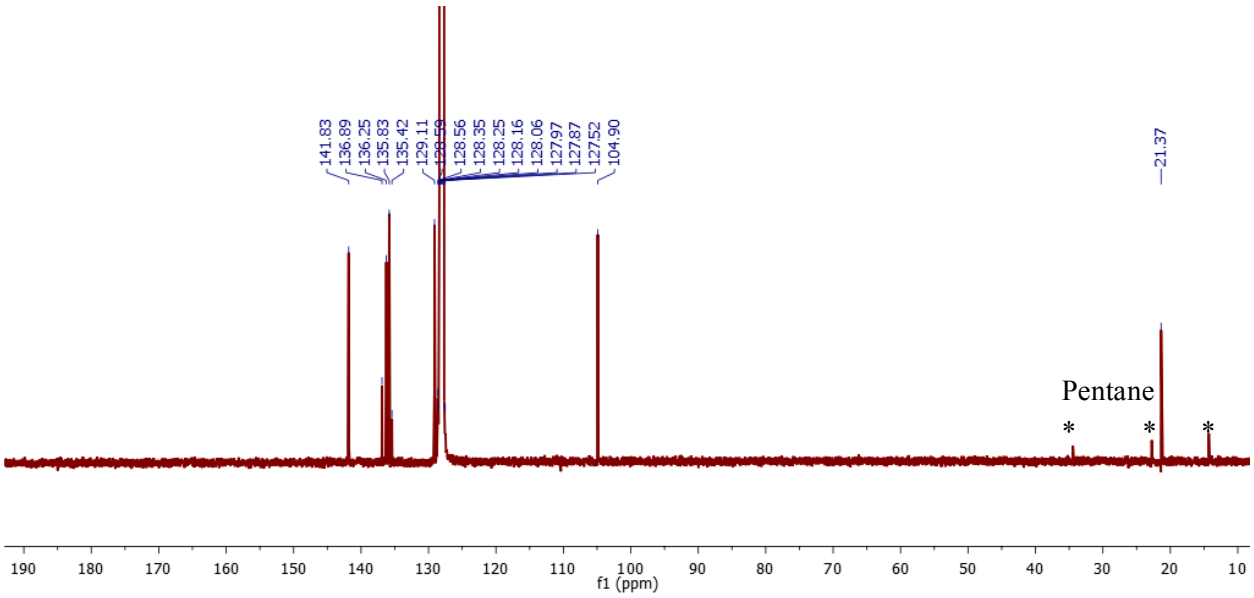

Figure S3. ^{13}C{^{1}H} NMR spectrum of **1** in C_6D_6.

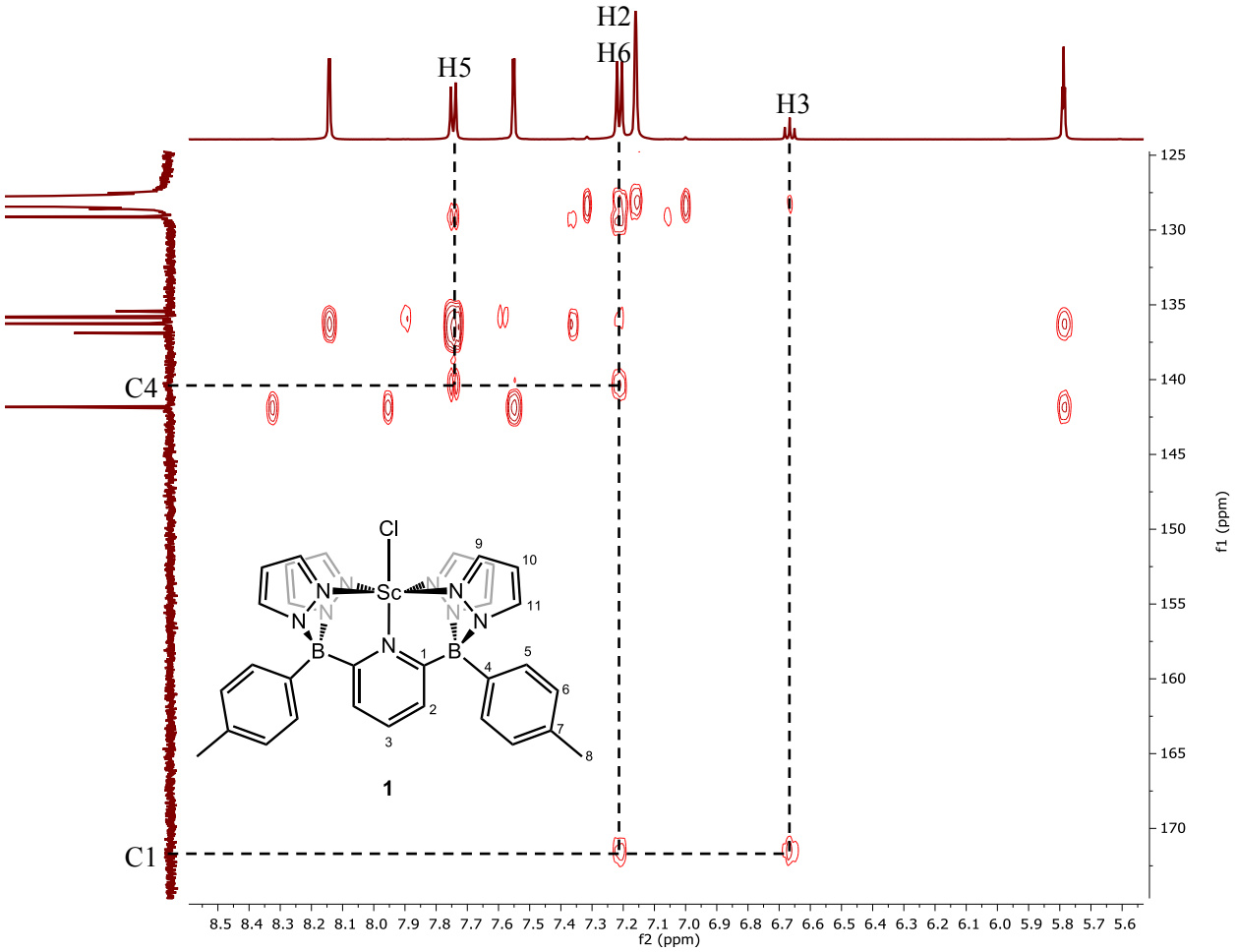

Figure S4. ^{1}H-^{13}C HMBC NMR spectrum of **1** for the determination of C1 and C4.

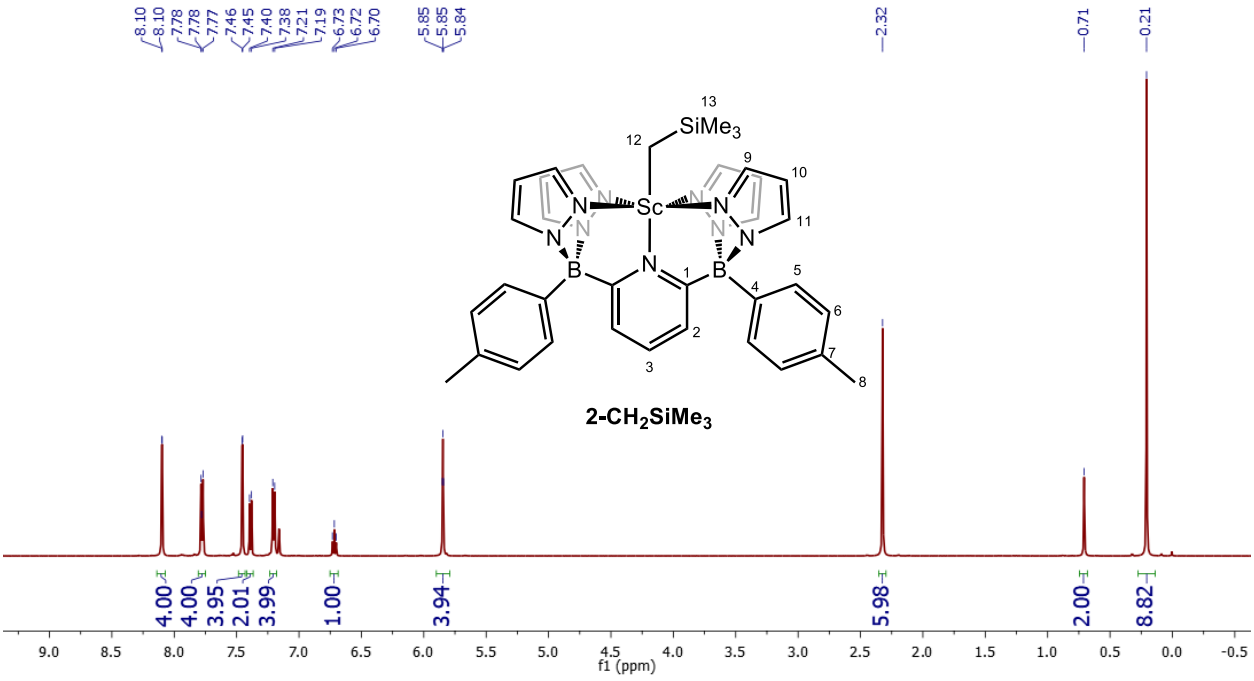

Figure S5. ^{1}H NMR spectrum of **2-CH_2SiMe_3** in C_6D_6.

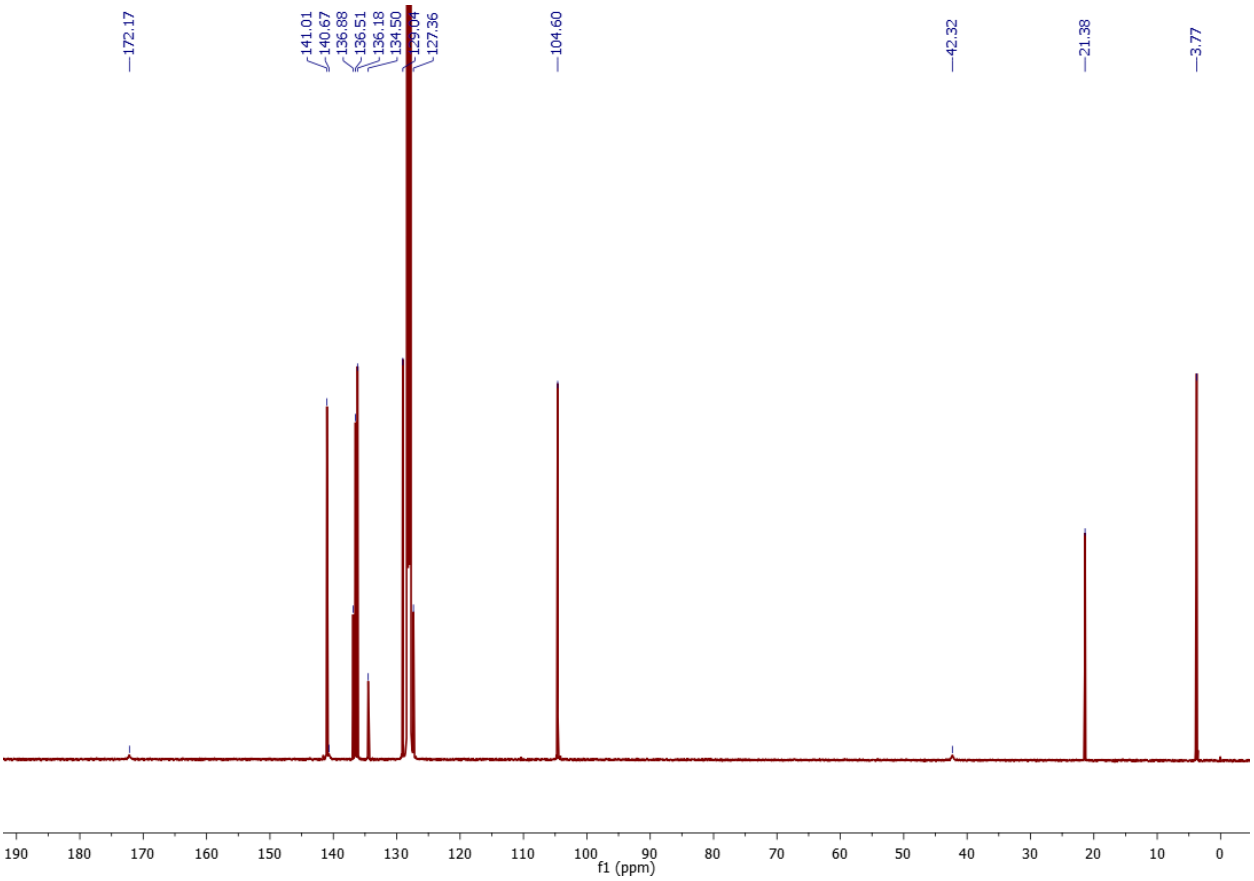

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **2-CH_2SiMe_3** in C_6D_6.

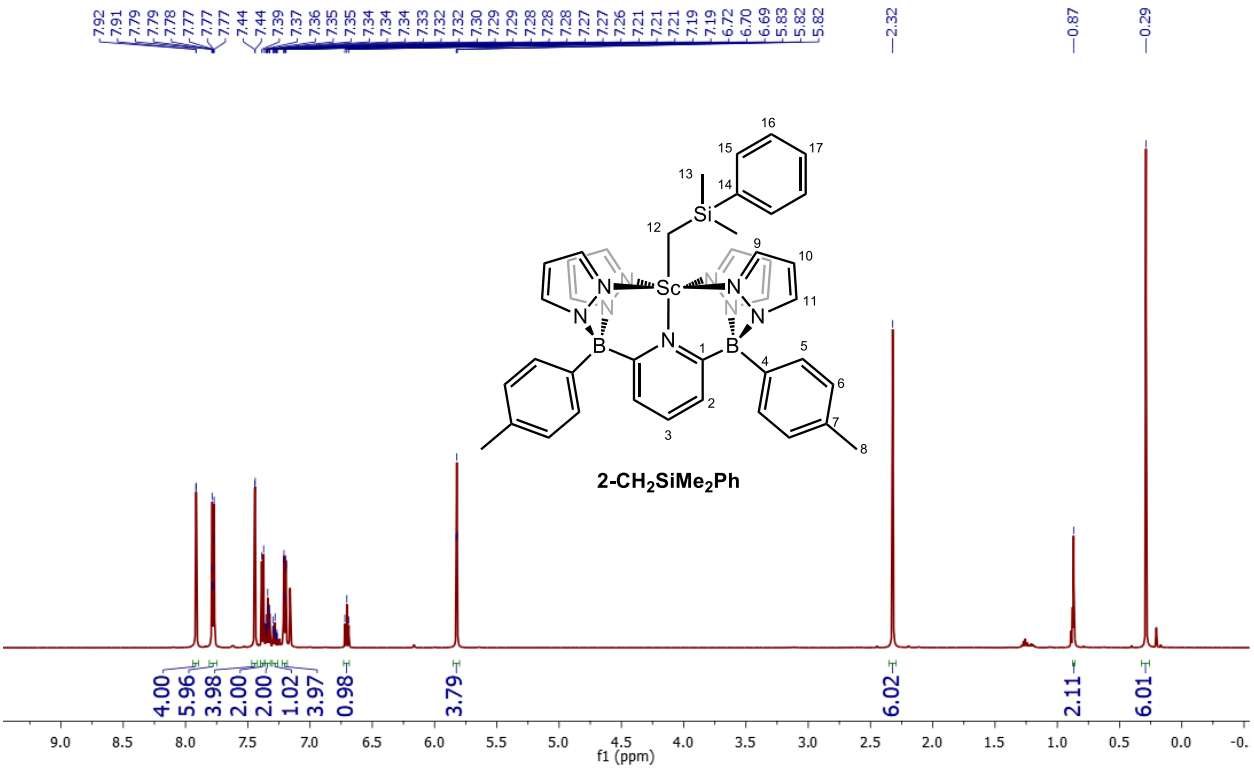

Figure S7. ^{1}H NMR spectrum of **2-CH$_2$SiMe$_2$Ph** in C_6D_6.

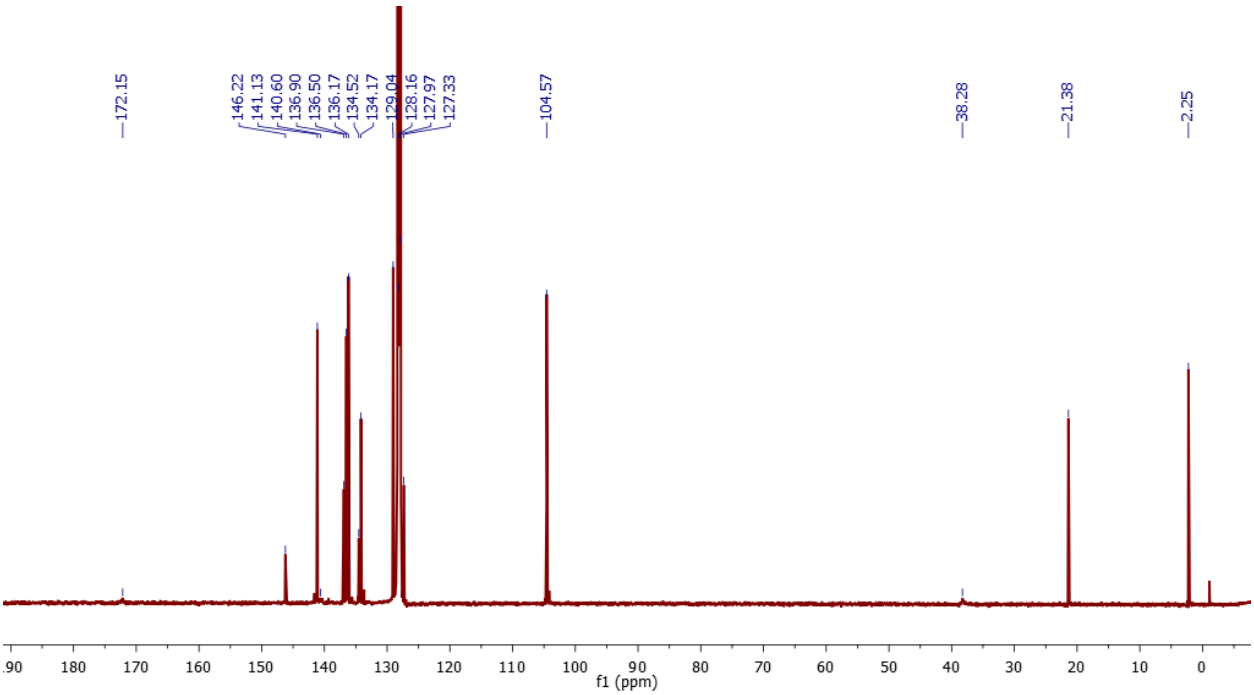

Figure S8. ^{13}C{^{1}H} NMR spectrum of **2-CH$_2$SiMe$_2$Ph** in C_6D_6.

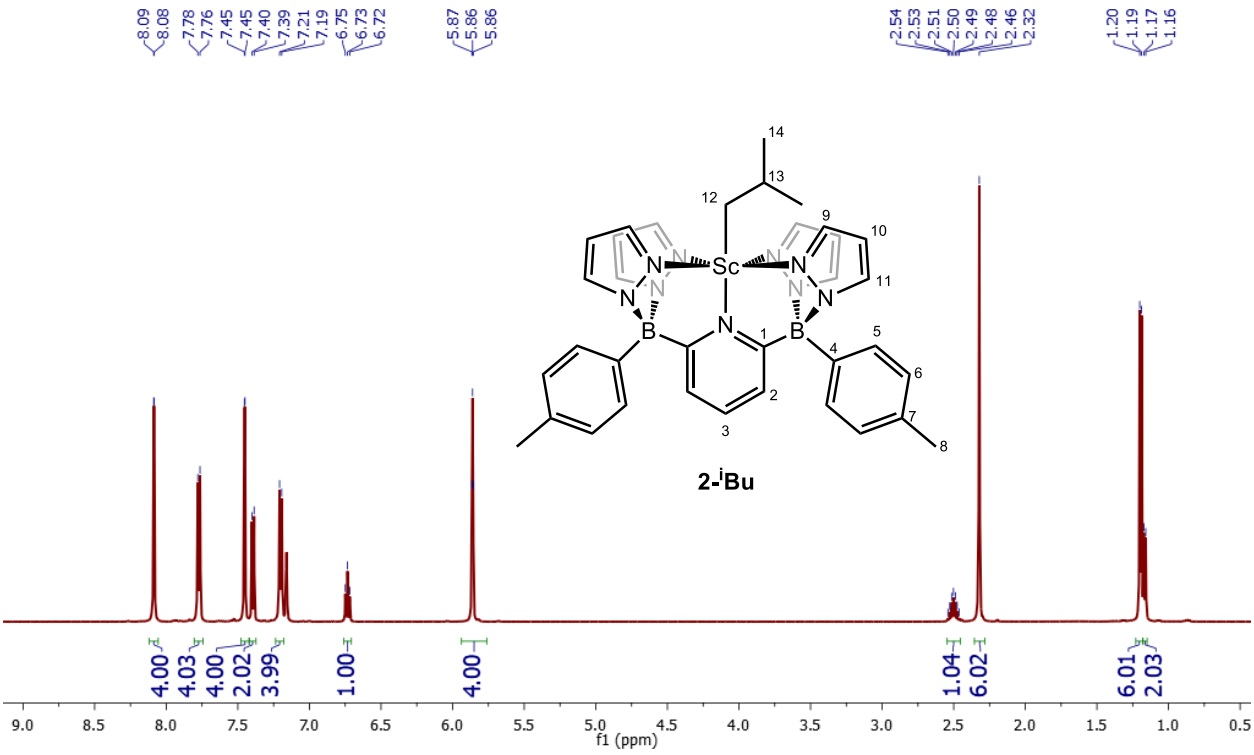

Figure S9. ^{1}H NMR spectrum of **2-^{i}Bu** in C_6D_6.

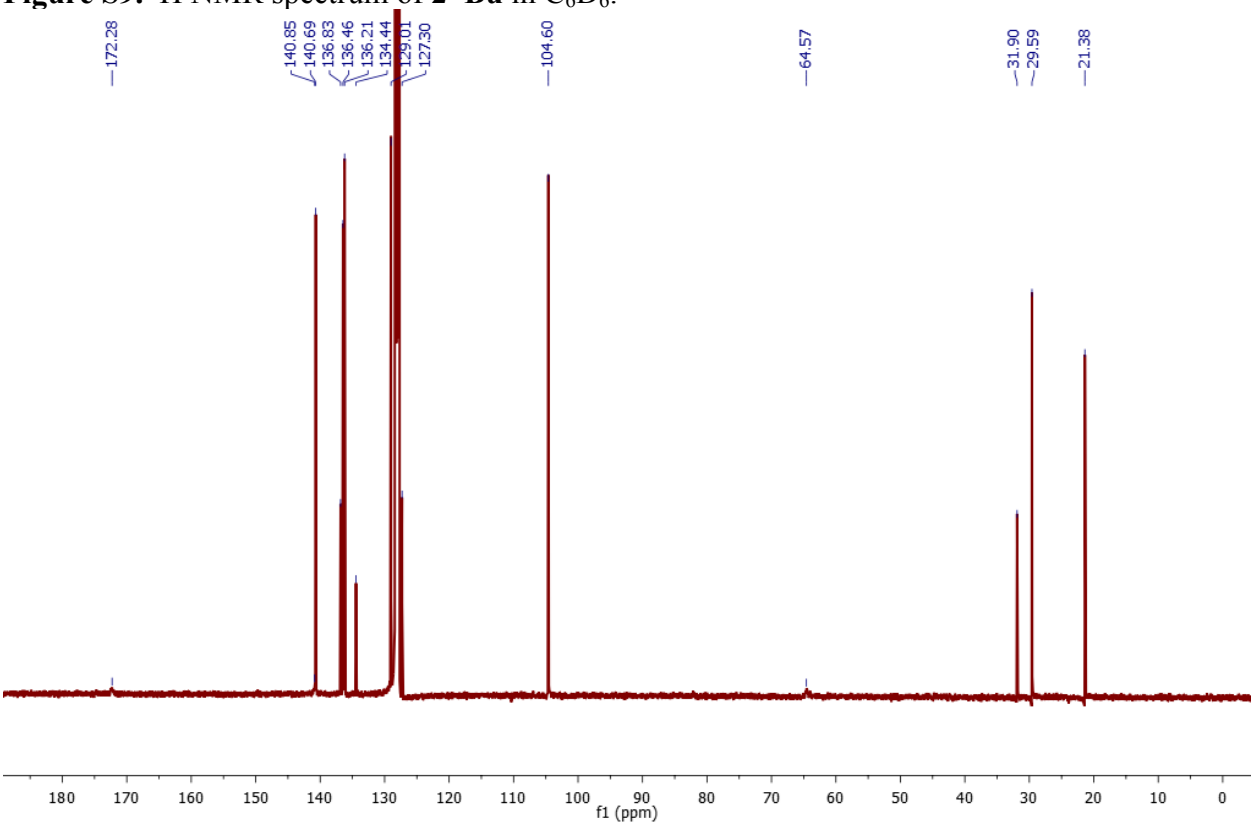

Figure S10. ^{13}C{^{1}H} NMR spectrum of **2-^{i}Bu** in C_6D_6.

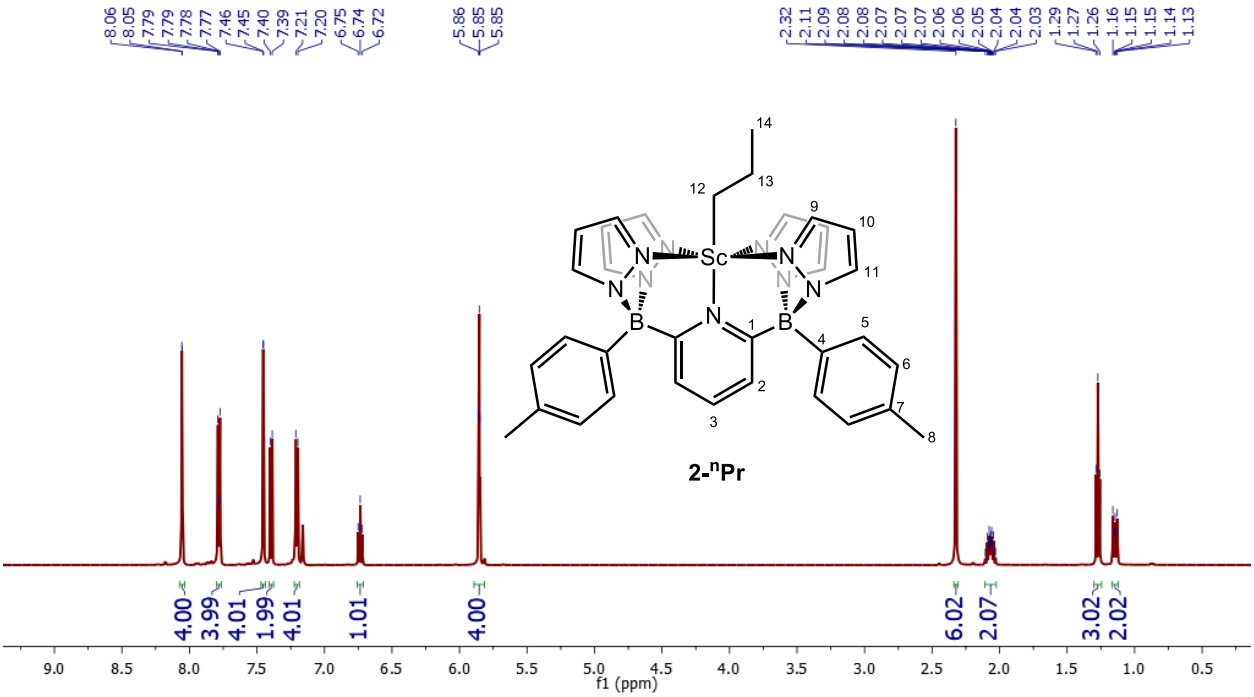

Figure S2. ^{1}H NMR spectrum of **2-^{n}Pr** in C_6D_6.

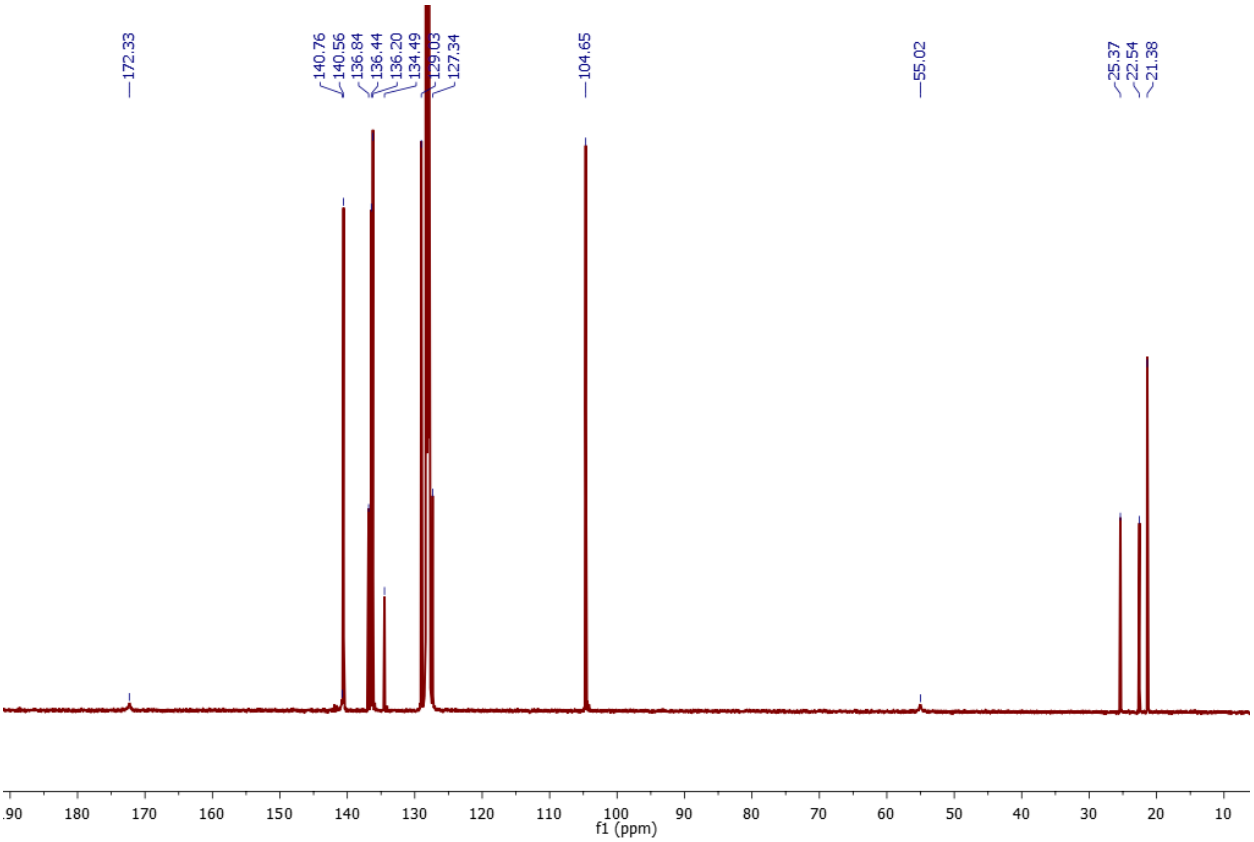

Figure S3. ^{13}C{^{1}H} NMR spectrum of **2-^{n}Pr** in C_6D_6.

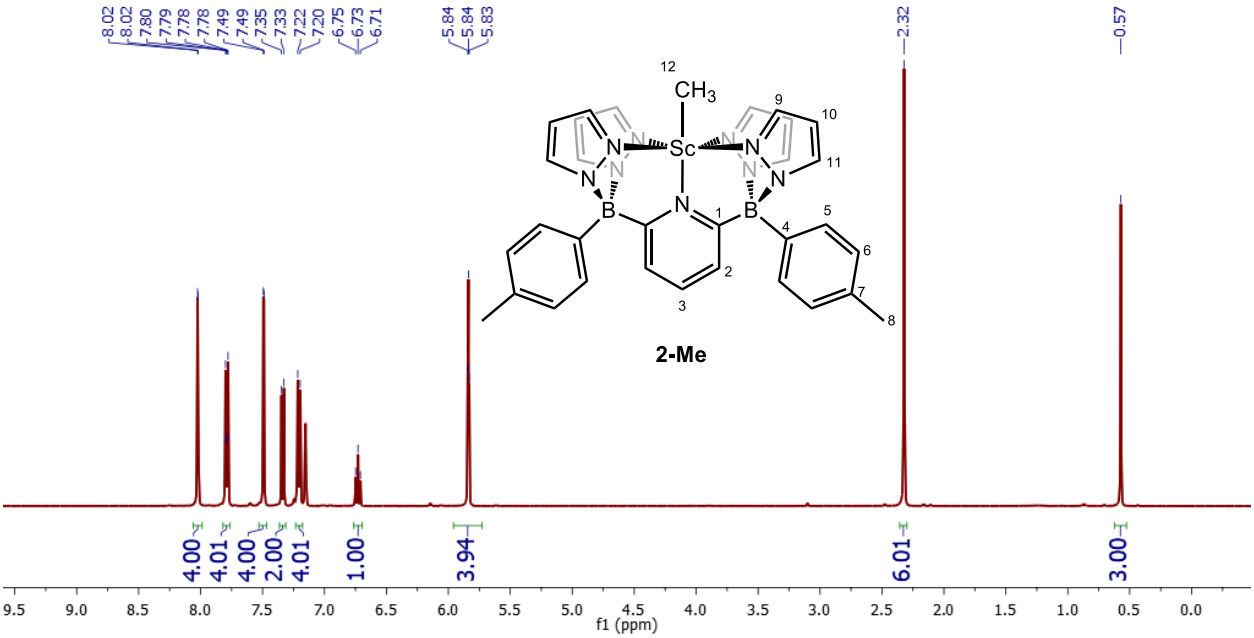

Figure S4. ^{1}H NMR spectrum of **2-Me** in C_6D_6.

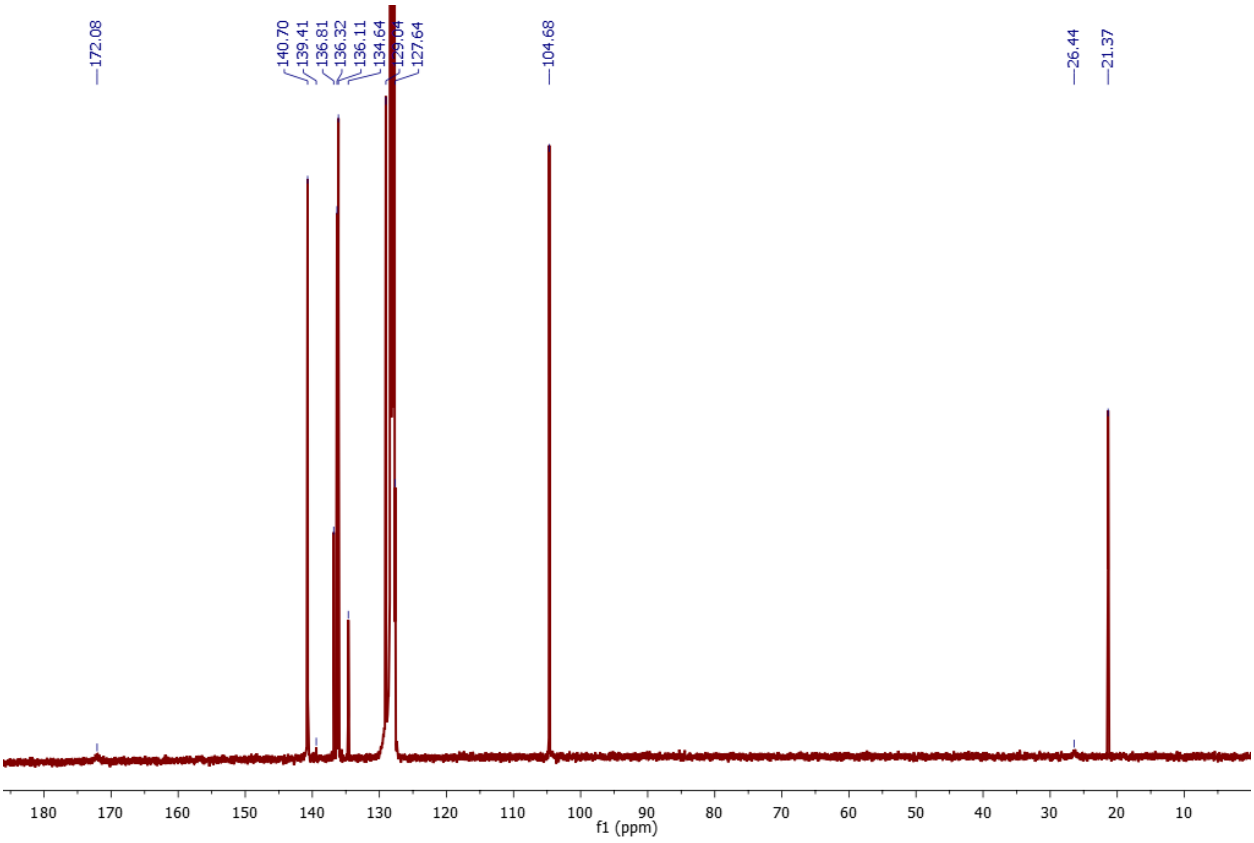

Figure S5. ^{13}C{^{1}H} NMR spectrum of **2-Me** in C_6D_6.

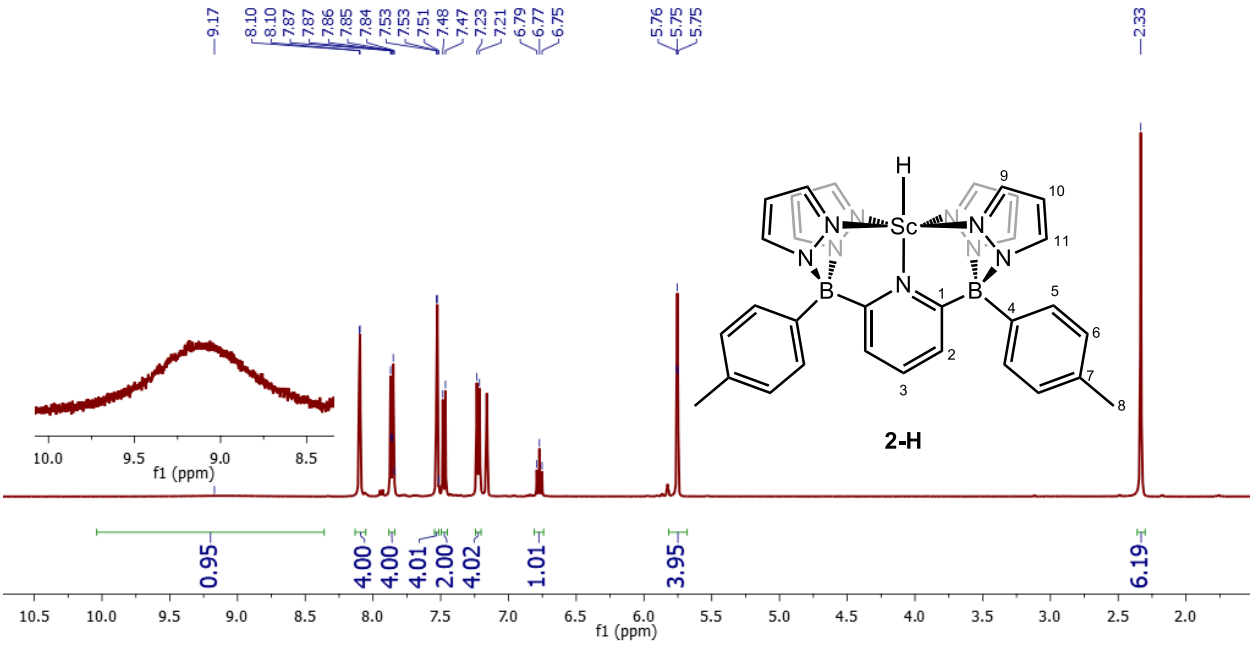

Figure S6. ^{1}H NMR spectrum of **2-H** in C_6D_6.

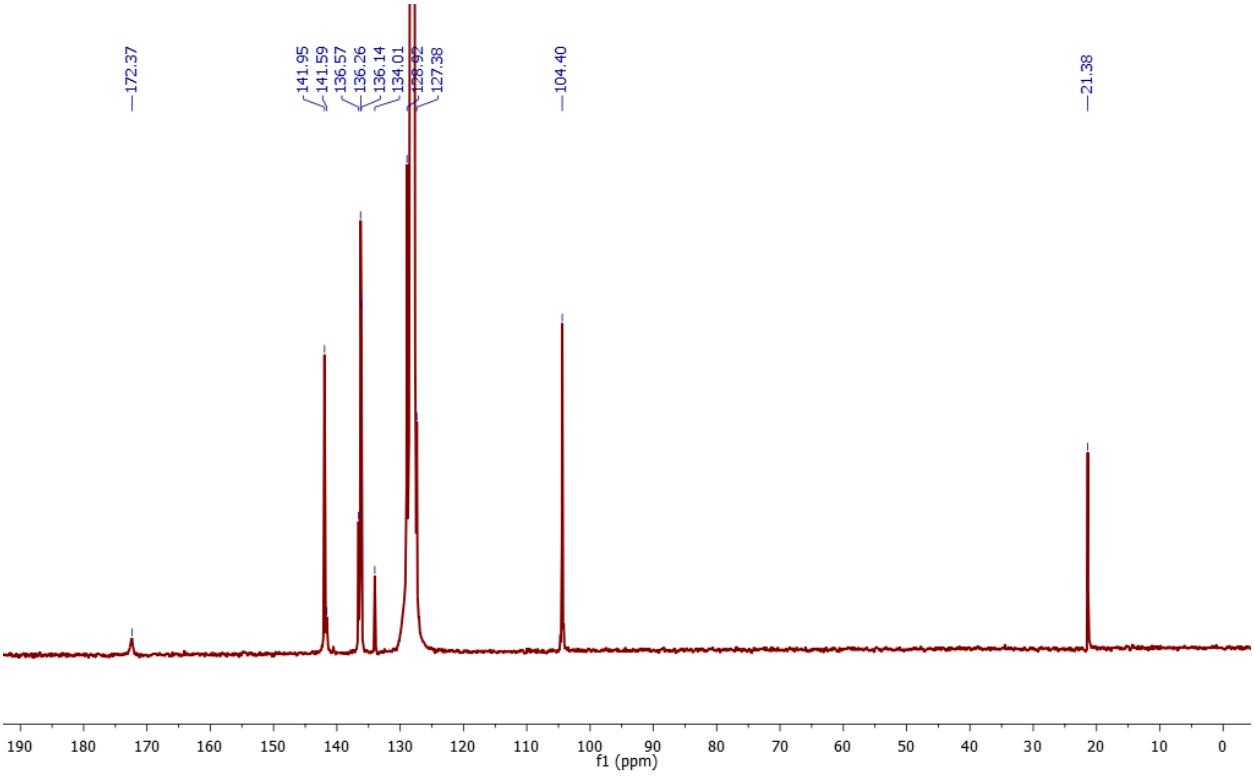

Figure S7. ^{13}C{^{1}H} NMR spectrum of **2-H** in C_6D_6.

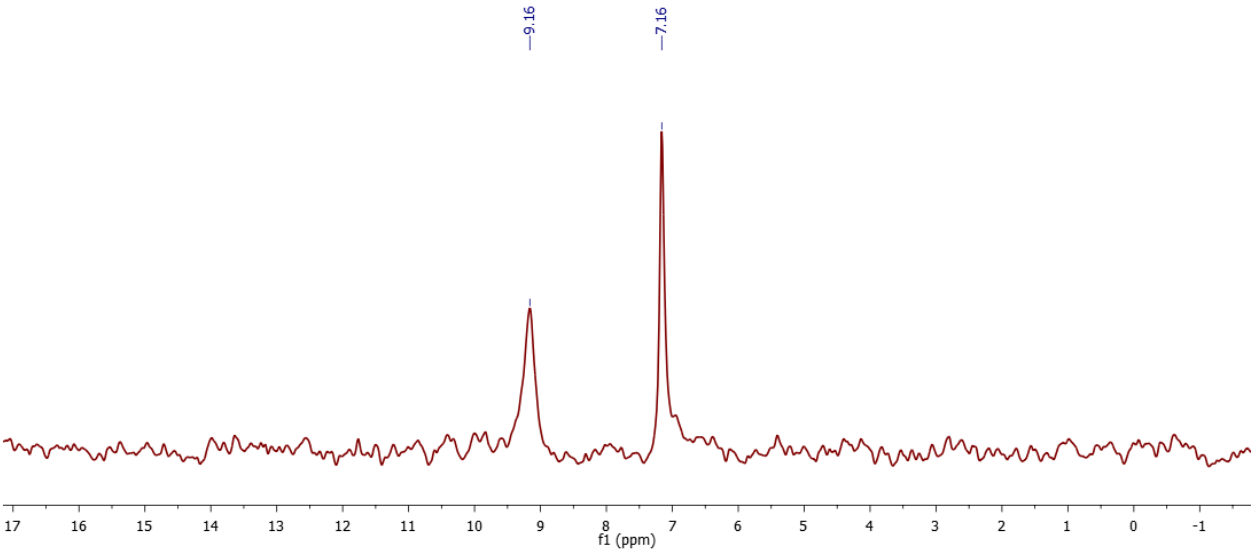

Figure S8. ^{2}H NMR spectrum of **2-D** in C_6H_6.

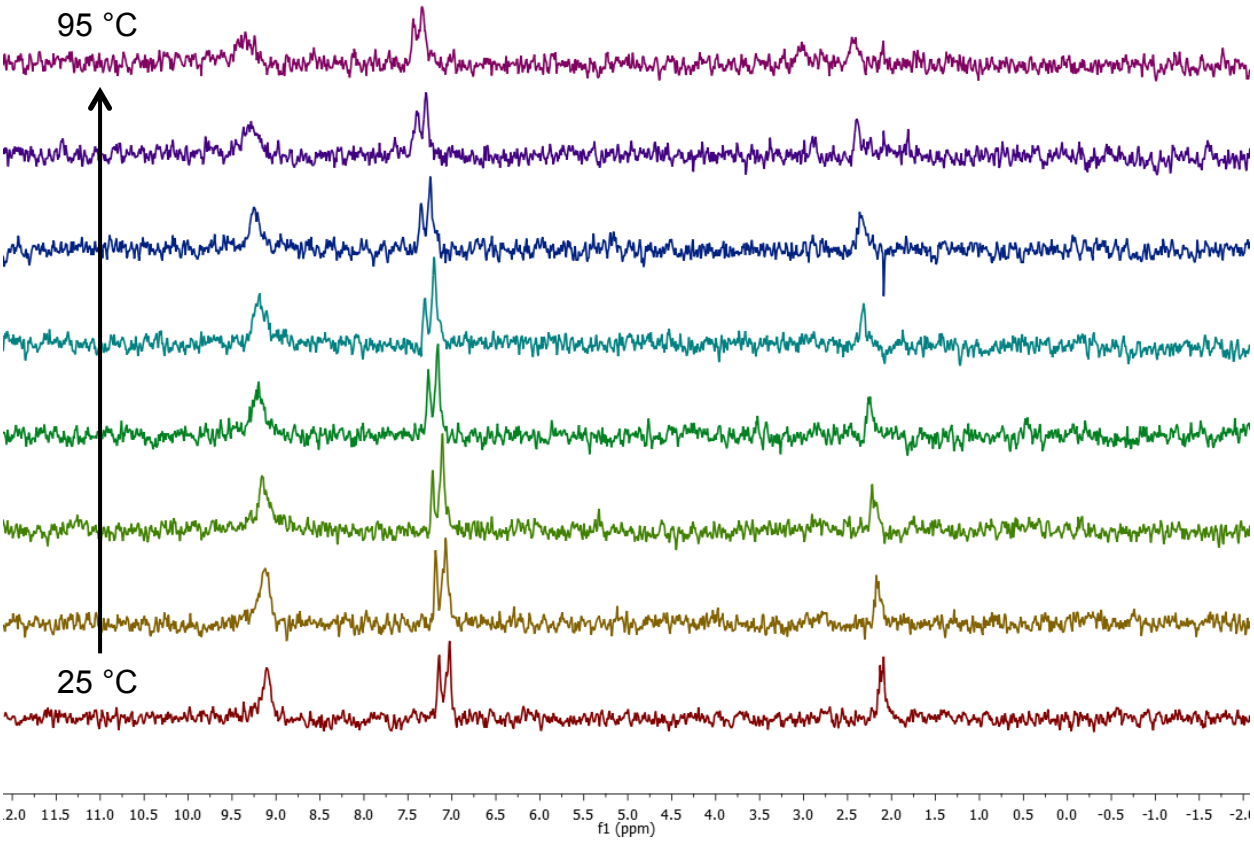

Figure S9. Variable temperature ^{2}H NMR spectra of **2-D** in toluene-H_8.

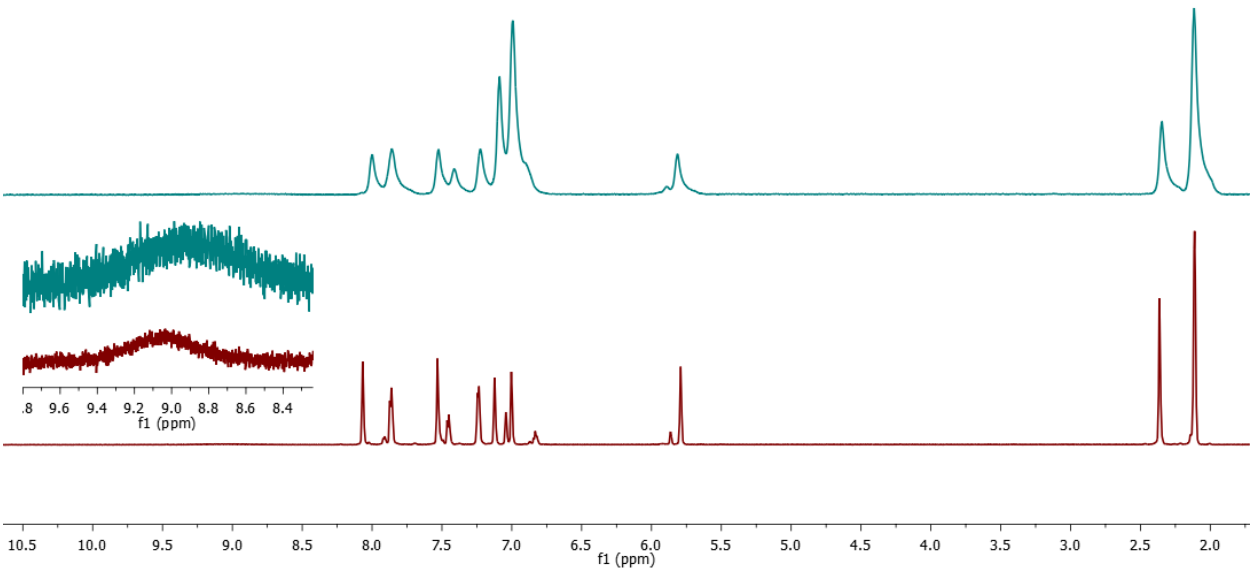

Figure S10. Stacked ^{1}H NMR spectra of **2-H** in toluene-d_8 at 368 K (top) and 298 K (bottom) with zoomed in region of the hydride (inset).

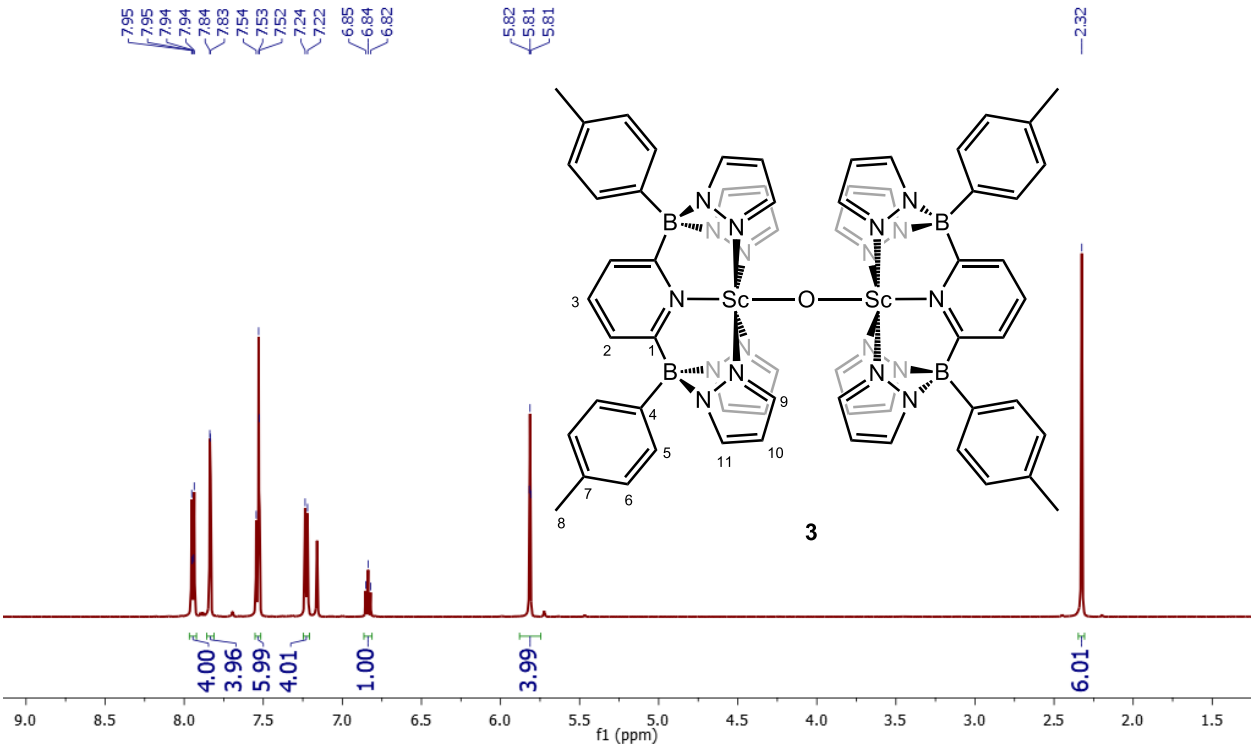

Figure S20. ^{1}H NMR spectrum of **3** in C_6D_6.

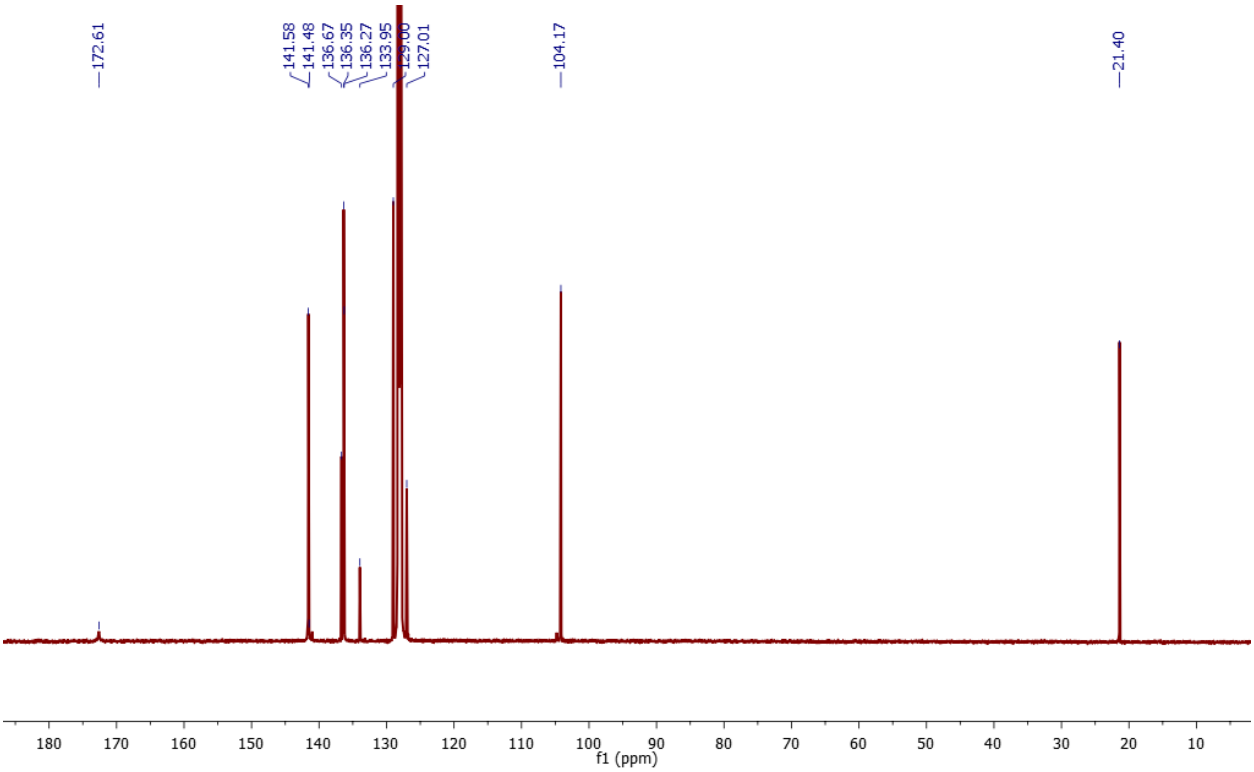

Figure S21. ^{13}C{^{1}H} NMR spectrum of **3** in C_6D_6.

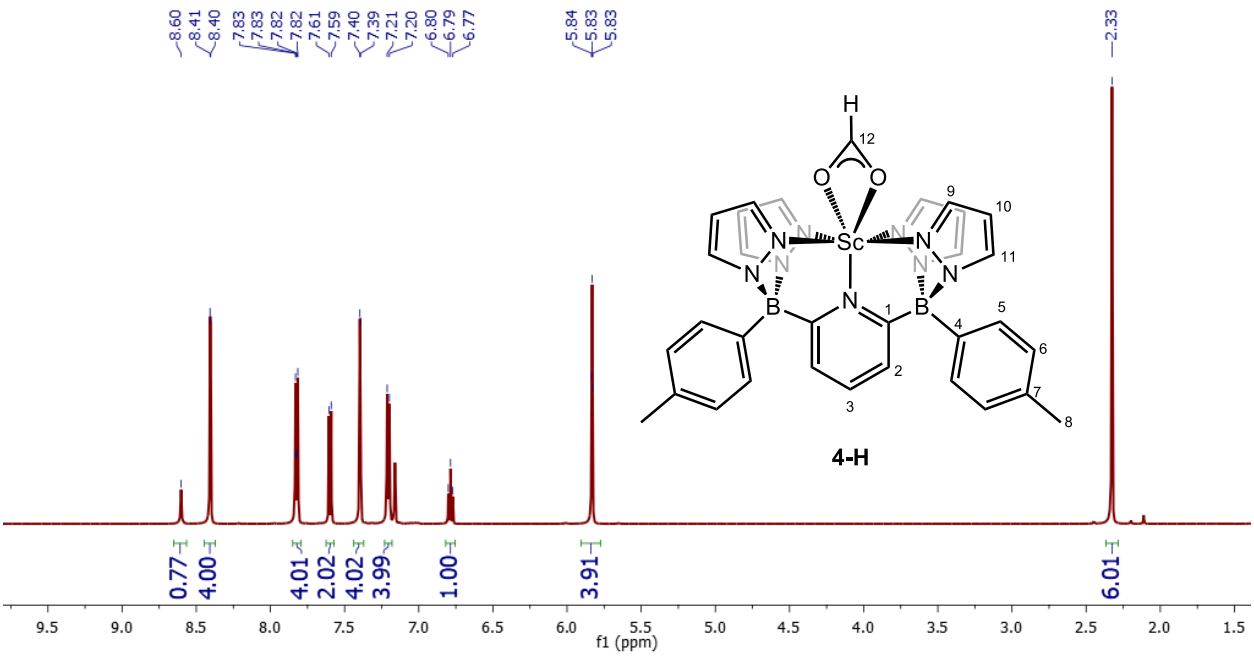

Figure S22. ^{1}H NMR spectrum of **4-H** in C_6D_6.

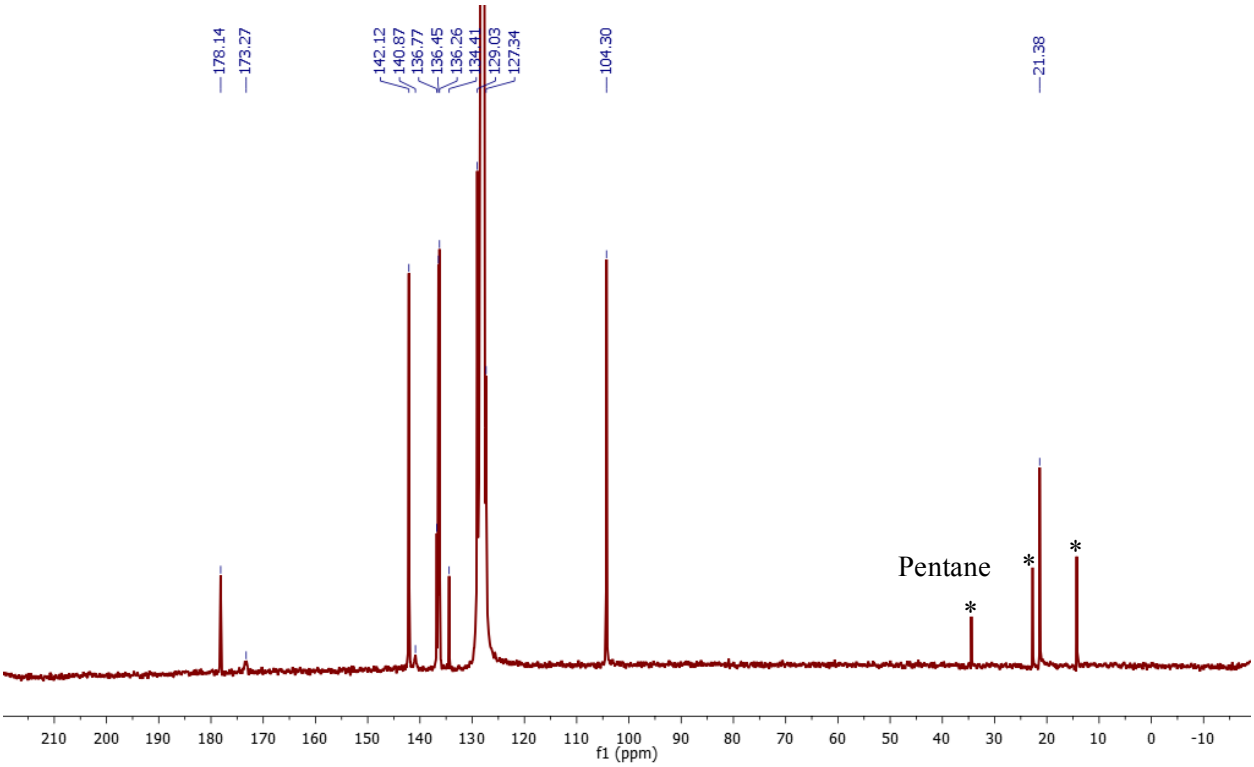

Figure S23. ^{13}C{^{1}H} NMR spectrum of **4-H** in C_6D_6.

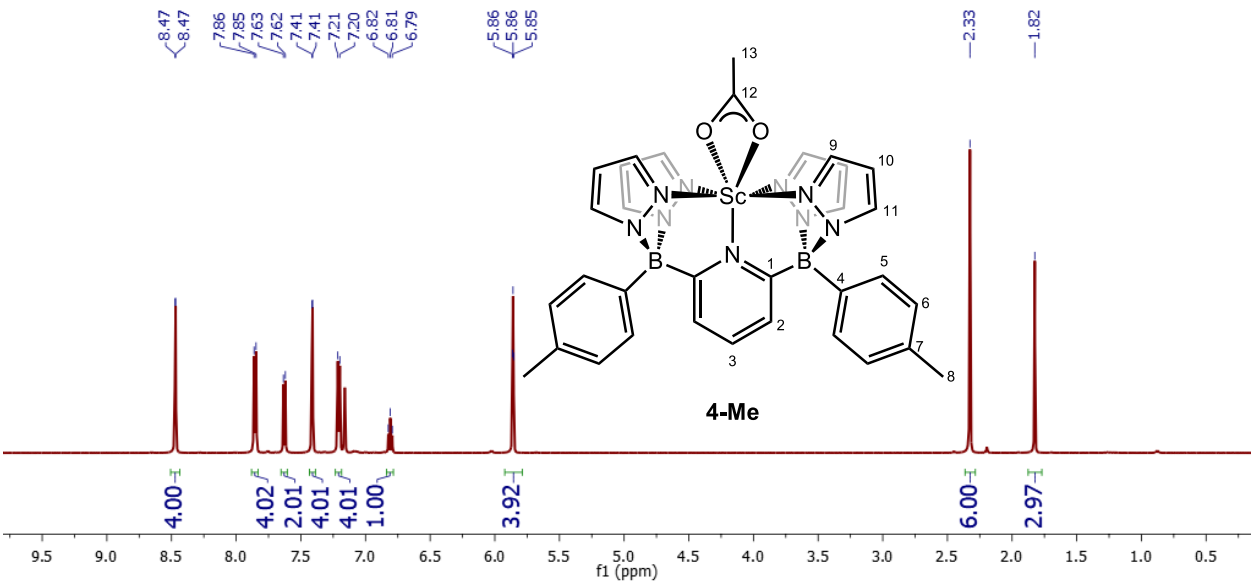

Figure S24. ^{1}H NMR spectrum of **4-Me** in C_6D_6.

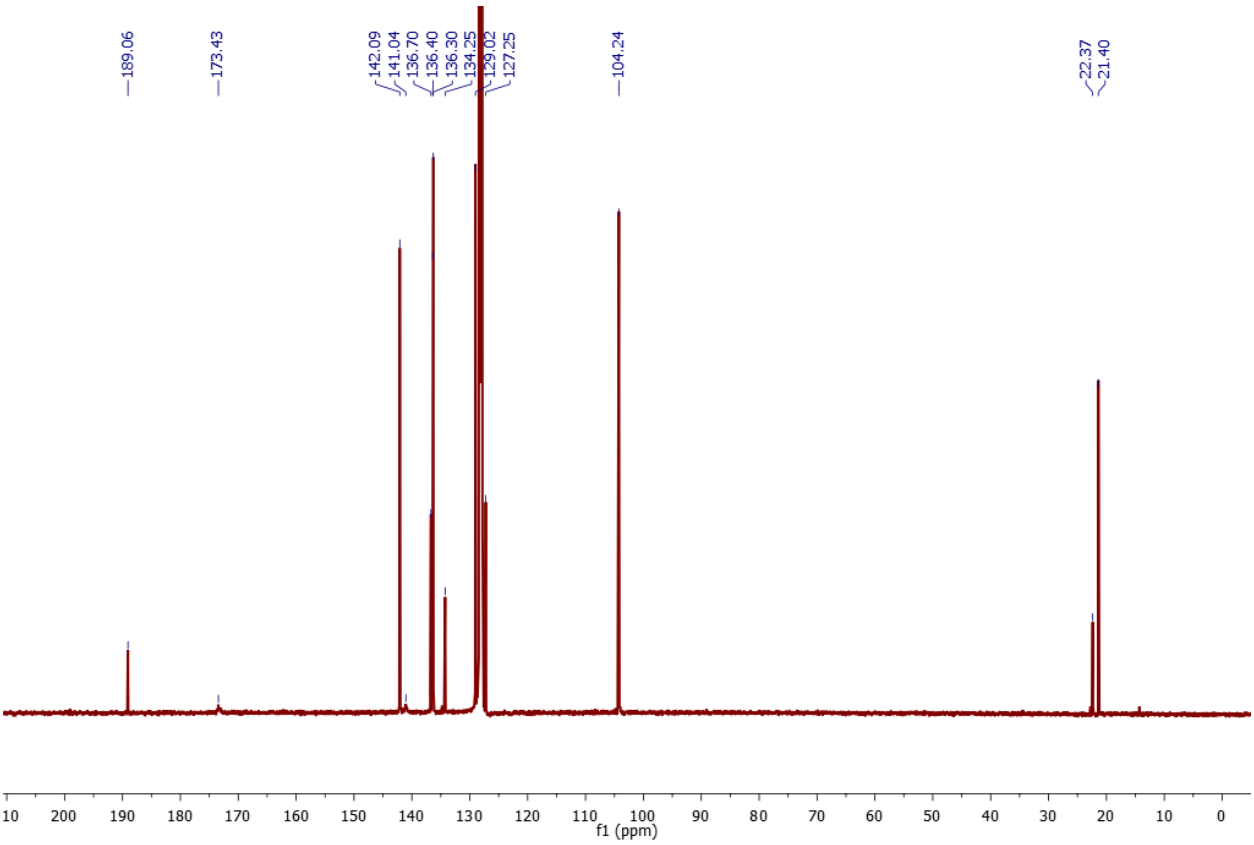

Figure S11. ^{1}H NMR spectrum of **4-Me** in C_6D_6.

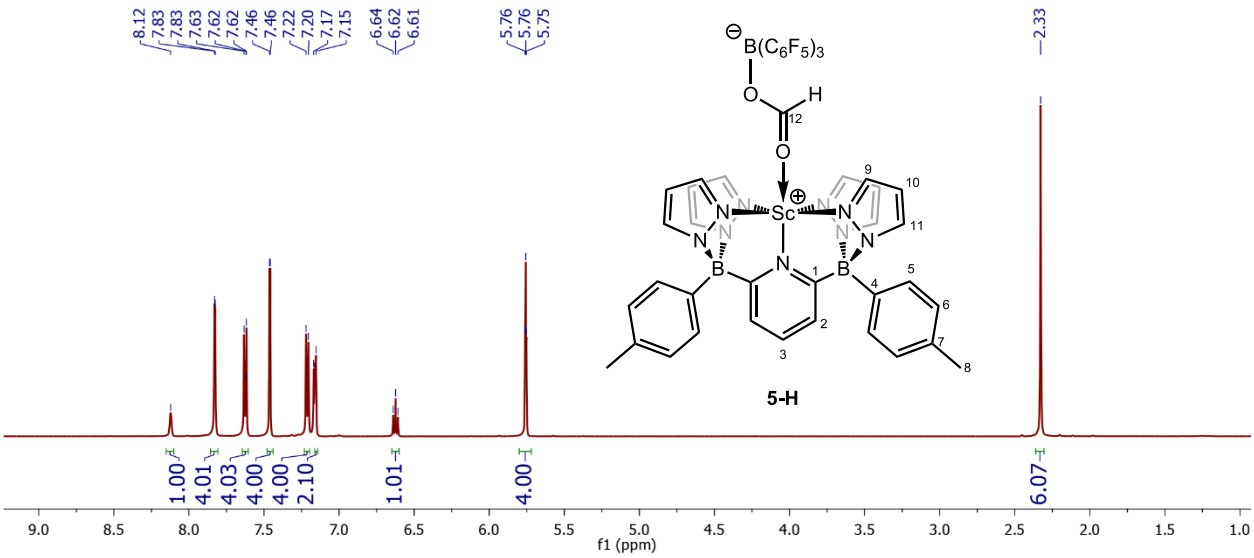

Figure S26. ^{1}H NMR spectrum of **5-H** in C_6D_6.

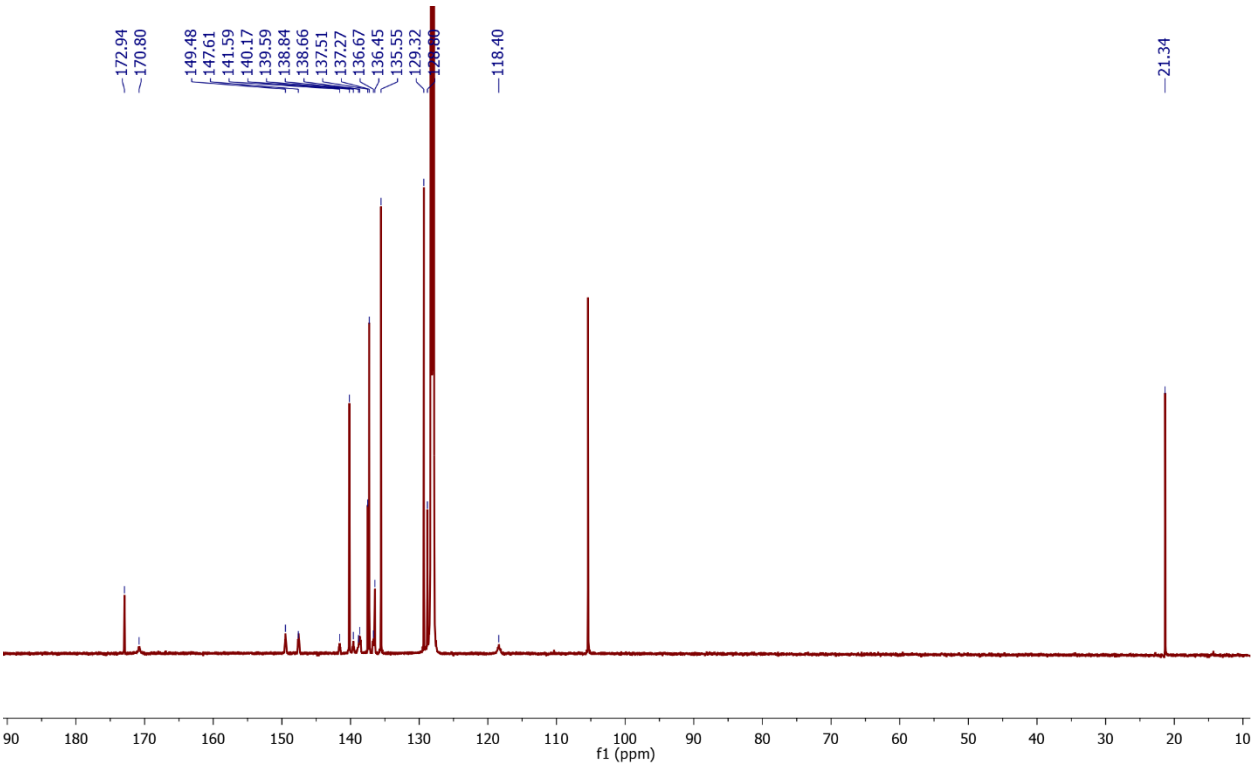

Figure S27. ^{13}C{^{1}H} NMR spectrum of **5-H** in C_6D_6.

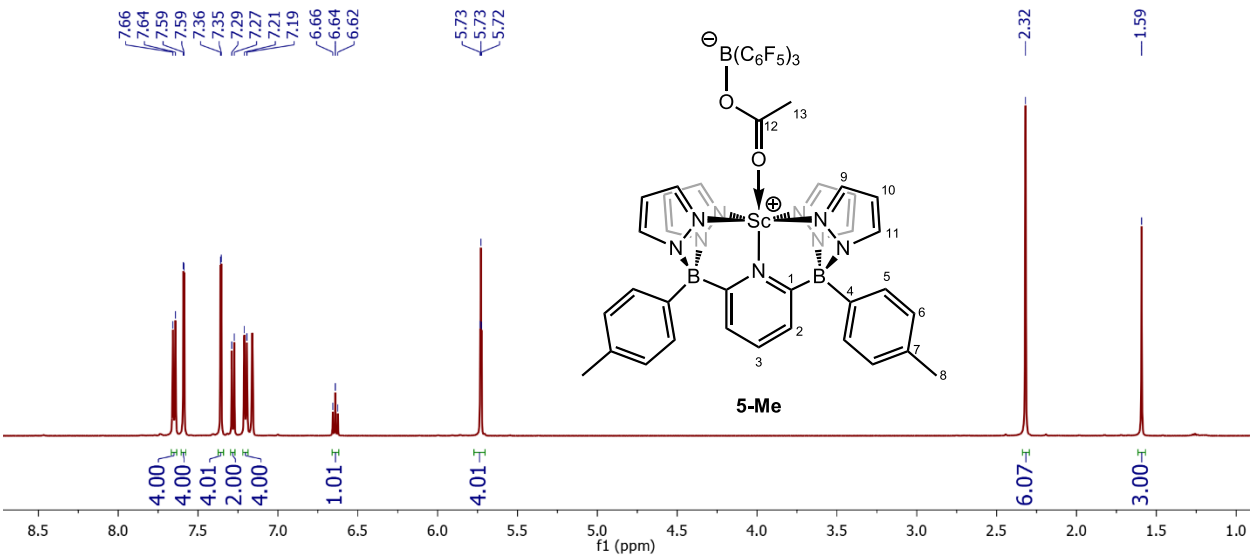

Figure S12. ^{1}H NMR spectrum of **5-Me** in C_6D_6.

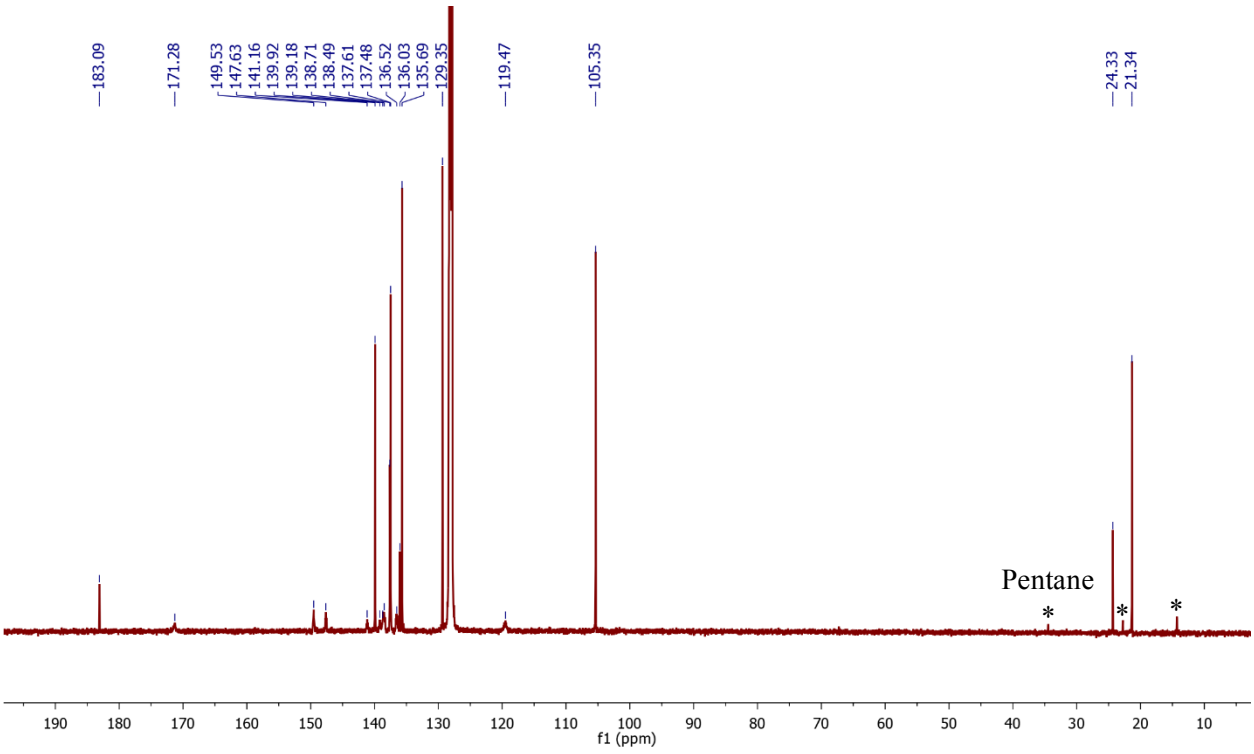

Figure S13. ^{13}C{^{1}H} NMR spectrum of **5-Me** in C_6D_6.

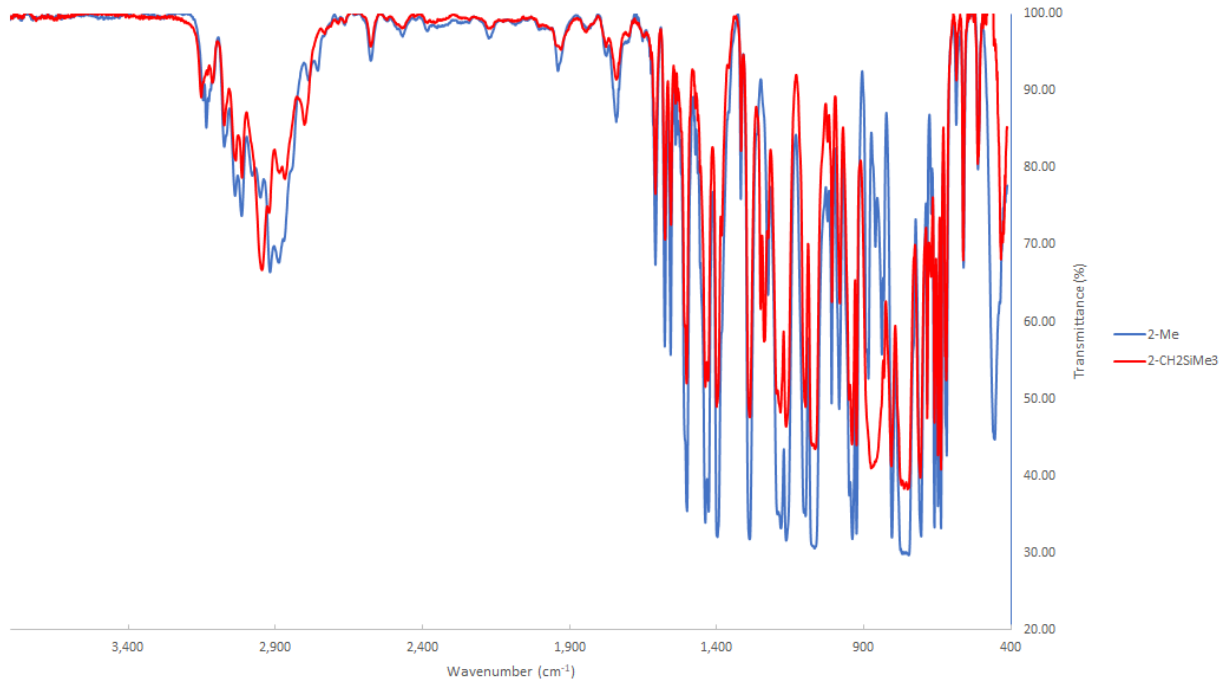

Figure S30. Superimposed FT-IR spectra of **2-Me** and **2-CH_2SiMe_3**, KBr pellet.

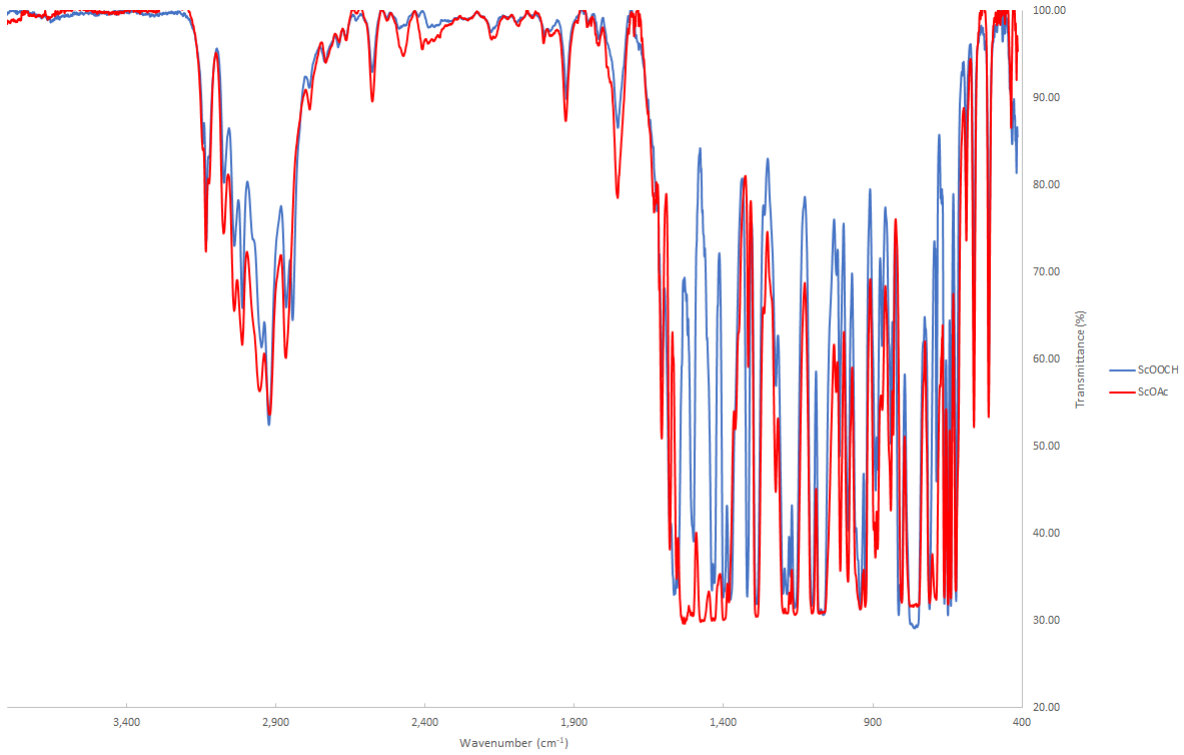

Figure S31. Superimposed FT-IR spectra of **4-H** and **4-Me**, KBr pellet.

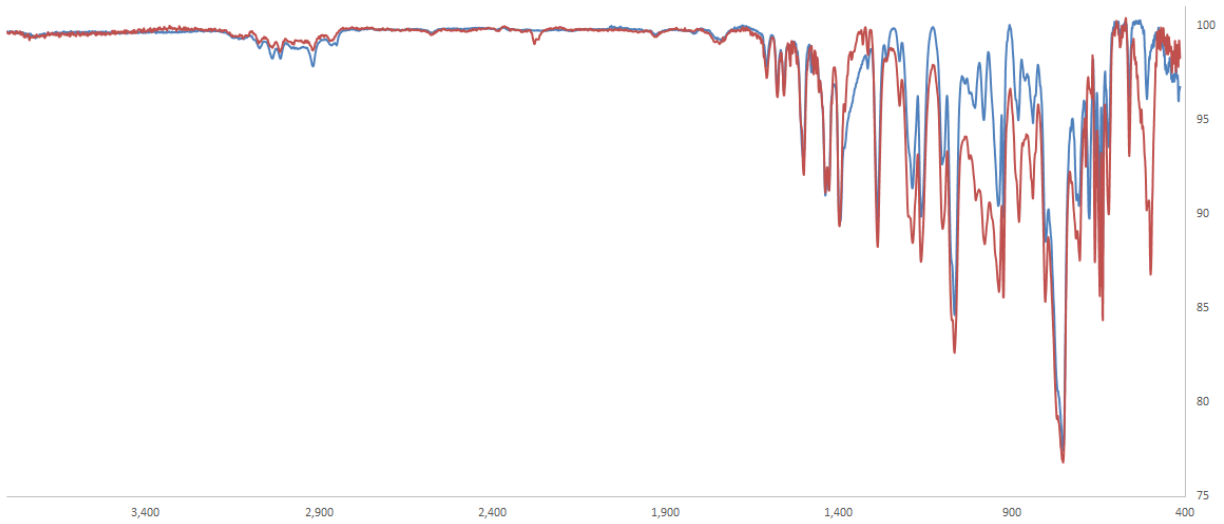

Figure S32. Superimposed FT-IR spectra of **2-H** and **2-D**, thin film on AgCl plates.

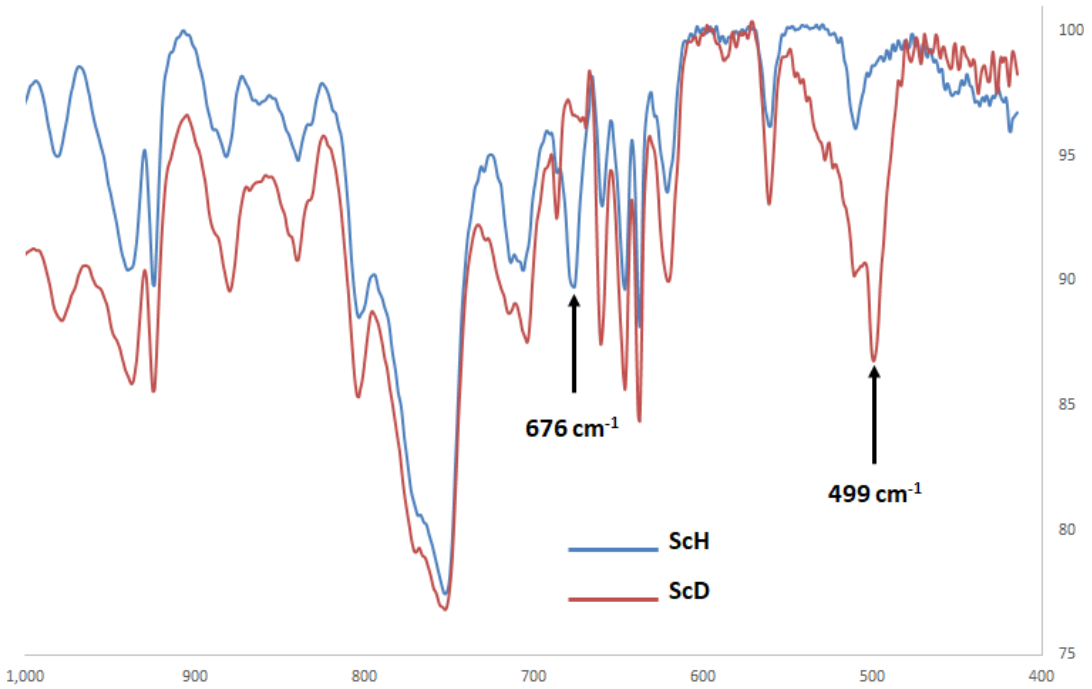

Figure S33. Zoomed in region of the superimposed FT-IR spectra of **2-H** and **2-D**.

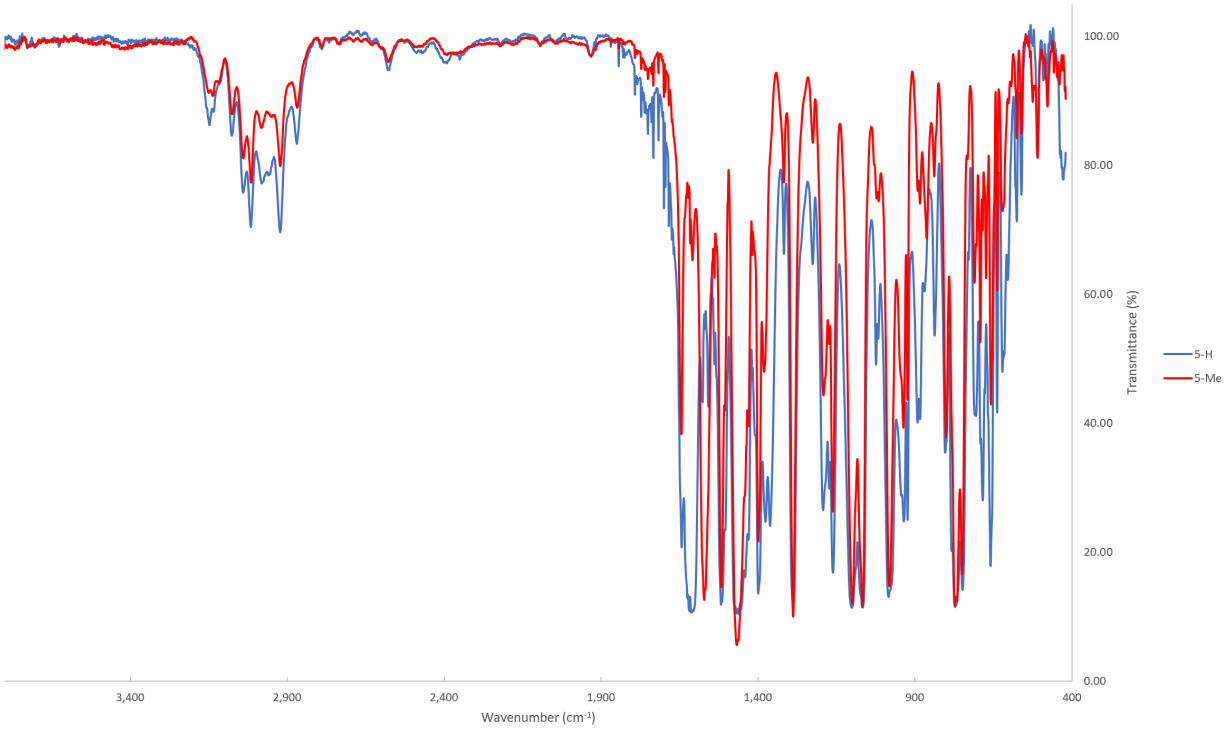

Figure S34. Superimposed FT-IR spectra of **5-H** and **5-Me**, KBr pellet.

$$MW_{ScH} = \frac{(mg_{ScH})(MW_{PhNNPh})(ml_{PhNNPh})}{(mg_{PhNNPh})(ml_{ScH})}$$

Mass of ScH = 10.1 mg
Mass of ScH = 10.2 mg
Molecular weight of azobenzene = 182.23 g/mol
V_i of ScH = 0.83 mL V_f of ScH = 0.24 mL
V_i of Azobenzene = 0.85 mL V_f of Azobenzene = 1.47 mL

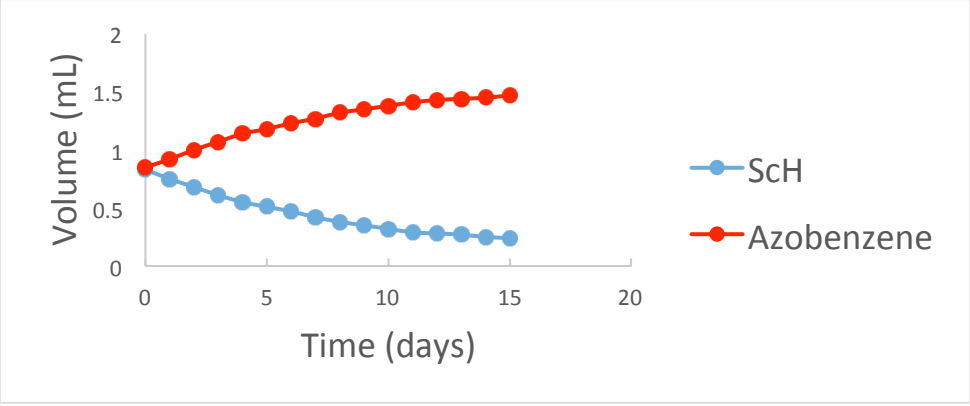

Figure S35. Signer method for the molecular weight determination of **2-H** in C_6H_6.

$$r = \frac{k_b T}{6\pi D\eta}$$

Where r = Hydrodynamic radius

k_b = Boltzmann constant = 1.38×10^{-23} J K^{-1}

T = Temperature = 298 K

D = Diffusion constant obtained from DOSY NMR spectrum

η = Viscosity of C_6D_6 at 298 K = 0.6392 mPa.s [8]

Complex	D (m^2/s)	r (Å)
2-H	4.80×10^{-10}	7.11
2-Me	6.88×10^{-10}	4.96
3	4.83×10^{-10}	7.07

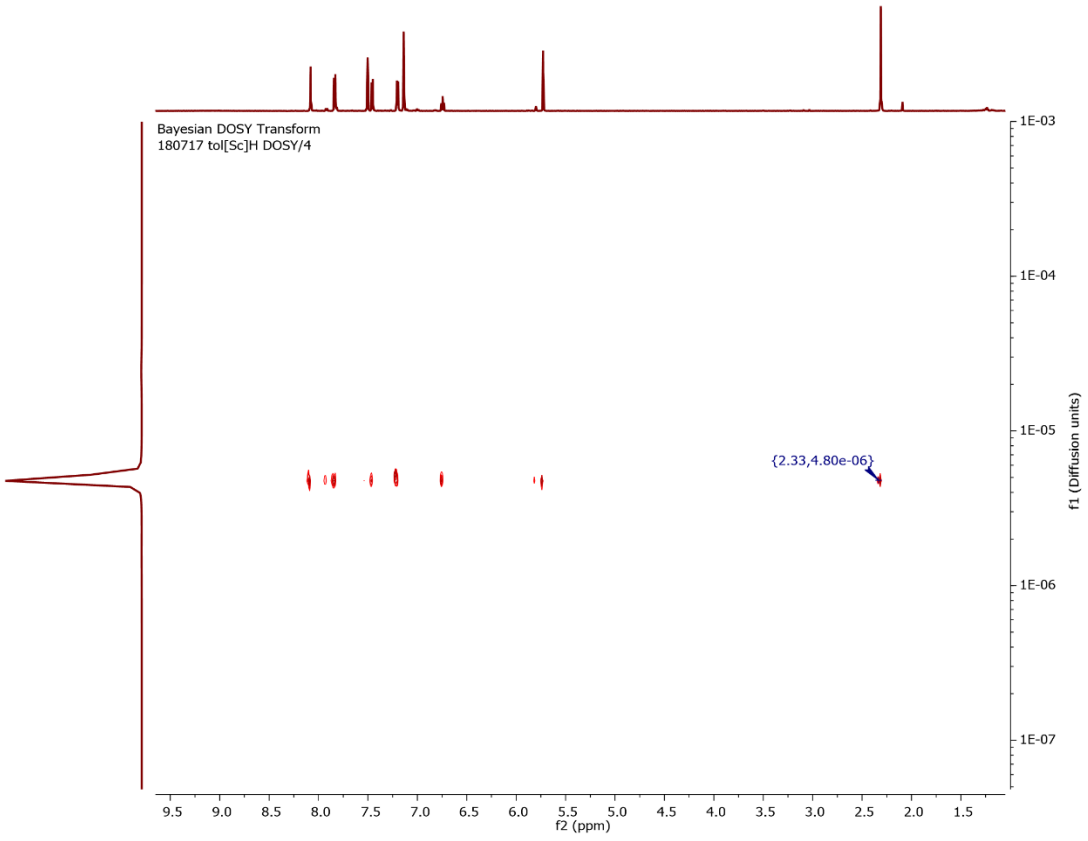

Figure S36. 2D DOSY spectrum of **2-H** in C_6D_6.

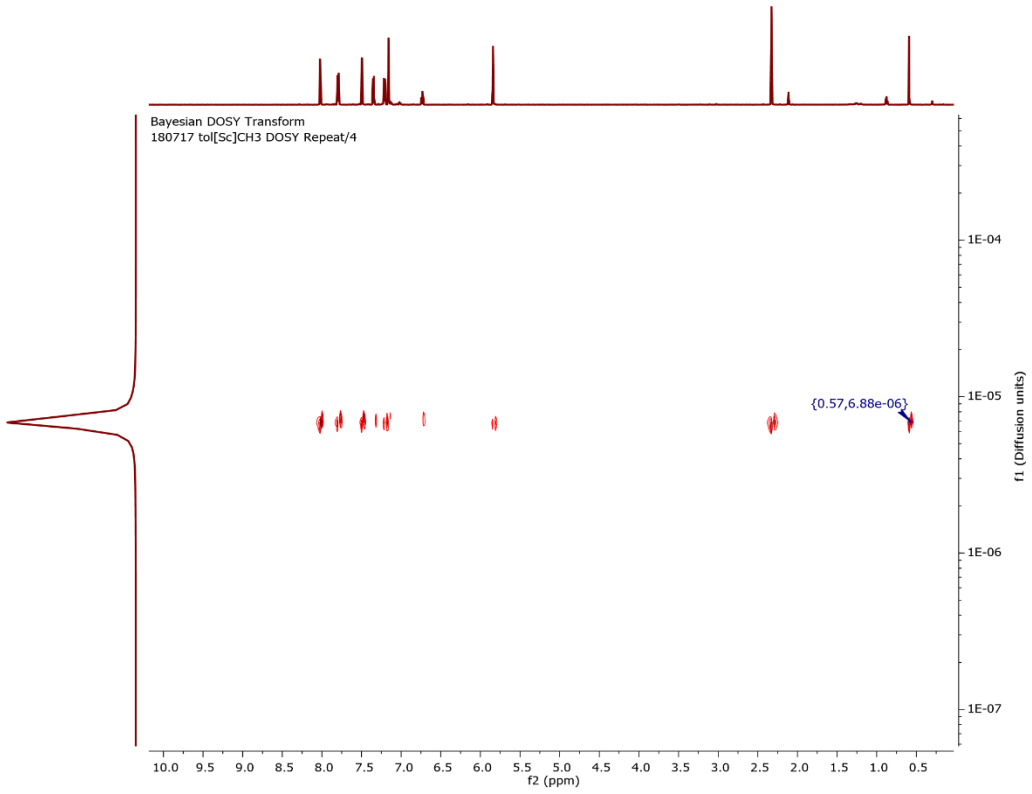

Figure S14. 2D DOSY spectrum of **2-Me** in C_6D_6.

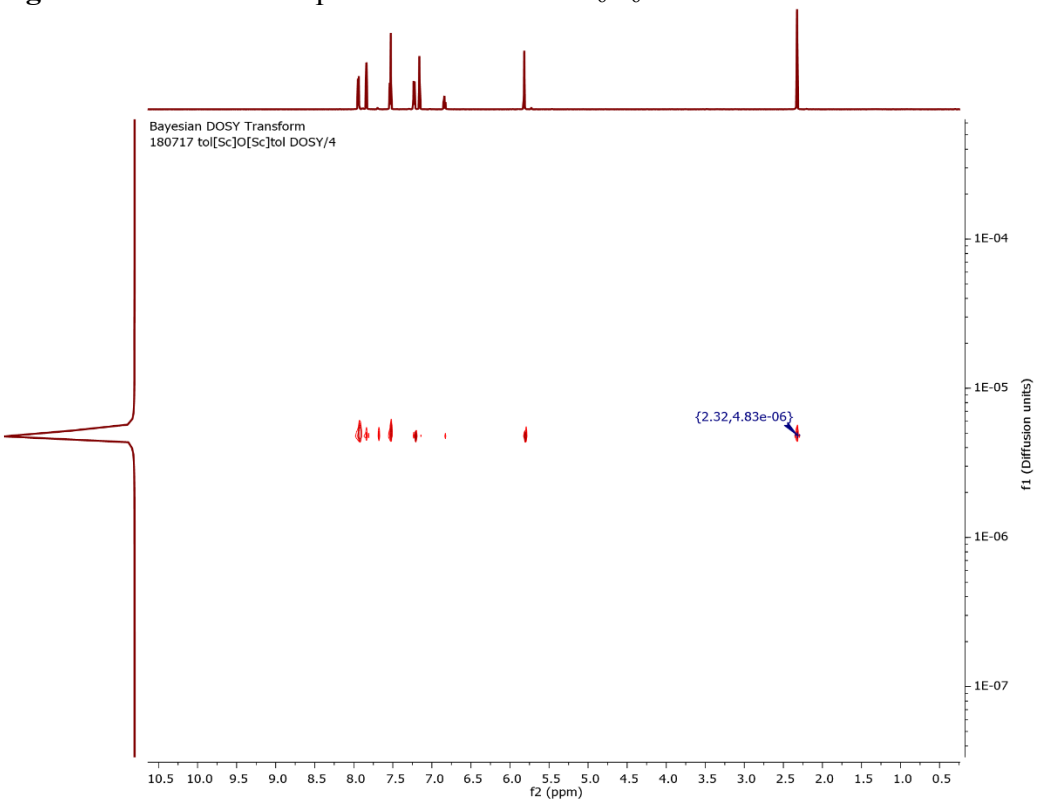

Figure S15. 2D DOSY spectrum of **3** in C_6D_6.

Table S1. Crystal data collection and refinement parameters for complexes.

	1	**2-Me**	**2-CH_2SiMe_3**
formula	$C_{31}H_{29}B_2ClN_9Sc$, $2(C_6H_6)$	$C_{32}H_{32}B_2N_9Sc$, $2(C_6H_6)$	$C_{35}H_{40}B_2N_9ScSi$
fw	785.88	765.46	681.43
crystal system	triclinic	triclinic	monoclinic
space group	P-1	P-1	C2/c
***a* (Å)**	10.2171(2)	10.2075(9)	39.5534(15)
***b* (Å)**	12.1118(4)	11.9288(10)	8.3472(3)
***c* (Å)**	18.2907(4)	18.5503(16)	27.4331(9)
α (deg)	103.202(2)	104.426(4)	90
β (deg)	92.4060(10)	92.714(5)	126.713(2)
γ (deg)	113.9310(10)	112.543(4)	90
***V* (Å^3)**	1990.99(9)	1994.4(3)	7260.7(5)
Z	2	2	8
***T* (K)**	173(2)	173(2)	173(2)
Wavelength (Å)	1.54178	0.71073	0.71073
ρ_{calcd} (g·cm^{-3})	1.311	1.275	1.247
***F*(000)**	820	804	2864
μ (mm^{-1})	2.539	0.229	0.274
crystal size, mm^3	0.198×0.111×0.053	0.2×0.2×0.2	0.27×0.20×0.16
transmission factors	0.646 – 0.754	0.6309 − 0.7461	0.6269 − 0.7456
***θ* range (deg)**	2.510 − 68.228	3.348 − 26.000	3.110 − 25.000
data/restraints/param	7007/0/507	7825/0/506	6319/525/468
GOF	1.024	1.004	1.023
R_1 [I > 2σ(I)]	0.0790	0.0421	0.0403
wR_2 [all data]	0.2498	0.1096	0.1135
residual density, e/Å^3	0.580 and -0.888	0.436 and -0.401	0.376 and -0.365

Table S2. Data collection and structure refinement details for complexes.

	3	**4-H**	**4-Me**
formula	$C_{62}H_{46}B_4N_{18}OSc_2$	$C_{32}H_{30}B_2N_9O_2Sc$, $2(C_6H_6)$	$C_{33}H_{32}B_2N_9O_2Sc$
fw	1204.42	795.45	653.25
crystal system	monoclinic	triclinic	orthorhombic
space group	P2/c	P-1	P212121
***a* (Å)**	17.2544(3)	12.9337(7)	13.860(4)
***b* (Å)**	11.7447(2)	13.0637(5)	14.896(5)
***c* (Å)**	15.3640(2)	13.3321(7)	15.506(5)
α (deg)	90	67.293(2)	90
β (deg)	104.3550(10)	82.797(3)	90
γ (deg)	90	75.727(2)	90
***V* (Å^3)**	3016.27(8)	2012.73(17)	3201.3(18)
Z	2	2	4
***T* (K)**	173(2)	173(2)	173(2)
Wavelength (Å)	1.54178	0.71073	0.71073
ρ_{calcd} (g·cm^{-3})	1.326	1.313	1.355
***F*(000)**	1252	832.0	1360
μ (mm^{-1})	2.400	0.233	0.277
crystal size, mm^3	0.21×0.13×0.12	0.522×0.462×0.38	0.130×0.130×0.100
transmission factors	0.6219 − 0.7533	0.7270 − 0.9984	0.5506 − 0.7455
***θ* range (deg)**	2.643 − 67.485	1.903 − 27.878	2.627 − 24.994
data/restraints/param	5307/0/395	9505/360/617	5646/0/428
GOF	1.058	1.021	1.013
R_1 [I > 2σ(I)]	0.0471	0.0550	0.0646
wR_2 [all data]	0.1355	0.1578	0.1452
residual density, e/Å^3	0.487 and -0.305	0.768 and -0.471	0.263 and -0.350

Table S3. Crystal data collection and refinement parameters for complex.

	5-H
formula	$C_{50}H_{30}B_3F_{15}N_9O_2Sc,2(C_3H_9O_{0.5}Si)$
fw	1313.60
crystal system	monoclinic
space group	C2/c
***a* (Å)**	36.353(4)
***b* (Å)**	12.6079(14)
***c* (Å)**	30.349(3)
α (deg)	90
β (deg)	116.768(3)
γ (deg)	90
***V* (Å^3)**	12419(2)
Z	8
***T* (K)**	173(2)
Wavelength (Å)	0.71073
ρ_{calcd} (g·cm^{-3})	1.405
***F*(000)**	5360
μ (mm^{-1})	0.253
crystal size, mm^3	0.300×0.200×0.100
transmission factors	0.6335 − 0.7455
***θ* range (deg)**	1.503 − 25.000
data/restraints/param	10596/0/820
GOF	1.016
R_1 [I > 2σ(I)]	0.0533
wR_2 [all data]	0.1482
residual density, e/Å^3	0.713 and -0.533

Cartesian coordinates of all optimized structures

ScH monomer **2-H**

73

C	7.99134	6.03529	5.56303
C	6.97736	6.44851	4.70778
N	5.88850	5.68562	4.91772
N	6.17092	4.75713	5.86249
C	7.43040	4.97301	6.26978
B	4.50846	5.60327	4.13501
C	4.62581	4.18139	3.32685
N	4.46018	3.00880	3.99684
C	4.60057	1.80606	3.37662
C	5.02144	1.76585	2.04198
C	5.26684	2.94497	1.35157
C	5.04724	4.15686	1.99214
Sc	4.78724	3.05389	6.33600
N	6.13918	1.30769	5.93074
N	5.83731	0.34583	5.02614
C	6.91131	-0.44545	4.84675
C	7.93473	-0.01592	5.68249
C	7.39529	1.08539	6.34488
B	4.45700	0.42133	4.24292
C	4.16039	-0.92482	3.38883
C	3.38630	-0.89947	2.21568
C	3.02031	-2.06147	1.53819
C	3.40451	-3.32234	2.00416
C	4.13874	-3.37106	3.19348
C	4.49586	-2.20493	3.86781
C	3.04827	-4.57699	1.25236

H	5.01240	3.09034	8.18684
N	3.27785	1.45753	6.28733
N	3.30676	0.50907	5.32351
C	2.26066	-0.32506	5.49769
C	1.53385	0.08695	6.60532
C	2.22008	1.20820	7.06920
N	3.30502	4.67231	6.21558
N	3.35424	5.58056	5.21466
C	2.31984	6.43653	5.34789
C	1.58017	6.08054	6.46642
C	2.24646	4.96879	6.97968
C	4.23837	6.91911	3.22685
C	4.59523	8.21102	3.65617
C	4.26015	9.35572	2.93541
C	3.52773	9.27302	1.74683
C	3.12270	8.00167	1.32956
C	3.46674	6.86106	2.05333
C	3.19470	10.50328	0.94568
H	2.18047	7.24352	4.64621
H	5.22818	5.09176	1.47374
H	2.02149	1.83681	7.92606
H	5.18216	0.80660	1.56299
H	5.12430	8.33821	4.59762
H	5.62443	2.91975	0.32462
H	7.83438	1.71882	7.10345
H	3.03867	0.05330	1.82459
H	2.03270	4.37826	7.85966
H	6.88485	-1.25722	4.13659
H	2.41914	-1.98621	0.63403
H	4.42538	-4.33677	3.60570

H	5.02547	-2.30452	4.81229
H	6.96709	7.23040	3.96444
H	3.10339	5.89975	1.69929
H	8.91877	-0.44574	5.79288
H	7.85621	4.36399	7.05545
H	2.10522	-1.15793	4.83063
H	0.69489	6.56425	6.85044
H	4.56273	10.33178	3.31016
H	0.64399	-0.36733	7.01388
H	2.52243	7.90143	0.42723
H	8.98308	6.45094	5.65755
H	2.11599	-4.45797	0.69202
H	2.93227	-5.43048	1.92729
H	3.83065	-4.83926	0.52913
H	3.08538	11.38300	1.58728
H	2.26511	10.37591	0.38273
H	3.98609	10.72777	0.21956

ScH dimer **[2-H]$_2$**

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C	8.02107	6.96586	11.95474
C	8.39582	5.73352	11.38955
C	9.68702	5.28178	11.71371
C	10.55980	6.02754	12.50436
C	10.18412	7.27147	13.02151
C	8.89019	7.72079	12.74056
B	7.33511	4.79975	10.59503
C	7.95728	3.80588	9.45030
N	7.21233	2.77636	8.96549
C	7.66706	2.00303	7.93960

C	8.84452	2.36002	7.27326
C	9.59203	3.44634	7.70544
C	9.16352	4.14590	8.82374
Sc	4.84563	2.76976	9.38048
H	3.28688	1.88706	10.19903
Sc	1.54920	2.75502	9.84586
H	3.11031	3.65374	9.05299
B	6.78105	0.72056	7.43452
C	7.56086	-0.41812	6.57733
C	6.87287	-1.29435	5.71716
C	7.50370	-2.35505	5.06936
C	8.86441	-2.61291	5.26176
C	9.55459	-1.78352	6.15073
C	8.91701	-0.72222	6.79131
C	9.55971	-3.73377	4.53589
C	11.13965	8.09762	13.84081
N	1.22119	1.00376	8.48292
N	0.11395	0.84100	7.71996
C	0.06096	-0.43015	7.28009
C	1.18280	-1.11216	7.73418
C	1.88173	-0.16542	8.48150
B	-0.96698	1.99187	7.64742
C	-1.57179	2.08940	9.16663
N	-0.83296	2.67391	10.15117
C	-1.33657	2.82922	11.40512
C	-2.59026	2.29022	11.72245
C	-3.31209	1.58912	10.76814
C	-2.80339	1.50376	9.47989
B	-0.38876	3.42329	12.60209
C	-1.15959	3.93680	13.93259

C	-2.40199	4.59073	13.85624
C	-3.02035	5.14827	14.97396
C	-2.42295	5.08599	16.23702
C	-1.17001	4.47185	16.32640
C	-0.55501	3.92286	15.20225
C	-3.10694	5.65009	17.45395
N	0.73233	3.86717	8.06856
N	-0.24164	3.34536	7.29284
C	-0.55127	4.22115	6.31214
C	0.24161	5.34922	6.45462
C	1.03049	5.07433	7.57314
N	1.43175	4.52772	11.14418
N	0.52785	4.62397	12.14693
C	0.60422	5.85688	12.68950
C	1.58464	6.58200	12.02826
C	2.07951	5.69911	11.06940
N	1.33182	1.71876	11.88669
N	0.54235	2.17517	12.88614
C	0.45601	1.24032	13.85378
C	1.23531	0.14990	13.49454
C	1.76239	0.50275	12.25081
C	-2.03430	1.73832	6.44906
C	-1.64598	1.17865	5.21759
C	-2.51822	1.07468	4.13527
C	-3.83204	1.54569	4.21791
C	-4.22286	2.14797	5.41763
C	-3.34576	2.24377	6.49668
C	-4.78929	1.40429	3.06450
N	4.68138	2.14109	7.23576
N	5.58966	1.35440	6.61041

C	5.38755	1.41459	5.28080
C	4.29372	2.23233	5.02678
C	3.88372	2.66024	6.28850
N	5.45559	0.61830	9.62709
N	6.18918	-0.02156	8.69189
C	6.42637	-1.28818	9.09707
C	5.83259	-1.47899	10.33502
C	5.23564	-0.24990	10.62166
N	5.42511	3.28332	11.43945
N	6.50986	4.04606	11.70985
C	6.69899	4.08124	13.04512
C	5.71068	3.32819	13.66220
C	4.93088	2.85275	12.60897
N	5.31525	5.00268	9.09278
N	6.32185	5.64893	9.72501
C	6.46023	6.88487	9.20388
C	5.49865	7.06681	8.22029
C	4.80741	5.85407	8.19102
H	2.82522	-0.24746	9.00356
H	1.45144	-2.13990	7.54192
H	-0.76736	-0.76990	6.67770
H	1.78638	5.67890	8.05208
H	0.24251	6.23577	5.83846
H	-1.31154	3.98611	5.58456
H	-0.62350	0.83459	5.08206
H	-2.16690	0.63050	3.20565
H	-5.22772	2.55650	5.50789
H	-3.69241	2.74961	7.39395
H	-4.26521	1.41663	2.10388
H	-5.53028	2.20947	3.05746

H	-5.33999	0.45694	3.12164
H	-3.34922	0.97246	8.70849
H	-4.26052	1.12135	11.02285
H	-2.96840	2.38694	12.73372
H	2.87289	5.82743	10.34583
H	1.89700	7.59650	12.22445
H	-0.03427	6.13527	13.51273
H	2.41995	-0.05010	11.59591
H	1.39377	-0.76024	14.05331
H	-0.15916	1.40458	14.72482
H	-2.89717	4.68435	12.89268
H	-3.98189	5.64588	14.86159
H	-0.66170	4.43307	17.28810
H	0.43881	3.49704	15.31954
H	-3.71340	6.52609	17.20372
H	-2.38356	5.94554	18.21994
H	-3.77830	4.91076	17.90855
H	3.05596	3.29477	6.57423
H	3.85916	2.47226	4.06816
H	6.03157	0.87820	4.60115
H	4.67064	0.05936	11.48858
H	5.83645	-2.37579	10.93616
H	6.99961	-1.96404	8.48271
H	5.80409	-1.16700	5.56313
H	6.92474	-3.00079	4.41154
H	10.60704	-1.97480	6.35220
H	9.49412	-0.12902	7.49563
H	8.87548	-4.56155	4.32567
H	10.40017	-4.12668	5.11608
H	9.96114	-3.39222	3.57349

H	9.15906	1.78736	6.40812
H	10.49872	3.74019	7.18123
H	9.73255	4.99168	9.19224
H	4.03611	2.24556	12.62133
H	5.57505	3.16171	14.72011
H	7.51530	4.64328	13.46992
H	3.97990	5.54488	7.56929
H	5.32902	7.94689	7.61833
H	7.23507	7.54790	9.55637
H	10.01937	4.31064	11.35476
H	11.54903	5.63256	12.72851
H	8.55288	8.66990	13.15314
H	7.01097	7.33991	11.80410
H	11.80707	7.46685	14.43620
H	10.60780	8.76768	14.52304
H	11.77275	8.72262	13.19854

ScMe Monomer **2-Me**

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C	3.47868	6.81762	2.10711
C	4.23673	6.85356	3.29032
C	4.58715	8.13721	3.74876
C	4.25802	9.29556	3.04740
C	3.53834	9.23541	1.84968
C	3.14044	7.97198	1.40256
B	4.50028	5.52058	4.17619
N	3.33393	5.47606	5.24297
N	3.27511	4.55801	6.23407
C	2.19439	4.83337	6.97448
C	1.52416	5.94077	6.45679

C	2.28474	6.31674	5.35945
Sc	4.77317	2.93812	6.37536
N	3.23536	1.35498	6.24450
N	3.27413	0.42598	5.26254
C	2.20876	-0.39256	5.38939
C	1.45783	0.00941	6.48412
C	2.15075	1.10852	6.98936
B	4.43831	0.34671	4.19544
C	4.14219	-0.98482	3.31754
C	3.38156	-0.93644	2.13634
C	3.01412	-2.08562	1.43812
C	3.38384	-3.35606	1.88978
C	4.10557	-3.42766	3.08553
C	4.46385	-2.27417	3.78076
C	3.02566	-4.59690	1.11619
C	3.21145	10.48090	1.06976
N	5.87384	5.59362	4.96914
C	6.96588	6.35234	4.75887
C	7.98348	5.92379	5.60161
C	7.42053	4.85739	6.30078
N	6.15633	4.65354	5.90187
C	4.62797	4.11499	3.34434
N	4.45629	2.93340	3.99478
C	4.59945	1.74307	3.35375
C	5.03366	1.72317	2.02261
C	5.28784	2.91303	1.35425
C	5.06213	4.11393	2.01320
N	6.11358	1.18537	5.91597
N	5.80994	0.24630	4.98886
C	6.88350	-0.54013	4.78571

C	7.90984	-0.13083	5.62751
C	7.37169	0.95336	6.31875
C	5.10745	2.94183	8.56689
H	2.15054	7.12806	4.66191
H	5.24793	5.05747	1.51226
H	1.93260	1.72463	7.85069
H	5.19685	0.77149	1.52929
H	5.10747	8.24599	4.69747
H	5.65553	2.90467	0.33055
H	7.81576	1.56892	7.08886
H	3.04604	0.02489	1.75582
H	6.85417	-1.33434	4.05607
H	2.42346	-1.99270	0.52865
H	4.38124	-4.40149	3.48603
H	4.98400	-2.39101	4.72858
H	6.95431	7.14232	4.02415
H	3.12144	5.86281	1.72998
H	8.89472	-0.56226	5.72342
H	7.85108	4.23614	7.07398
H	2.05726	-1.20811	4.70044
H	0.62315	6.40817	6.82409
H	4.55518	10.26446	3.44449
H	0.54831	-0.43619	6.85748
H	2.55048	7.88879	0.49170
H	8.97874	6.33174	5.69301
H	2.09482	-4.46579	0.55605
H	2.90571	-5.46122	1.77650
H	3.80862	-4.84932	0.39009
H	3.09977	11.34865	1.72705
H	2.28474	10.36546	0.49947

H	4.00699	10.71774	0.35214
H	1.96285	4.23066	7.84178
H	4.66779	2.06156	9.06049
H	6.17901	2.92992	8.82645
H	4.68897	3.83577	9.05428

CO2

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O	2.95015	0.13859	4.64268
C	2.09914	0.17047	5.43646
O	1.24678	0.20232	6.22920

ScH CO2 insertion adduct

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C	-1.12263	-3.96182	-2.40047
C	-0.34060	-3.96580	-1.23231
C	0.00898	-5.23684	-0.73951
C	-0.34289	-6.41441	-1.39644
C	-1.08562	-6.38700	-2.58117
C	-1.48331	-5.13543	-3.06061
B	-0.05273	-2.60715	-0.39515
N	-1.19713	-2.51754	0.68730
N	-1.22242	-1.55764	1.63895
C	-2.27024	-1.80339	2.43519
C	-2.95416	-2.93440	1.99121
C	-2.23577	-3.35649	0.88176
Sc	0.26784	0.05217	1.65442
N	1.66009	1.74853	1.16591
N	1.36747	2.66469	0.21037
C	2.45738	3.41731	-0.02798

C	3.48214	3.01230	0.81807
C	2.92802	1.96348	1.54955
B	-0.01855	2.57713	-0.56409
N	-1.16619	2.57060	0.51863
N	-1.20536	1.67336	1.52902
C	-2.25540	1.97803	2.30160
C	-2.92688	3.08421	1.78240
C	-2.19855	3.42889	0.65281
C	-1.43692	-7.65414	-3.31410
N	1.63964	-1.68872	1.27580
C	2.90557	-1.89422	1.67106
C	3.44557	-2.99460	1.00790
C	2.41441	-3.44045	0.19067
N	1.33406	-2.66090	0.38147
N	-0.07038	-0.02079	-0.67050
C	0.07440	-1.23059	-1.27705
C	0.48945	-1.28446	-2.61292
C	0.72643	-0.11302	-3.31884
C	0.50710	1.10530	-2.69086
C	0.09161	1.14470	-1.35476
C	-0.28950	3.88249	-1.48687
C	-1.07068	3.81238	-2.65334
C	-1.41911	4.94531	-3.38704
C	-1.00909	6.22064	-2.98728
C	-0.26654	6.31555	-1.80591
C	0.07287	5.17855	-1.07509
C	-1.34770	7.44247	-3.79895
O	2.96331	0.13880	4.65003
C	2.07792	0.16987	5.41697
O	1.25484	0.20272	6.24134

H	0.26536	0.11308	3.51810
H	-2.34392	4.22920	-0.05540
H	0.68405	2.03477	-3.22020
H	-2.45997	-1.16537	3.28684
H	0.65283	-2.24877	-3.08062
H	0.61004	5.31537	-0.13957
H	1.07865	-0.14909	-4.34731
H	3.34962	-1.25277	2.41981
H	-1.48128	-3.01721	-2.80135
H	2.38626	-4.25642	-0.51464
H	-2.09119	-5.07675	-3.96151
H	-0.04529	-7.37232	-0.97390
H	0.54621	-5.31995	0.20229
H	2.44005	4.18683	-0.78403
H	-1.43851	2.84775	-2.99355
H	4.43600	-3.41269	1.10556
H	3.36302	1.36625	2.33908
H	-2.39135	-4.19935	0.22734
H	-3.80795	3.57243	2.17045
H	0.04051	7.29533	-1.44474
H	-3.83694	-3.38912	2.41445
H	-2.02695	4.83583	-4.28320
H	4.47749	3.42379	0.89055
H	-0.65652	-7.92086	-4.03780
H	-2.37293	-7.54911	-3.87102
H	-1.54356	-8.49917	-2.62709
H	-0.56160	7.65920	-4.53311
H	-1.45227	8.32889	-3.16582
H	-2.28140	7.30938	-4.35370
H	-2.45573	1.39725	3.19094

ScH CO2 insertion TS

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C	7.40690	1.18582	6.27681
N	6.12328	1.37502	5.93110
N	5.80536	0.40414	5.03692
C	6.89140	-0.35475	4.80174
C	7.94232	0.10063	5.58677
Sc	4.72309	3.11950	6.32329
O	6.66060	3.17845	8.69067
C	5.82392	3.21012	9.52461
O	5.18290	3.24402	10.49879
B	4.41636	0.45411	4.26370
C	4.54108	1.83682	3.39345
N	4.39703	3.04593	4.00443
C	4.55912	4.21017	3.31550
C	4.97561	4.16969	1.97992
C	5.19609	2.95292	1.35088
C	4.95689	1.78344	2.05795
B	4.45117	5.64831	4.09334
C	4.18968	6.95033	3.16224
C	3.40919	6.88103	1.99530
C	3.06654	8.01389	1.25866
C	3.48173	9.28830	1.65594
C	4.22346	9.38261	2.83789
C	4.55708	8.24575	3.57155
C	3.14942	10.50982	0.84119
N	3.27096	4.75913	6.17908
C	2.21340	5.05708	6.94536
C	1.53178	6.15204	6.41526

C	2.26179	6.49961	5.28772
N	3.30322	5.65093	5.16492
N	3.25302	1.49022	6.29052
N	3.27208	0.53429	5.33612
C	2.22446	-0.29565	5.51926
C	1.50361	0.13069	6.62540
C	2.19713	1.25192	7.07967
N	6.14347	4.81848	5.82177
N	5.83891	5.73265	4.86556
C	6.93377	6.46326	4.58601
C	7.97731	6.04828	5.40267
C	7.42805	5.01577	6.15941
C	4.13773	-0.90225	3.41871
C	4.49363	-2.17259	3.90875
C	4.14790	-3.35049	3.24919
C	3.40501	-3.32422	2.06453
C	3.00074	-2.07365	1.58802
C	3.35538	-0.89964	2.25082
C	3.06051	-4.59150	1.32859
H	4.19907	3.18313	8.11327
H	2.11336	7.29563	4.57516
H	5.15279	5.09996	1.45232
H	2.01482	1.89034	7.93182
H	5.11972	0.81827	1.59210
H	5.09487	8.38189	4.50689
H	5.54980	2.91660	0.32296
H	7.86923	1.82932	7.01080
H	2.99142	0.04396	1.85226
H	6.85206	-1.16406	4.08935
H	2.39246	-2.01607	0.68732

H	4.45052	-4.30781	3.66952
H	5.03233	-2.25463	4.84989
H	6.90558	7.22540	3.82287
H	3.03702	5.91738	1.65697
H	8.94245	-0.30109	5.64713
H	7.88095	4.41622	6.93536
H	2.06639	-1.13537	4.86122
H	0.64366	6.63276	6.79671
H	4.53445	10.36184	3.19720
H	0.61356	-0.31639	7.04162
H	2.45909	7.90505	0.36215
H	8.98157	6.44235	5.44062
H	3.84368	-4.85400	0.60631
H	2.12542	-4.48923	0.76963
H	2.95555	-5.43811	2.01393
H	3.93933	10.72411	0.11038
H	3.04378	11.39724	1.47276
H	2.21799	10.37801	0.28236
H	2.02135	4.47755	7.83654

ScH CO_2 k^1 kinetic insertion product

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C	2.81944	-1.88742	1.75376
N	1.56640	-1.69694	1.31012
N	1.30335	-2.66613	0.40057
C	2.39924	-3.43237	0.24446
C	3.39366	-2.97784	1.10129
Sc	0.21944	0.05270	1.64423
O	0.47260	0.11509	3.61705
C	1.40446	0.13841	4.52870

O	2.60950	0.12592	4.32407
B	-0.05459	-2.60816	-0.40902
C	0.09508	-1.23050	-1.28441
N	-0.03171	-0.02084	-0.67163
C	0.11048	1.14482	-1.36172
C	0.51560	1.10554	-2.70056
C	0.73775	-0.11209	-3.32847
C	0.49954	-1.28340	-2.62311
B	-0.02541	2.57771	-0.57733
C	-0.28946	3.87921	-1.50714
C	-1.06813	3.80498	-2.67543
C	-1.40908	4.93432	-3.41782
C	-0.99437	6.21055	-3.02522
C	-0.25507	6.30981	-1.84235
C	0.07756	5.17611	-1.10301
C	-1.32463	7.42834	-3.84629
N	-1.29481	1.64333	1.46935
C	-2.37614	1.94257	2.20055
C	-3.01769	3.06243	1.67481
C	-2.24016	3.41970	0.58260
N	-1.20819	2.55773	0.47646
N	-1.30814	-1.53221	1.57644
N	-1.23349	-2.50957	0.64446
C	-2.26892	-3.35718	0.81395
C	-3.03653	-2.92538	1.88603
C	-2.38545	-1.77734	2.33328
N	1.58318	1.76417	1.20066
N	1.33115	2.67506	0.23005
C	2.43444	3.41936	0.02747
C	3.42299	3.01151	0.91407

C	2.83728	1.97084	1.63406
C	-0.33312	-3.96355	-1.25401
C	0.02552	-5.23551	-0.77083
C	-0.31621	-6.41052	-1.43797
C	-1.05672	-6.37956	-2.62382
C	-1.46388	-5.12726	-3.09379
C	-1.11387	-3.95646	-2.42337
C	-1.39574	-7.64331	-3.36825
H	1.00611	0.17223	5.56059
H	-2.35266	4.23069	-0.11919
H	0.68211	2.03542	-3.23219
H	-2.62848	-1.12526	3.16067
H	0.65361	-2.24770	-3.09354
H	0.61306	5.31694	-0.16733
H	1.08726	-0.14775	-4.35783
H	3.21201	-1.24186	2.52947
H	-1.47963	-3.01149	-2.81711
H	2.40666	-4.24515	-0.46515
H	-2.07039	-5.06613	-3.99545
H	-0.01138	-7.36937	-1.02280
H	0.56208	-5.32216	0.17082
H	2.45046	4.18491	-0.73273
H	-1.43978	2.83984	-3.01018
H	4.38452	-3.38546	1.23328
H	3.22238	1.37283	2.45061
H	-2.38997	-4.21201	0.16795
H	-3.91233	3.54883	2.03282
H	0.05563	7.29050	-1.48686
H	-3.93099	-3.38254	2.28108
H	-2.01457	4.82162	-4.31518

H	4.41746	3.41744	1.02191
H	-0.61279	-7.89556	-4.09435
H	-2.33277	-7.54242	-3.92425
H	-1.49387	-8.49562	-2.68902
H	-0.53733	7.63340	-4.58251
H	-1.42230	8.32047	-3.22015
H	-2.25953	7.29770	-4.39962
H	-2.62916	1.34694	3.06661

ScH eta2 coordination **$TS_{2\text{-}H}$**

76

C	-1.13747	-3.95450	-2.41891
C	-0.33409	-3.96367	-1.26511
C	0.02426	-5.23674	-0.78451
C	-0.33990	-6.41134	-1.44035
C	-1.10393	-6.37872	-2.61119
C	-1.51014	-5.12492	-3.07781
B	-0.03396	-2.60777	-0.42798
N	-1.18642	-2.50428	0.64762
N	-1.22273	-1.52972	1.58326
C	-2.27708	-1.76685	2.37413
C	-2.95287	-2.90709	1.94306
C	-2.22345	-3.34354	0.84637
Sc	0.30038	0.05486	1.62222
N	1.66478	1.76213	1.13565
N	1.38018	2.67254	0.17164
C	2.47738	3.41257	-0.07274
C	3.49685	3.00512	0.77821
C	2.93523	1.96773	1.52044
B	0.00347	2.57699	-0.60550

N	-1.15238	2.56085	0.47123
N	-1.20375	1.65091	1.46904
C	-2.26050	1.94955	2.23542
C	-2.92270	3.06485	1.72526
C	-2.18253	3.42090	0.60685
C	-1.46852	-7.64252	-3.34339
N	1.64076	-1.70106	1.25449
C	2.90782	-1.89964	1.65390
C	3.45438	-2.99202	0.98268
C	2.42935	-3.43978	0.15909
N	1.34302	-2.66924	0.35255
O	0.26223	0.12752	3.64205
C	1.29213	0.14885	4.43582
O	2.46677	0.12770	4.08381
N	-0.01435	-0.02120	-0.69358
C	0.10164	-1.23167	-1.30681
C	0.48379	-1.28789	-2.65196
C	0.71151	-0.11868	-3.36401
C	0.50282	1.10015	-2.73403
C	0.12019	1.14247	-1.38863
C	-0.27705	3.87826	-1.53104
C	-1.07711	3.80381	-2.68460
C	-1.43445	4.93350	-3.41885
C	-1.01540	6.21006	-3.03230
C	-0.25399	6.30941	-1.86348
C	0.09481	5.17546	-1.13210
C	-1.36414	7.42835	-3.84498
H	1.02647	0.18961	5.50892
H	-2.31893	4.22971	-0.09333
H	0.66256	2.02905	-3.26947

H	-2.48179	-1.11647	3.21269
H	0.62849	-2.25365	-3.12247
H	0.64756	5.31602	-0.20638
H	1.04283	-0.15684	-4.39928
H	3.32907	-1.25735	2.41534
H	-1.50360	-3.00809	-2.80881
H	2.40868	-4.25082	-0.55224
H	-2.13409	-5.06219	-3.96738
H	-0.03458	-7.37112	-1.02769
H	0.57855	-5.32430	0.14681
H	2.46755	4.17530	-0.83589
H	-1.45310	2.83840	-3.01365
H	4.44700	-3.40481	1.08103
H	3.34751	1.37098	2.32273
H	-2.37100	-4.19614	0.20291
H	-3.80643	3.55033	2.11068
H	0.06116	7.29031	-1.51250
H	-3.83844	-3.35738	2.36517
H	-2.05650	4.82071	-4.30480
H	4.49555	3.40884	0.84868
H	-0.70013	-7.90718	-4.08056
H	-2.41324	-7.53421	-3.88476
H	-1.56503	-8.49019	-2.65813
H	-1.45978	8.31773	-3.21458
H	-2.30519	7.29330	-4.38669
H	-0.58769	7.64124	-4.59043
H	-2.47690	1.35796	3.11362

ScH final product **4-H**

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Sc	11.67243	5.23640	6.69306
O	13.00013	3.56231	7.30802
O	12.04764	4.79940	8.85614
N	13.40399	5.62569	5.37019
N	13.61885	6.82761	4.79123
N	12.29795	7.27874	7.44959
N	12.68507	8.30116	6.65079
N	10.59477	6.57456	5.04847
N	9.55285	5.09128	7.48571
N	8.45703	4.94623	6.70352
N	10.88121	3.63027	5.39305
N	9.65127	3.68786	4.83622
C	14.36112	4.79387	4.93551
H	14.39430	3.77767	5.29857
C	15.20757	5.45736	4.04899
H	16.06859	5.06471	3.52952
C	14.69992	6.74680	3.98920
H	15.04049	7.60841	3.43731
C	12.17308	7.77263	8.69183
H	11.90448	7.11363	9.50389
C	12.45344	9.13799	8.69932
H	12.44039	9.81681	9.53868
C	12.76250	9.43132	7.37762
H	13.02523	10.36863	6.91214
C	13.40847	9.32085	4.30328
C	14.52165	10.00113	4.83065
H	14.89177	9.74160	5.81968
C	15.20529	10.98191	4.11430
H	16.05917	11.48011	4.56975
C	14.82310	11.32529	2.81383

C	13.74777	10.62775	2.25531
H	13.44273	10.84524	1.23338
C	13.06562	9.65207	2.98063
H	12.25439	9.12099	2.48905
C	15.53610	12.40767	2.04788
H	15.06470	13.38472	2.21276
H	15.51599	12.21651	0.97058
H	16.58191	12.49638	2.35736
C	11.14543	7.78208	4.73917
C	10.33219	8.81394	4.25675
H	10.77055	9.78720	4.06807
C	8.97541	8.60464	4.05999
H	8.33094	9.41385	3.72399
C	8.46104	7.33745	4.28994
H	7.40860	7.13437	4.12855
C	9.28720	6.31353	4.76733
C	3.73530	3.11254	2.17035
H	3.44030	2.09545	2.44661
H	3.89187	3.13828	1.08775
H	2.88357	3.76802	2.39140
C	4.96627	3.55287	2.91679
C	5.22508	3.10817	4.21728
H	4.54432	2.39946	4.68544
C	6.34799	3.54490	4.91764
H	6.52456	3.13113	5.90762
C	7.26593	4.46238	4.37351
C	7.01034	4.86397	3.05070
H	7.71212	5.52327	2.54607
C	5.89243	4.42765	2.34128
H	5.74135	4.76883	1.31882

C	9.11892	5.32647	8.73454
H	9.83330	5.43792	9.53656
C	7.72600	5.36405	8.76296
H	7.08067	5.53205	9.61198
C	7.35008	5.12872	7.44692
H	6.37063	5.08638	6.99628
C	11.46350	2.50149	4.96446
H	12.45154	2.24160	5.31351
C	10.60733	1.81630	4.10413
H	10.78275	0.88066	3.59506
C	9.46735	2.60477	4.05399
H	8.54042	2.46248	3.52154
C	12.79793	3.83897	8.52452
H	13.28346	3.23311	9.30623
B	12.71506	8.08114	5.08665
B	8.64209	4.85688	5.13679

ScMe CO2 insertion adduct

79

C	3.79911	2.85121	0.46051
C	2.74039	3.28694	-0.32609
N	1.64749	2.55761	-0.03285
N	1.96712	1.62936	0.89958
C	3.25789	1.81162	1.21501
B	0.22632	2.49896	-0.73757
C	0.27142	1.07239	-1.54226
N	0.11756	-0.08967	-0.85311
C	0.19295	-1.29786	-1.47208
C	0.53849	-1.35852	-2.82771
C	0.77468	-0.19082	-3.54017

C	0.61827	1.03002	-2.89817
Sc	0.57586	-0.03888	1.49999
N	1.85245	-1.82839	1.00337
N	1.47382	-2.78205	0.12009
C	2.51749	-3.59449	-0.13065
C	3.60201	-3.18695	0.63577
C	3.12879	-2.07642	1.33266
B	0.05754	-2.67073	-0.58787
C	-0.31879	-4.01531	-1.41377
C	-1.15390	-3.97751	-2.54396
C	-1.58868	-5.13413	-3.18933
C	-1.21565	-6.40160	-2.73234
C	-0.41887	-6.46157	-1.58456
C	0.00684	-5.30054	-0.94187
C	-1.64812	-7.65182	-3.45095
C	1.08209	0.01223	3.66172
N	-0.99695	-1.59119	1.50873
N	-1.03567	-2.54279	0.54755
C	-2.10771	-3.33508	0.75702
C	-2.78302	-2.89284	1.88471
C	-2.04027	-1.79719	2.32269
N	-0.89045	1.61098	1.41475
N	-0.87280	2.50441	0.39920
C	-1.89951	3.36618	0.55476
C	-2.60171	3.02985	1.70263
C	-1.92261	1.92249	2.20903
C	-0.06152	3.81895	-1.63550
C	0.34053	5.10350	-1.22403
C	-0.00500	6.25486	-1.92881
C	-0.79351	6.18706	-3.08208

C	-1.24195	4.92420	-3.47970
C	-0.88727	3.77651	-2.77203
C	-1.13919	7.42430	-3.86705
H	-2.06067	4.16277	-0.15398
H	0.79208	1.95688	-3.43322
H	-2.19570	-1.15899	3.18155
H	0.64847	-2.32483	-3.30704
H	0.91650	5.21911	-0.30886
H	1.07534	-0.23161	-4.58477
H	3.63174	-1.45237	2.05845
H	-1.49519	-3.01844	-2.92508
H	2.42716	-4.40484	-0.83719
H	-2.23539	-5.04925	-4.06065
H	-0.13708	-7.43172	-1.17941
H	0.58474	-5.40719	-0.02686
H	2.69992	4.06319	-1.07432
H	-1.28562	2.82279	-3.10840
H	4.58270	-3.63591	0.68050
H	3.72241	1.19545	1.97246
H	-2.31690	-4.16198	0.09752
H	-3.47254	3.52172	2.10877
H	0.33408	7.22466	-1.56921
H	-3.67767	-3.30982	2.32168
H	-1.88480	4.83622	-4.35355
H	4.80689	3.23756	0.48125
H	-1.75700	-8.49436	-2.76117
H	-0.91161	-7.94639	-4.20906
H	-2.60315	-7.50883	-3.96555
H	-1.22387	8.30131	-3.21791
H	-2.08510	7.30712	-4.40437

H	-0.36657	7.64719	-4.61360
O	-2.17353	0.18676	5.58435
C	-1.41579	0.22376	6.47463
O	-0.67736	0.26182	7.37589
H	-2.11501	1.34574	3.10309
H	0.63710	-0.83608	4.20422
H	2.16561	-0.04112	3.85446
H	0.73482	0.94059	4.14060

ScMe CO2 insertion **$TS_{2\text{-}Me}$**

79

C	7.84234	6.08898	5.92649
C	6.92036	6.42542	4.94255
N	5.81403	5.67896	5.10438
N	5.99455	4.82982	6.14527
C	7.21161	5.08732	6.65828
B	4.53402	5.56474	4.18212
C	4.68906	4.14363	3.38611
N	4.46357	2.98056	4.05872
C	4.45784	1.78700	3.40893
C	4.78497	1.73518	2.04748
C	5.14664	2.89075	1.37131
C	5.08685	4.10212	2.04578
Sc	4.73496	3.00936	6.46959
N	6.19128	1.42385	5.66258
N	5.80052	0.37097	4.90423
C	6.88836	-0.31922	4.50337
C	8.02020	0.27688	5.03646
C	7.52600	1.36651	5.75489
B	4.35430	0.39711	4.26708

C	4.01984	-0.94763	3.42762
C	3.13684	-0.93419	2.33419
C	2.74404	-2.10102	1.67988
C	3.21147	-3.35295	2.09079
C	4.06055	-3.38981	3.20176
C	4.44338	-2.21963	3.85449
C	2.82411	-4.61163	1.36119
C	5.95441	2.40094	8.38994
N	3.31854	1.33864	6.44734
N	3.28717	0.43961	5.43682
C	2.25881	-0.40840	5.63982
C	1.60484	-0.05852	6.81300
C	2.31334	1.04267	7.28562
N	3.08572	4.48928	6.00686
N	3.25769	5.47204	5.09446
C	2.11839	6.18808	4.98644
C	1.17421	5.65830	5.85074
C	1.83236	4.59544	6.46798
C	4.34314	6.90711	3.28548
C	4.63339	8.18068	3.81027
C	4.36015	9.35699	3.11494
C	3.75879	9.32731	1.85305
C	3.41771	8.07428	1.33531
C	3.69773	6.90209	2.03599
C	3.49414	10.59256	1.08154
H	2.05524	7.02103	4.30468
H	5.35257	5.02523	1.54336
H	2.16499	1.63250	8.17937
H	4.80907	0.77637	1.54286
H	5.06298	8.26637	4.80543

H	5.46469	2.84866	0.33201
H	8.06559	2.10507	6.32911
H	2.72577	0.01201	1.99037
H	6.78881	-1.17597	3.85551
H	2.05747	-2.03722	0.83778
H	4.41838	-4.34978	3.56939
H	5.06824	-2.30879	4.74034
H	6.98235	7.14890	4.14428
H	3.37624	5.95948	1.60170
H	9.04735	-0.03468	4.92158
H	7.55049	4.54801	7.53064
H	2.06167	-1.20875	4.94489
H	0.16201	5.99780	6.01035
H	4.60722	10.31558	3.56747
H	0.74640	-0.54027	7.25591
H	2.91624	8.01294	0.37120
H	8.81946	6.51845	6.08799
H	2.76478	-5.46763	2.04050
H	3.56104	-4.86233	0.58791
H	1.85539	-4.50510	0.86384
H	3.33597	11.44435	1.74998
H	2.61217	10.49526	0.44107
H	4.34135	10.84319	0.43087
O	3.54951	3.74648	8.56776
C	4.52235	4.16979	9.11614
O	5.20748	4.82979	9.79783
H	1.46880	3.91362	7.22134
H	5.69231	1.35607	8.15580
H	7.02928	2.50941	8.20683
H	5.84351	2.46216	9.47921

ScMe CO2 insertion product **4-Me**

79

C	-0.99684	3.86270	-2.85454
C	-0.19517	3.92715	-1.70169
C	0.19194	5.22012	-1.30294
C	-0.14211	6.35810	-2.03473
C	-0.90424	6.26783	-3.20389
C	-1.33987	4.99663	-3.58927
B	0.07204	2.62392	-0.77448
N	-1.05919	2.63716	0.32168
N	-1.09699	1.74643	1.33924
C	-2.13616	2.06263	2.12452
C	-2.80036	3.17283	1.60334
C	-2.08283	3.50480	0.46338
Sc	0.34467	0.10699	1.46165
O	0.65079	0.17777	3.41143
C	0.01990	0.23280	4.56381
O	-1.20098	0.25686	4.66913
C	-1.23720	7.49004	-4.01730
N	1.47294	2.69620	-0.02458
C	2.56874	3.43517	-0.27865
C	3.60176	3.01228	0.54843
C	3.04303	1.96911	1.28465
N	1.76699	1.77323	0.92155
C	0.15570	1.18411	-1.55322
N	0.00672	0.02493	-0.85368
C	0.11311	-1.18910	-1.46160
C	0.48830	-1.25464	-2.80848
C	0.72211	-0.09094	-3.52729

C	0.53204	1.13231	-2.90025
B	-0.01631	-2.56195	-0.57581
N	-1.14270	-2.45622	0.52006
N	-1.14898	-1.48981	1.46694
C	-2.19044	-1.71715	2.27957
C	-2.88764	-2.84558	1.84843
C	-2.18773	-3.28270	0.73341
N	1.71043	-1.64209	1.05068
N	1.38418	-2.62299	0.17597
C	2.45493	-3.41383	-0.02286
C	3.50321	-2.96452	0.77040
C	2.98044	-1.85190	1.42707
C	-0.32937	-3.92106	-1.40355
C	-1.13693	-3.91545	-2.55428
C	-1.52018	-5.08846	-3.20261
C	-1.12111	-6.34139	-2.72784
C	-0.35363	-6.37027	-1.55914
C	0.02072	-5.19311	-0.91390
C	-1.49740	-7.60831	-3.44866
C	0.93210	0.26471	5.77036
H	-2.23009	4.30160	-0.24845
H	0.70282	2.05713	-3.43931
H	-2.34799	-1.07125	3.13397
H	0.62435	-2.22362	-3.27493
H	0.74439	5.35461	-0.37603
H	1.04681	-0.13669	-4.56439
H	3.44600	-1.19974	2.15314
H	-1.49882	-2.96983	-2.94981
H	2.40841	-4.23930	-0.71589
H	-2.14746	-5.02821	-4.09000

H	-0.05469	-7.32896	-1.13930
H	0.57529	-5.27768	0.01764
H	2.54931	4.20823	-1.03091
H	-1.38636	2.90240	-3.18250
H	4.49262	-3.38760	0.85618
H	3.48658	1.35804	2.05867
H	-2.36033	-4.12750	0.08582
H	-3.67277	3.67122	1.99811
H	0.18455	7.33518	-1.68355
H	-3.77013	-3.28837	2.28484
H	-1.96413	4.89129	-4.47457
H	4.60437	3.40832	0.60506
H	-1.59780	-8.44971	-2.75624
H	-0.73363	-7.88460	-4.18640
H	-2.44324	-7.49741	-3.98752
H	-1.32736	8.37987	-3.38670
H	-2.17693	7.36444	-4.56351
H	-0.45520	7.69607	-4.75892
H	-2.31523	1.48857	3.02468
H	1.56645	-0.62714	5.77726
H	1.59505	1.13339	5.70904
H	0.34701	0.30988	6.68901

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C	0.00668	-5.27661	-1.07004
C	-0.34880	-3.98999	-1.51583
C	-1.18438	-3.94905	-2.64559
C	-1.58955	-5.10203	-3.31621
C	-1.18524	-6.36927	-2.88613

C	-0.38936	-6.43383	-1.73801
B	-0.00546	-2.65576	-0.65996
N	1.40823	-2.74539	0.05466
N	1.75071	-1.78907	0.94837
C	3.02473	-2.01223	1.30249
C	3.53347	-3.10914	0.60896
C	2.47237	-3.53527	-0.18030
Sc	0.41992	-0.04488	1.45281
N	-1.08857	-1.63469	1.44532
N	-1.10552	-2.57197	0.46801
C	-2.15932	-3.39020	0.66689
C	-2.84220	-2.97992	1.80251
C	-2.12626	-1.87479	2.25989
C	-1.58503	-7.61430	-3.63207
N	-1.02504	1.60172	1.40565
N	-1.00794	2.51457	0.40574
C	-2.03527	3.37119	0.57995
C	-2.73497	3.01144	1.72258
C	-2.05691	1.89531	2.20993
B	0.09607	2.53141	-0.72124
C	0.15727	1.11337	-1.53949
N	0.02748	-0.06339	-0.86621
C	0.10959	-1.26026	-1.51065
C	0.44635	-1.29068	-2.86889
C	0.66534	-0.10885	-3.56224
C	0.49505	1.09732	-2.89767
C	-0.19377	3.85974	-1.60551
C	-1.02222	3.82906	-2.74065
C	-1.37833	4.98376	-3.43593
C	-0.92937	6.24263	-3.02630

C	-0.14011	6.29873	-1.87306
C	0.20692	5.14026	-1.18069
C	-1.27605	7.48767	-3.79832
N	1.51153	2.58277	-0.00615
C	2.60496	3.32619	-0.25781
C	3.64924	2.87747	0.54122
C	3.09925	1.81630	1.25851
N	1.81758	1.63406	0.90870
O	1.10771	-0.03696	3.33735
C	0.40548	-0.00737	4.44461
C	1.22805	-0.00784	5.71351
O	-0.82393	0.01852	4.46577
H	-2.19808	4.18106	-0.11333
H	0.65256	2.03593	-3.41646
H	-2.26751	-1.25390	3.13372
H	0.56483	-2.24718	-3.36490
H	0.78153	5.24766	-0.26379
H	0.96216	-0.12749	-4.60850
H	3.49798	-1.38125	2.04167
H	-1.55069	-2.99122	-3.00609
H	2.41218	-4.34345	-0.89243
H	-2.23776	-5.01461	-4.18612
H	-0.08490	-7.40508	-1.35239
H	0.58347	-5.38894	-0.15512
H	2.57533	4.12029	-0.98753
H	-1.42226	2.87918	-3.08590
H	4.52232	-3.53792	0.66971
H	3.54818	1.18427	2.01183
H	-2.35093	-4.21118	-0.00547
H	-3.60461	3.49605	2.13993

H	0.19819	7.26489	-1.50313
H	-3.72558	-3.42519	2.23451
H	-2.02301	4.90450	-4.30924
H	4.65376	3.26943	0.59305
H	-2.53633	-7.48010	-4.15575
H	-1.68608	-8.47100	-2.95869
H	-0.83379	-7.88129	-4.38592
H	-1.35935	8.35817	-3.14033
H	-2.22289	7.37611	-4.33516
H	-0.50457	7.71766	-4.54389
H	-2.22024	1.30084	3.09809
H	1.89842	0.85713	5.71836
H	0.58003	0.02065	6.58962
H	1.85598	-0.90363	5.74467

ScMe final product **4-Me**

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Sc	3.74187	10.40085	5.38870
O	4.52826	11.40401	3.59620
O	2.38159	10.99927	3.74740
N	5.53254	7.79818	5.41372
N	2.34808	12.03946	7.80241
N	3.04424	7.24165	5.44378
N	5.03545	11.92105	6.35335
N	4.02395	9.38202	7.53547
N	2.63327	8.45549	5.00821
N	4.87802	12.30372	7.63938
N	5.44654	9.05734	4.93136
N	2.18421	11.58303	6.53851
C	4.67241	4.60829	5.53490

H	4.15448	4.84957	4.60971
C	2.05912	6.34297	5.26011
H	2.18247	5.31892	5.57680
C	1.16793	12.48218	8.27451
H	1.08400	12.85716	9.28275
C	5.17543	3.31687	5.68356
H	5.00963	2.58413	4.89592
C	6.70248	7.25213	5.02339
H	6.95918	6.24332	5.30488
C	0.20744	12.34804	7.28055
H	-0.83469	12.62562	7.33041
C	5.90312	2.95110	6.82002
C	7.39850	8.17959	4.26247
H	8.36522	8.05661	3.79794
C	0.98242	6.97498	4.65210
H	0.04305	6.53429	4.35387
C	4.82668	12.82870	12.17576
H	5.44289	12.41234	12.97052
C	3.26776	8.11109	9.88934
H	2.92142	7.61498	10.79324
C	5.83532	13.19935	7.95673
H	5.87791	13.63155	8.94380
C	4.61389	12.08770	11.01461
H	5.09157	11.11466	10.93240
C	6.08986	12.58692	5.86283
H	6.37805	12.44778	4.83178
C	3.65582	7.37475	8.78016
H	3.62776	6.29140	8.80245
C	3.34291	9.49429	9.82386
H	3.06637	10.09994	10.67929

C	5.61500	5.22623	7.63056
H	5.84105	5.96266	8.39764
C	4.05313	8.02180	7.60423
C	6.12675	3.93881	7.78415
H	6.71660	3.69999	8.66723
C	3.82983	12.56555	9.94968
C	0.89793	11.78231	6.20983
H	0.55379	11.52020	5.22046
C	4.84649	5.60269	6.51477
C	3.31836	13.86655	10.10873
H	2.76793	14.33115	9.29419
C	6.56317	9.29518	4.22943
H	6.69021	10.24456	3.73128
C	1.39568	8.29911	4.51222
H	0.88626	9.14427	4.07397
C	3.52102	14.61167	11.26917
H	3.10043	15.61291	11.34286
C	6.63866	13.40922	6.84579
H	7.49087	14.06701	6.76519
C	6.41822	1.54819	7.00224
H	5.69300	0.92815	7.54407
H	7.34926	1.53366	7.57722
H	6.60599	1.06131	6.04043
C	3.74295	10.12708	8.64110
C	4.26933	14.10122	12.33435
C	3.36414	11.46283	3.08850
C	3.16053	12.03767	1.71612
H	3.92071	12.78989	1.49995
H	2.15858	12.45940	1.62255
H	3.26124	11.22922	0.98362

C	4.46048	14.88680	13.60440
H	3.66872	14.66292	14.33035
H	4.43336	15.96475	13.41796
H	5.41521	14.64917	14.08355
B	3.71344	11.75920	8.54588
B	4.38759	7.13990	6.26908