Supporting Information for

An Unusual Hydrogen Migration/C–H Activation Reaction with Group 3 Metals

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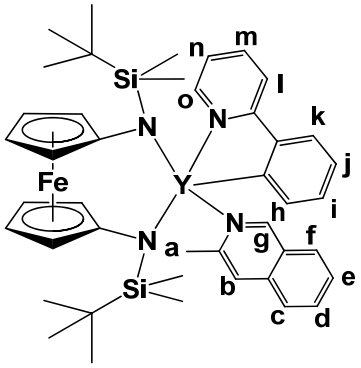
Experimental

All experiments were performed under a dry nitrogen atmosphere using standard Schlenk techniques or in an MBraun inert-gas glovebox. Solvents were purified using a two-column solid-state purification system by the method of Grubbs[1] and transferred to the glovebox without exposure to air. NMR solvents were obtained from Cambridge Isotope Laboratories, degassed, and stored over activated molecular sieves prior to use. **1^{Y}-py^{Ph}**, **1^{Lu}-py^{Ph}**, 2-phenyl-d_5-pyridine, and 2-(*p*-tolyl)-d_4-pyridine were prepared following published procedures.[2-4] ^{1}H, ^{2}H, and ^{13}C NMR spectra were recorded on Bruker300 or Bruker500 spectrometers (supported by the NSF grant CHE-9974928) at room temperature in C_6D_6 (except for ^{2}H NMR spectra) unless otherwise specified. Chemical shifts are reported with respect to solvent residual peak, 7.16 ppm (C_6D_6). CHN analyses were performed by Midwest Microlab, LLC, 7212 N. Shadeland Avenue, Suite 110, Indianapolis, IN 46250.

Synthesis of 2^{Y}-Phpy-iqn. 1^{Y}-py^{Ph} (149.8 mg, 0.198 mmol) was dissolved in a minimal amount of C_6H_6 and stirred in a Schlenk tube for 2 weeks at 50 ºC. The solution was then transferred to a 20-mL vial and the volatiles were removed under reduced pressure. The resulting dark-green material was dissolved in minimal hexanes. 1 equiv of 3-methylisoquinoline (28.5 mg, 0.199 mmol) was added to the hexanes solution and the mixture was stirred for 30 min. The solution was filtered through Celite and the volatiles removed under reduced pressure. A dark-brown powder was collected the following morning from hexanes. Yield: 115.2 mg, 70%.



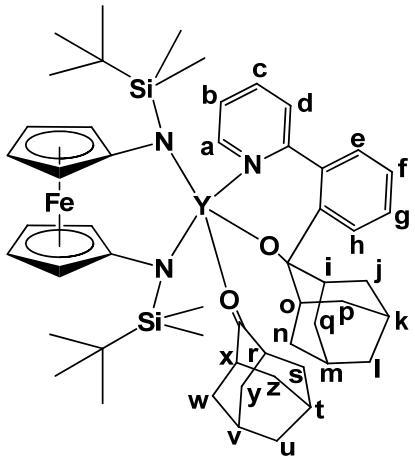
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 10.53 (s, 1H, *g*), 8.57 (br s, 1H, *o*), 7.95 (br s, 1H, *h*), 7.77 (d, 1H, *k*), 7.62 (d, 1H, *l*), 7.25 (br d, 1H, *m*), 7.21 (dd, 2H, *i, j*), 7.17 (d, 1H, *b*), 7.05 (m, 4H, *c, d, e, f*), 6.67 (dd, 1H, *n*), 4.22 (br s, 2H, fc-C*H*), 3.78 (br s, 2H, fc-C*H*), 3.74 (br s, 2H, fc-C*H*), 3.23 (s, 3H, *a*), 3.14 (br s, 2H, fc-C*H*), 0.96 (s, 18H, SiC(CH_3)$_3$), 0.04 and -0.12 (s, 12H, Si(CH_3)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 196.9 (iqn), 165.1 (iqn), 147.3 (phpy), 139.1 (phpy), 138.1 (phpy), 133.0 (phpy), 132.1 (phpy), 126.5 (phpy), 125.7 (iqn), 125.6 (iqn), 124.0 (iqn), 121.0 (phpy), 120.1 (iqn), 119.5 (phpy), 105.2 (fc), 77.4 (fc), 73.0 (fc), 70.7 (fc), 67.2 (fc), 66.7 (fc), 64.5 (fc), 64.1 (fc), 27.6 (t-Bu), 27.5 (t-Bu), 20.4 (iqn), -2.2 (Me), -3.1 (Me). Anal. (%): Calcd. for $C_{43}H_{55}FeN_4Si_2Y$: C, 57.46; H, 6.84; N, 6.65. Found: C, 57.29; H 6.51; N 6.46.

Synthesis of 2^{Lu}-Phpy. 1^{Lu}-py^{Ph} (133.5 mg, 0.143 mmol) was dissolved in a minimal amount of C_6H_6 and stirred in a Schlenk tube for 19 days at 50 ºC. The solution was then transferred to a 20-mL vial and the volatiles were removed under reduced pressure. The resulting black material was dissolved in *n*-pentane and filtered through Celite. The remaining solid on the Celite was washed with three 1 mL portions of *n*-pentane. The filtrate was concentrated under

reduced pressure and stored at -35 °C, giving small black crystals. Yield: 71.2 mg. ^{1}H NMR spectroscopy data indicates that only about 50% conversion from **1^{Lu}-py^{Ph}** to **2^{Lu}-Phpy** occurred, and the products simply co-crystallized. Although over a dozen attempts were made, full conversion to **2^{Lu}-Phpy** was never achieved, and its separation from **1^{Lu}-py^{Ph}** proved difficult.

^{1}H NMR (300 MHz, C_6D_6): δ, ppm: 8.66 (d, 1H, phpy), 7.91 (d, 1H, phpy), 7.84 (d, 1H, phpy), 7.58 (d, 1H, phpy), 7.51 (t, 1H, phpy), 7.09 (br s, 1H, phpy), 6.89 (br s, 1H, phpy), 6.61 (dd, 1H, phpy), 4.15 (br, 4H, OC*H*$_2$CH$_2$), 4.05 (br s, 2H, fc-C*H*), 3.97 (br s, 2H, fc-C*H*), 3.65 (br s, 2H, fc-C*H*), 3.21 (br s, 2H, fc-C*H*), 1.43 (br, 4H, OCH$_2$C*H*$_2$), 0.88 (s, 18H, SiC(C*H*$_3$)$_3$), 0.07 and -0.16 (s, 12H, Si(C*H*$_3$)$_2$).

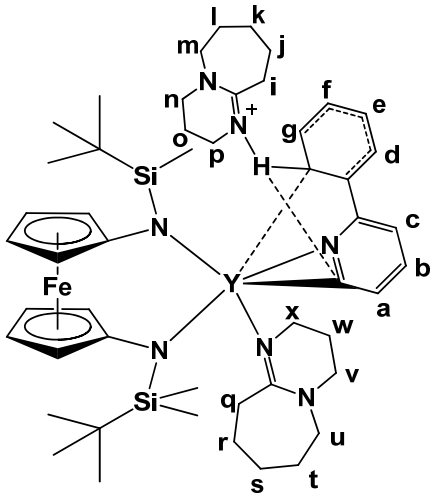
Synthesis of 3. 2^{Y}-Phpy-iqn (115.2 mg, 0.139 mmol) was combined with 2.03 equiv of 2-adamantanone (42.3 mg, 0.282 mmol) in hexanes (5 mL) and stirred for 2 h at ambient temperature. The volatiles were then removed under reduced pressure. A clean golden-brown powder was obtained the next morning from hexanes. Yield: 95.2 mg, 69%.



^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 9.62 (br s, 1H, *a*), 7.77 (br s, 1H, *d*), 7.25 (dd, 1H, *b*), 7.08 (dd, 1H, *c*), 6.99 (br s, 1H, *e*), 6.92 (dd, 2H, *f, g*), 6.75 (br s, 1H, *h*), 4.23 (br s, 2H, fc-C*H*), 3.88 (br s, 2H, fc-C*H*), 3.81 (br s, 2H, fc-C*H*), 3.31 (br s, 2H, *i, o*), 2.93 (br s, 2H, *r*, *x*), 2.88 (br s, 2H, fc-C*H*), 2.56 (br s, 1H, *k*), 2.40 (br s, 1H, *m*), 2.04 (br s, 4H, *j, p*), 1.92 (br s, 2H, *t, v*), 1.75 (m, 8H, *n, q, s, z*), 1.61 (br s, 2H, *l*), 1.49 and 1.46 (br s, 4H, *w, y*), 1.34 (t, 2H, *u*), 1.03 (s, 18H, SiC(C*H*$_3$)$_3$), 0.29 and 0.13 (s, 12H, Si(C*H*$_3$)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 164.5 (ad), 149.9 (ad), 148.5 (phpy), 138.2 (phpy), 137.4 (phpy), 133.5 (phpy), 125.9 (phpy), 121.0 (phpy), 107.8 (fc), 79.3 (fc), 79.2 (fc), 67.3 (fc), 65.9 (fc), 64.1 (fc), 63.2 (fc), 46.5 (ad), 39.1 (ad), 38.5 (ad), 38.2 (ad), 37.3 (ad), 36.5 (ad), 35.6 (ad), 34.1 (ad), 33.6 (ad), 33.4 (ad), 27.9 (t-Bu), 27.0 (ad), 26.1 (ad), 22.2 (ad), 20.3 (ad), 13.7 (ad), -0.7 (Me), -1.6 (Me). Found: C, 63.83; H, 7.21; N, 3.97.

Synthesis of 4^{Y}. 1^{Y}-py^{Ph} (186.4 mg, 0.246 mmol) was combined with 2 equiv of 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU; 74.8 mg, 0.491 mmol) in C_6H_6 (5 mL) and stirred for 2 d at ambient temperature. The volatiles were then removed under reduced pressure, resulting in a golden-brown oil. Attempts to precipitate the product out as a solid were unsuccessful, even from concentrated *n*-pentane at -78 ºC. Spectroscopic methods indicate a mix of **4^{Y}** and **2^{Y}-Phpy-DBU**

in the oil, with a maximum ratio of 9:1 obtained. Keeping $\mathbf{4^Y}$ in solution led to its slow conversion to $\mathbf{2^Y}$**-Phpy-DBU**, which then precipitated from solution.



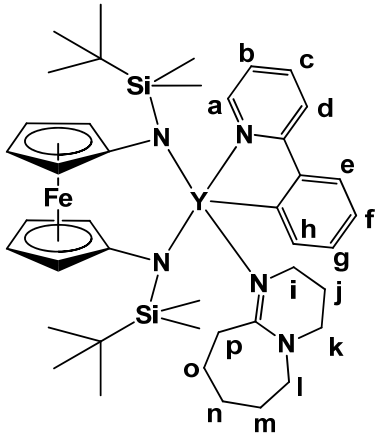
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.57 (br s, 1H, *a*), 8.13 (d, 1H, *g*), 7.34 (d, 1H, *d*), 7.26 (dd, 1H, *f*), 7.17 (dd, 1H, *e*), 7.13 (d, 1H, *c*) 6.68 (dd, 1H, *b*), 4.15 (br s, 2H, fc-C*H*), 4.07 (br s, 2H, fc-C*H*), 3.64 (br s, 2H, fc-C*H*), 3.32 (br s, 2H, fc-C*H*), 3.07 (br s, 4H, *i, p*), 2.74 (br s, 4H, *q, x*), 2.65 (br s, 3H, *h, r*), 2.50 (br s, 6H, *u, v, w*), 2.29 (br s, 2H, *o*), 1.73 (br s, 4H, *j, k*), 1.66 (br s, 2H, *n*), 1.42 (br s, 2H, *l*), 1.30 (br s, 2H, *m*), 1.16 (br s, 4H, *s, t*), 1.09 (s, 18H, SiC(CH_3)$_3$), 0.36 and 0.32 (s, 12H, Si(CH_3)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 169.2 ($C_{DBU\alpha}$9), 165.6 ($C_{DBU\beta}$9), 159.8 (C_{Ph}1), 157.0 (C_{py}1), 149.5 (C_{py}2), 139.4 (C_{Ph}6), 135.9 (C_{py}4), 128.7 (C_{Ph}3), 128.4 (C_{Ph}4), 127.9 (C_{Ph}2), 126.8 (C_{py}5), 121.6 (C_{py}3), 119.6 (C_{Ph}5), 105.7 (C_{fc}), 66.6 (C_{fc}), 65.9 (C_{fc}), 65.5 (C_{fc}), 65.0 (C_{fc}), 54.0 ($C_{DBU\alpha}$8), 52.7 ($C_{DBU\beta}$3), 52.2 ($C_{DBU\beta}$7), 50.3 ($C_{DBU\alpha}$1), 48.0 ($C_{DBU\beta}$4), 47.7 ($C_{DBU\beta}$8), 37.1 ($C_{DBU\beta}$2), 36.8 ($C_{DBU\beta}$1), 29.5 ($C_{DBU\beta}$5), 29.0 ($C_{DBU\beta}$6), 28.4 ($C_{DBU\alpha}$4), 27.9 ($C_{DBU\alpha}$6), 27.6 ($C_{t\text{-}Bu}$), 26.1 ($C_{DBU\alpha}$2), 25.6 ($C_{DBU\alpha}$3), 22.8 ($C_{DBU\alpha}$7), 21.5 ($C_{DBU\alpha}$5), -2.4 (C_{Me}), -2.9 (C_{Me}).

Synthesis of $\mathbf{4^{Lu}}$. $\mathbf{1^{Lu}}$**-py^{Ph}** (84.8 mg, 0.0912 mmol) was combined with 2 equiv DBU (27.8 mg, 0.182 mmol) in toluene (5 mL) and stirred for 30 h at ambient temperature. The yellowish-brown solution was filtered through Celite, and the volatiles were then removed under reduced pressure. ^{1}H NMR spectroscopy was used at this time to assess the purity of the product. Attempts at crystallization resulted in the decomposition of the product to an intractable mixture.

^{1}H NMR (300 MHz, C_6D_6): δ, ppm: 8.58 (d, 1H, *py^{Ph} ring*), 8.16 (d, 1H, *py^{Ph} ring*), 7.32 (d, 1H, *py^{Ph} ring*), 7.25 (t, 2H, *py^{Ph} ring*), 7.09 (m, 1H, *py^{Ph} ring*), 6.64 (m, 1H, *py^{Ph} ring*), 4.12 (br s, 2H, fc-C*H*), 4.08 (br s, 2H, fc-C*H*), 3.76 (br s, 2H, fc-C*H*), 3.54 (br s, 2H, *DBU*), 3.44 (br s, 2H, fc-C*H*), 3.05 (br s, 2H, *DBU*), 3.00 (q, 2H, *DBU*), 2.85 (br s, 2H, *DBU*), 2.56 (br s, 2H, *DBU*), 2.44 (m, 5H, *DBU*), 2.29 (br s, 2H, *DBU*), 2.13 (br s, 1H, *DBU*), 1.71 (br s, 6H, *DBU*), 1.63 (br s, 2H, *DBU*), 1.53 (br s, 1H, *DBU*), 1.44 (br s, 2H, *DBU*), 1.12 (s, 18H, SiC(CH_3)$_3$), 0.38 and 0.33 (s, 12H, Si(CH_3)$_2$).

Synthesis of $\mathbf{2^Y}$-Phpy-DBU: Method A. $\mathbf{2^Y}$-Phpy-iqn (80.8 mg, 0.0975 mmol) was combined with 1 equiv of DBU (14.9 mg, 0.0979 mmol) and was stirred in a minimal amount of C_6H_6 (2 mL) for 1 h at RT. The volatiles were then removed under reduced pressure and the

resulting yellow-orange powder was dissolved in a minimal amount of diethyl ether. Yellow-orange crystals formed overnight at -30 ºC. Yield: 76.4 mg, 93.5%. **Method B: 1^{Y}-py^{Ph}** (107.0 mg, 0.141 mmol) was combined with 2 equiv of DBU (44.3 mg, 0.291 mmol) in a minimal amount of C_6H_6 (4 mL) in a Schlenk tube. The solution was stirred for 2 d at ambient temperature, then for 2 d at 70 ºC. The volatiles were then removed under reduced pressure and the resulting yellow-orange solid was dissolved in diethyl ether. A yellow-orange precipitate formed overnight at -30 ºC. Yield: 69.4 mg, 58.7%.



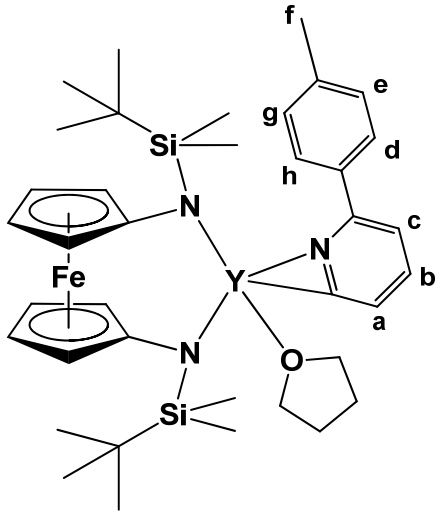
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.72 (br s, 1H, *a*), 8.05 (d, 1H, *h*), 7.86 (d, 1H, *e*), 7.65 (d, 1H, *d*), 7.46 (dd, 1H, *g*), 7.34 (dd, 1H, *f*), 7.16 (dd, 1H, *c*) 6.71 (dd, 1H, *b*), 4.31 (br s, 2H, fc-C*H*), 3.99 (br s, 2H, fc-C*H*), 3.95 (br s, 2H, *p*), 3.82 (br s, 2H, fc-C*H*), 3.42 (br s, 2H, fc-C*H*), 3.05 (br s, 2H, *i*), 2.49 (br s, 4H, *m, n*), 1.73 (br s, 2H, *j*), 1.52 (br s, 2H, *o*), 1.25 (br s, 2H, *k*), 1.01 (br s, 2H, *l*), 0.92 (s, 18H, SiC(CH_3)$_3$), -0.06 and -0.13 (s, 12H, Si(CH_3)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 191.8 (C_{Ph}1), 166.2 (C_{DBU}9), 164.7 (C_{py}5), 148.0 (C_{py}1), 146.8 (C_{Ph}6), 138.8 (C_{py}3), 138.7 (C_{Ph}2), 128.1 (C_{Ph}3), 125.5 (C_{Ph}4), 123.8 (C_{Ph}5), 120.0 (C_{py}2), 119.0 (C_{py}4), 106.0 (C_{fc}), 67.1 (C_{fc}), 66.8 (C_{fc}), 64.0 (C_{fc}), 63.1 (C_{fc}), 52.3 (C_{DBU}5), 47.8 (C_{DBU}6), 43.7 (C_{DBU}8), 36.8 (C_{DBU}1), 28.9 (C_{DBU}3), 27.5 ($C_{t\text{-}Bu}$), 26.8 (C_{DBU}4), 25.5 (C_{DBU}2), 21.4 (C_{DBU}7), 20.3, -2.3 (C_{Me}), -3.3 (C_{Me}). Anal. (%): Calcd. for $C_{42}H_{62}FeN_5Si_2Y$: C, 60.20; H, 7.46; N, 8.36. Found: C, 59.84; H 7.07; N 7.99.

Reaction of 1^{Lu}-py^{Ph} with 2 equiv of DBU. 1^{Lu}-py^{Ph} (29.0 mg, 0.0312 mmol) was split into two equal portions (14.5 mg, 0.0156 mmol each). One of the portions was combined with 2 equiv of DBU (4.7 mg, 0.0308 mmol). The second portion served as a control reaction and had no DBU added to it. Both portions were dissolved in 0.6 mL of C_6D_6 and heated at 50 ºC in J-Young tubes.

^{1}H NMR spectroscopy was used to measure the progress of each reaction. After 21 hours of heating, in the portion without DBU, 33% conversion to the product **2^{Lu}-Phpy** was observed. In the portion that included DBU, no conversion to the product **2^{Lu}-Phpy-DBU** was observed, as determined by comparison with the analogous experiment with yttrium. Instead, complete conversion to the product **4^{Lu}** was observed, again as determined by comparison with the analogous experiment with yttrium.

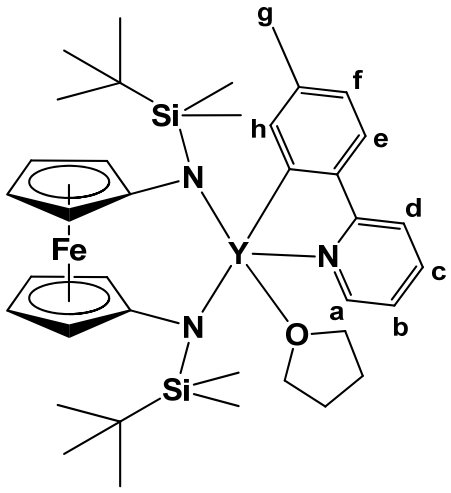
After 6 days of heating at 50 ºC, the reaction without DBU showed 40% conversion to the product **2^{Lu}-Phpy**. The reaction that included 2 equiv of DBU still showed no conversion to **2^{Lu}-Phpy-DBU**.

Synthesis of 1^{Y}-py^{tol}. 1^{Y}-CH_2Ph (119.9 mg, 0.175 mmol) was combined with 0.95 equiv 2-tolylpyridine (28.1 mg, 0.166 mmol) in toluene and stirred in a Schlenk tube for 1.5 h at 50 ºC. The volatiles were removed under reduced pressure; the resulting solid was dissolved in a minimal amount of hexanes and kept overnight at -30 ºC. A tan powder was separated from the solution and identified to be $\mathbf{1^{Y}\text{-}py^{tol}}$. Yield: 87.4 mg, 68.2%.



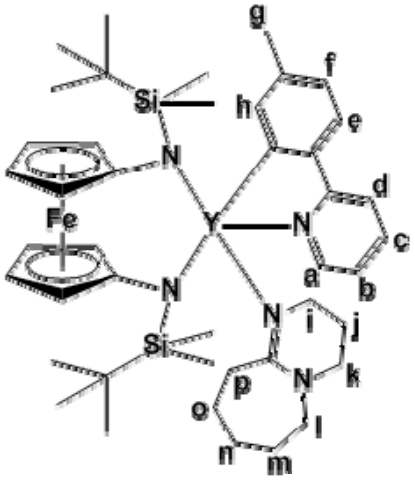
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.00 and 7.97 (m, 3H, *a, b, c*), 7.36 and 7.31 (d, 4H, *d, e, g, h*), 4.01 (br s, 4H, fc-C*H*), 3.99 (br s, 4H, fc-C*H*), 3.93 (br s, 4H, THF), 2.74 (s, 3H, *f*), 1.37 (br s, 4H, THF), 0.87 (s, 18H, SiC(CH_3)$_3$), -0.05 (s, 12H, Si(CH_3)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 152.9 (tolpy), 139.7 (tolpy), 133.7 (tolpy), 130.2 (tolpy), 128.9 (tolpy), 118.0 (tolpy), 104.9 (fc), 71.5 (fc), 66.2 (fc), 34.0 (THF), 26.8 (t-Bu), 24.7 (THF), 20.0 (tolpy), -3.7 (Me).

Synthesis of 2^{Y}-tolpy. 1^{Y}-py^{tol} (27.4 mg, 0.0355 mmol) was dissolved in C_6D_6 and heated in a J-Young tube for 20 d at 50 ºC. The reaction was determined to be complete when no more starting material could be detected by ^{1}H NMR spectroscopy. The solution was transferred to a 20-mL vial, the volatiles were removed under reduced pressure, and the residue was suspended in a minimal amount of *n*-pentane, and kept for 1 h at -78 ºC. A brown solid was quickly separated from the solution before melting into an oil and the solid was confirmed to be the desired product via ^{1}H NMR spectroscopy. Yield: 20.1 mg, 73.4%.



^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.53 (br s, 1H, *a*), 7.77 (s, 1H, *h*), 7.75 (d, 1H, *e*), 7.58 (d, 1H, *d*), 7.31 (d, 1H, *f*), 6.99 (br s, 1H, *c*) 6.55 (dd, 1H, *b*), 4.20 (br s, 4H, THF), 4.08 (br s, 2H, fc-C*H*), 4.04 (br s, 2H,fc-C*H*), 3.59 (br s, 2H, fc-C*H*), 3.15 (br s, 2H, fc-C*H*), 2.47 (s, 3H, *g*), 1.45 (br s, 4H, THF), 0.89 (s, 18H, SiC(CH_3)$_3$), -0.02 and -0.09 (s, 12H, Si(CH_3)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 151.0 (tolpy), 145.5 (tolpy), 139.9 (tolpy), 123.7 (tolpy), 122.0 (tolpy), 114.9 (tolpy), 110.2 (tolpy), 104.2 (fc), 66.5 (fc), 66.2 (fc), 64.5 (fc), 30.6 (THF), 27.5 (t-Bu), 20.6 (THF), 15.3 (tolpy), -2.7 (Me), -3.1 (Me).

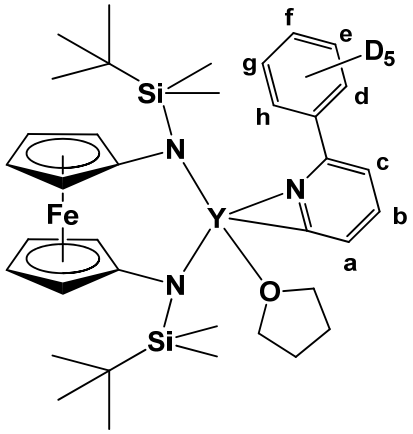
Synthesis of 2^{Y}-tolpy-DBU. 1^{Y}-py^{tol} (21.4 mg, 0.0251 mmol) was combined with 1 equiv DBU (3.9 mg, 0.0256 mmol), dissolved in a minimum amount of C_6D_6, and heated in a J-Young NMR tube at 70 ºC for 3 d. The reaction was monitored via ^{1}H NMR spectroscopy until completion. The volatiles were removed under reduced pressure and the resulting solid was filtered and dissolved in a minimum amount of diethyl ether. After leaving the solution overnight at -30 ºC, the ether layer was separated and dried, resulting in a tan-orange solid. Yield: 13.0 mg, 60.7%.



^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.68 (br s, 1H, *a*), 7.97 (s, 1H, *h*), 7.80 (d, 1H, *e*), 7.65 (d, 1H, *d*), 7.29 (d, 1H, *f*), 7.05 (dd, 1H, *c*) 6.69 (dd, 1H, *b*), 4.17 (br s, 2H, fc-C*H*), 4.09 (br s, 2H, fc-C*H*), 3.84 (br s, 2H, *p*), 3.69 (br s, 2H, fc-C*H*), 3.40 (br s, 2H, fc-C*H*), 3.07 (br s, 2H, *i*), 2.50

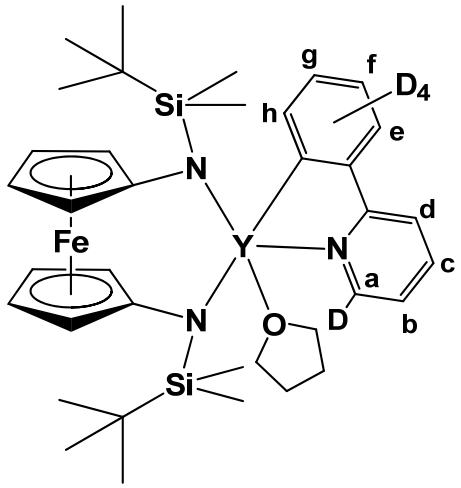
(br s, 4H, *m, n*), 2.44 (s, 3H, *g*), 1.76 (br s, 2H, *j*), 1.51 (br s, 2H, *o*), 1.28 (br s, 2H, *k*), 1.03 (br s, 2H, *l*), 0.92 (s, 18H, SiC(CH_3)$_3$), -0.05 and -0.12 (s, 12H, Si(CH_3)$_2$).

Synthesis of 1^{Y}-py^{Ph}-d_5. 1^{Y}-CH_2Ph (87.4 mg, 0.131 mmol) was combined with 0.95 equiv 2-pentadeuterophenylpyridine (19.9 mg, 0.124 mmol) in toluene and stirred in a Schlenk tube for 1 h at 50 ºC. Solvent was removed via vacuum and the resulting green-yellow solid was dissolved in minimal hexanes. Storing overnight at -30 ºC yielded a yellow-green powder. Yield: 55.7 mg, 58.9%.



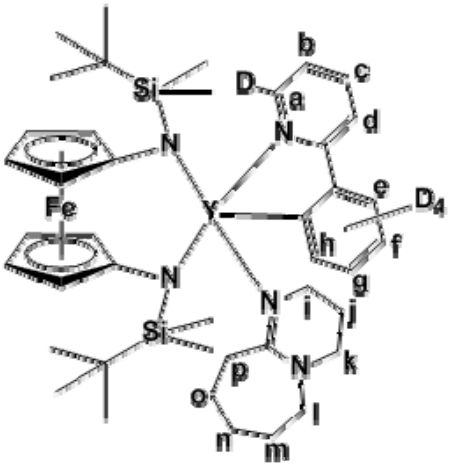
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.02 (d, 2H, *a, c*), 7.97 (dd, 1H, *b*), 4.15 (br s, 4H, fc-C*H*), 4.06 (br s, 4H, THF), 3.43 (br s, 4H, fc-C*H*), 1.40 (br s, 4H, THF) 0.86 (s, 18H, SiC(CH_3)$_3$), -0.07 (s, 12H, Si(CH_3)$_2$). ^{2}H NMR (500 MHz, C_6H_6): δ, ppm: 7.36 (br s, 1D, *h*), 7.30 (br s, 2D, *e,g*), 7.27 (br s, 1D, *d*), 7.18 (br s, 1D, *f*).

Synthesis of 2^{Y}-Phpy-d_5. 1^{Y}-py^{Ph}-d_5 (23.5 mg, 0.0308 mmol) was dissolved in minimal C_6D_6 and heated in a J-Young for 21 d. The reaction was determined to be complete via ^{1}H and ^{2}H NMR, though some decomposition occurred. The solution was removed and the resulting solid was dissolved in minimal pentane. After an overnight at -30 ºC, the *n*-pentane layer was separated and dried, resulting in a brown oil. Yield: 20.3 mg, 86.4%.



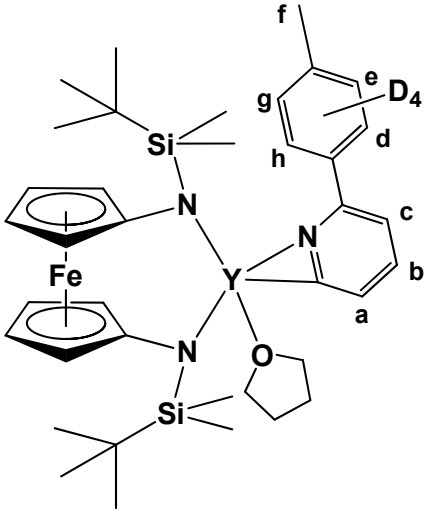
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 7.58 (d, 1H, *d*), 7.35 (br s, 1H, *c*), 6.58 (d, 1H, *b*), 4.20 (br s, 2H, fc-C*H*), 4.08 (br s, 4H, THF), 3.93 (br s, 2H, fc-C*H*), 3.58 (br s, 2H, fc-C*H*), 3.14 (br s, 2H, fc-C*H*), 1.40 (br s, 4H, THF) 0.88 (s, 18H, SiC(CH_3)$_3$), -0.03 and -0.10 (s, 12H, Si(CH_3)$_2$). ^{2}H NMR (500 MHz, C_6H_6): δ, ppm: 8.59 (br s, 1D, *a*), 7.95 (br s, 1D, *h*), 7.81 (br s, 1D, *e*), 7.48 (br s, 1D, *g*), 7.37 (br s, 1D, *f*).

Synthesis of 2^{Y}-Phpy-*d*$_5$-DBU. 1^{Y}-py^{Ph}-*d*$_5$ (18.7 mg, 0.0222 mol) was combined with 1 equiv DBU (3.4 mg, 0.0223 mmol), dissolved in a minimum amount of C_6H_6, and heated in a J-Young NMR tube at 70 ºC for 3 d. The reaction was monitored via ^{2}H NMR spectroscopy until completion. The volatiles were removed under reduced pressure and the resulting solid was filtered and dissolved in a minimum amount of diethyl ether. After leaving the solution for 2 days at -30 ºC, the ether layer was separated and dried, resulting in a yellow-orange powder. Yield: 11.6 mg, 62.0%.



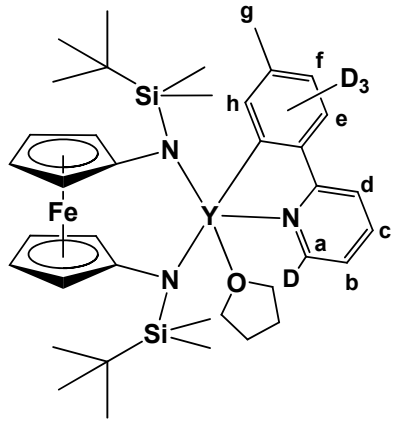
^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 7.65 (d, 1H, *d*), 7.16 (dd, 1H, *c*), 6.72 (d, 1H, *b*), 4.31 (br s, 2H, fc-C*H*), 3.99 (br s, 2H, fc-C*H*), 3.95 (br s, 2H, *p*), 3.82 (br s, 2H, fc-C*H*), 3.42 (br s, 2H, fc-C*H*), 3.05 (br s, 2H, *i*), 2.49 (br s, 4H, *m, n*), 1.73 (br s, 2H, *j*), 1.51 (br s, 2H, *o*), 1.25 (br s, 2H, *k*), 1.01 (br s, 2H, *l*), 0.93 (s, 18H, SiC(CH_3)$_3$), -0.06 and -0.13 (s, 12H, Si(CH_3)$_2$). ^{2}H NMR (500 MHz, C_6H_6): δ, ppm: 8.72 (br s, 1D, *a*), 8.05 (br s, 1D, *h*), 7.86 (br s, 1D, *e*), 7.46 (br s, 1D, *g*), 7.34 (br s, 1D, *f*).

Synthesis of 1^{Y}-py^{tol}-*d*$_4$. 1^{Y}-CH$_2$Ph (48.9 mg, 0.0716 mmol) was combined with 0.95 equiv 2-(2,3,5,6-*d*$_4$-tolyl)pyridine (11.8 mg, 0.0682 mmol) in C_6D_6 and heated in a J-Young for 2 h at 50 ºC. The solution was dried via vacuum and dissolved in minimal hexanes. After 48 h at -30 ºC, a brown powder was separated from the solution. Yield: 37.4 mg, 70.7%.



^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 8.02, 8.00, and 7.97 (m, 3H, *a, b, c*), 4.01 (br s, 4H, fc-C*H*), 3.99 (br s, 4H, fc-C*H*), 3.96 (br s, 4H, THF), 2.74 (s, 3H, *f*), 1.39 (br s, 4H, THF), 0.87 (s, 18H, SiC(CH_3)$_3$), -0.05 (s, 12H, Si(CH_3)$_2$). ^{2}H NMR (500 MHz, C_6H_6): δ, ppm: 7.37 (br s, 2D, *d, h*), 7.32 (br s, 2D, *e, g*).

Synthesis of 2^{Y}-tolpy-d_4. 1^{Y}-py^{tol}-d_4 (22.3 mg, 0.0289 mmol) was dissolved in a minimum amount of C_6D_6 and heated in a J-Young NMR tube for 32 d. The reaction was monitored by ^{1}H and ^{2}H NMR spectroscopy; some decomposition was observed. The volatiles were removed under reduced pressure and the resulting solid was dissolved in a minimum amount of *n*-pentane. After leaving the solution overnight at -30 ºC, the *n*-pentane layer was separated and dried, resulting in a brown oil. Yield: 16.9 mg, 75.8%.



^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 7.58 (d, 1H, *d*), 7.00 (t, 1H, *c*), 6.55 (d, 1H, *b*), 4.19 (br s, 4H, THF), 4.05 (m, 4H, fc-C*H*), 3.58 (br s, 2H, fc-C*H*), 3.15 (br s, 2H, fc-C*H*), 2.47 (s, 3H, *g*), 1.21 (br s, 4H, THF), 0.88 (s, 18H, SiC(CH_3)$_3$), -0.03 (s, 12H, Si(CH_3)$_2$). ^{2}H NMR (500 MHz, C_6H_6): δ, ppm: 8.52 (s, 1D, *a*), 7.76 (br s, 2D, *h,e*), 7.30 (s, 1D, *f*).

Crossover experiment #1: 1^{Y}-py^{tol} and 1^{Y}-py^{Ph}. 1^{Y}-py^{Ph} (13.6 mg, 0.0179 mmol) and **1^{Y}-py^{tol}** (13.9 mg, 0.0180 mmol) were combined in minimal C_6D_6 and heated in a J-Young for 21 d. After the reaction was considered complete, by ^{1}H NMR spectroscopy, the solution was

dried under reduced pressure, the resulting solid was dissolved in minimal hexanes and left for 48 h at -30 ºC. The hexanes solution was separated from the precipitate, dried down, and the resulting brown oil was identified to be **2^{Y}-Phpy** and **2^{Y}-tolpy** by ^{1}H NMR spectroscopy. The ^{1}H NMR spectrum of this mixture shows a clear resolution of a peak at 8.60 ppm for **2^{Y}-Phpy** and 8.53 ppm for **2^{Y}-tolpy**.

Crossover experiment #2: 1^{Y}-py^{tol} and 1^{Y}-py^{Ph}-*d*$_5$. **1^{Y}-py^{Ph}-*d*$_5$** (14.7 mg, 0.0193 mmol) and **1^{Y}-py^{tol}** (14.6 mg, 0.0189 mmol) were combined in minimal C_6D_6 and heated in a J-Young for 24 d. After the reaction was considered complete, by ^{1}H NMR spectroscopy, the solution was dried under reduced pressure, the resulting solid was dissolved in minimal hexanes and left for 48 h at -30 ºC. The hexanes solution was separated from the precipitate, dried down, and the resulting brown oil was identified to be **2^{Y}-Phpy-*d*$_5$** and **2^{Y}-tolpy** by ^{1}H and ^{2}H NMR spectroscopy. The presence of a peak at 8.53 ppm in the ^{1}H NMR spectrum and a peak at 8.60 ppm in the ^{2}H NMR spectrum, and the absence of these peaks in the other's spectrum favors an intramolecular mechanism.

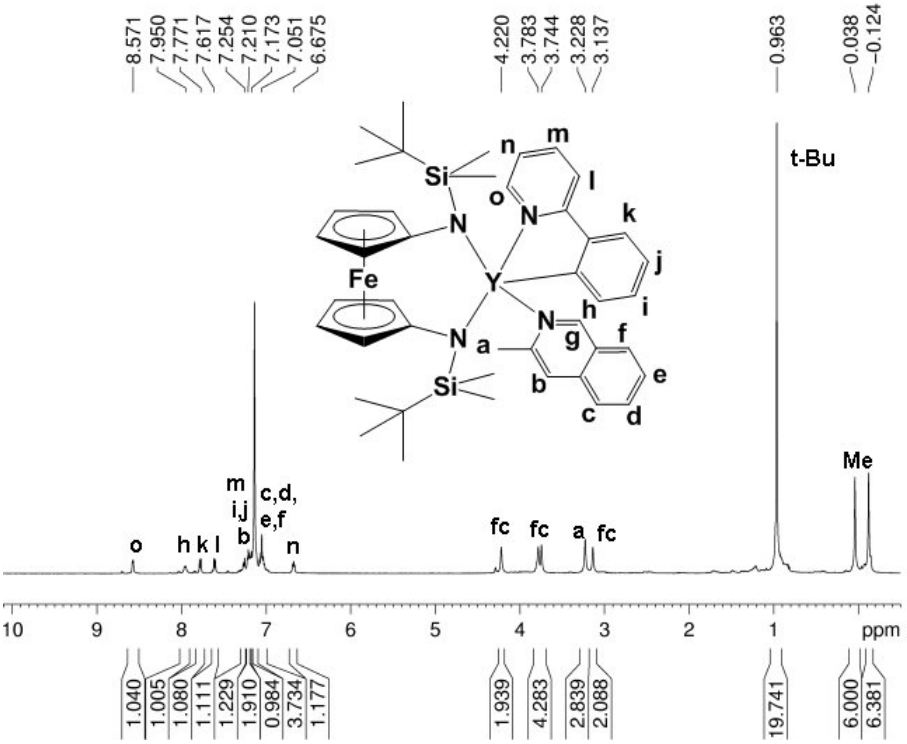
Crossover experiment #3: 1^{Y}-py^{tol}-*d*$_4$ and 1^{Y}-py^{Ph}-*d*$_5$. **1^{Y}-py^{Ph}-*d*$_5$** (13.1 mg, 0.0172 mmol) and **1^{Y}-py^{tol}-*d*$_4$** (13.3 mg, 0.0171 mmol) were combined in a minimum amount of C_6H_6 and heated in a J-Young NMR tube for 34 d. The reaction mixture was monitored by ^{1}H NMR spectroscopy. After completion, the volatiles were removed under reduced pressure, the resulting solid was dissolved in a minimum amount of hexanes and left for 48 h at -30 ºC. Decanting of the hexanes solution allowed the separation of a precipitate, which was dried and the resulted in a brown oil. The oil was determined to be **2^{Y}-Phpy-*d*$_5$** and **2^{Y}-tolpy-*d*$_4$** by ^{1}H and ^{2}H NMR spectroscopy. The ^{1}H NMR spectrum showed no peaks in the 8.5-8.6 ppm region, while the ^{2}H NMR spectrum showed two peaks at 8.60 ppm and 8.53 ppm, corresponding to each product.

Crossover experiment #4: 1^{Y}-py^{tol} and 1^{Y}-py^{Ph}-*d*$_5$ with 4 equiv DBU. **1^{Y}-py^{Ph}-*d*$_5$** (18.2 mg, 0.0216 mmol) and **1^{Y}-py^{tol}** (18.6 mg, 0.0218 mmol) were combined with 4 equiv DBU (13.4 mg, 0.0880 mmol) in a minimum amount of C_6D_6 and heated in a J-Young tube for 3.5 d. After completion, the volatiles were removed under reduced pressure, the resulting solid was dissolved in hexanes, and was left overnight at -30 ºC. The resulting tan-brown solid was separated, dried, and was determined to be **2^{Y}-tolpy-DBU** and **2^{Y}-Phpy-*d*$_5$-DBU** via ^{1}H and ^{2}H NMR spectroscopy; **2^{Y}-tolpy-DBU** shows no peaks in the ^{2}H NMR spectrum. In addition, **2^{Y}-Phpy-*d*$_5$-DBU** shows the expected 5 deuterium signals observed with the non-DBU-catalyzed intramolecular reaction mechanism.

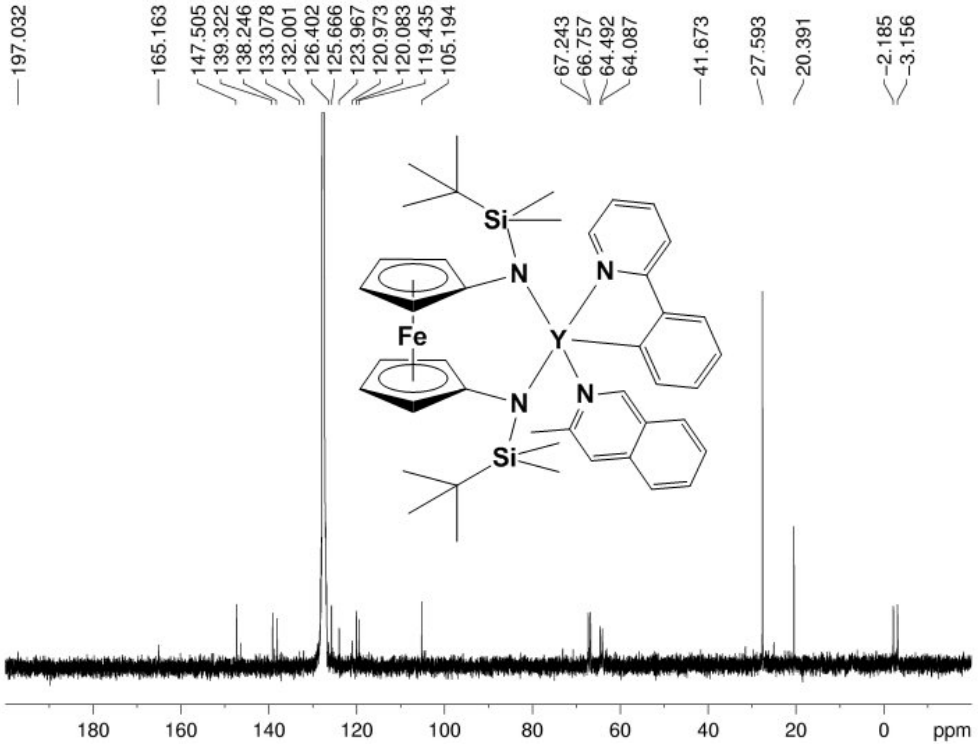
NMR Spectra

2^{Y}-Phpy-iqn

^{1}H NMR (500 MHz, C_6D_6)



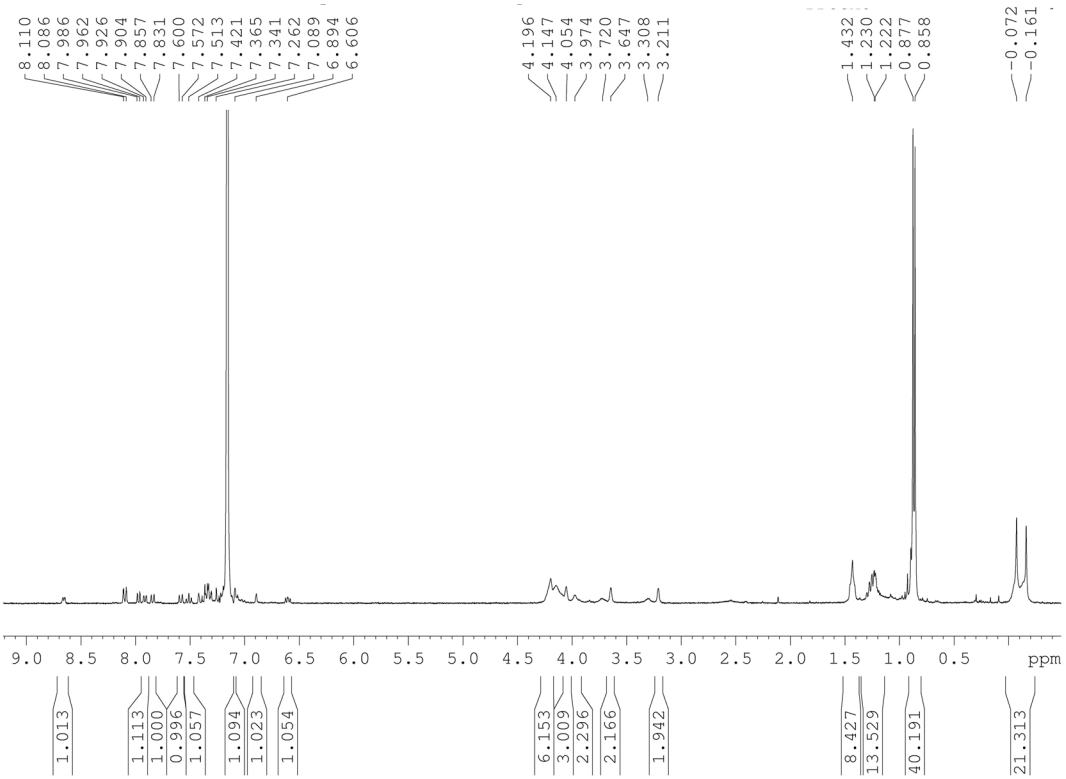
^{13}C NMR (126 MHz, C_6D_6)



2^{Lu}-Phpy

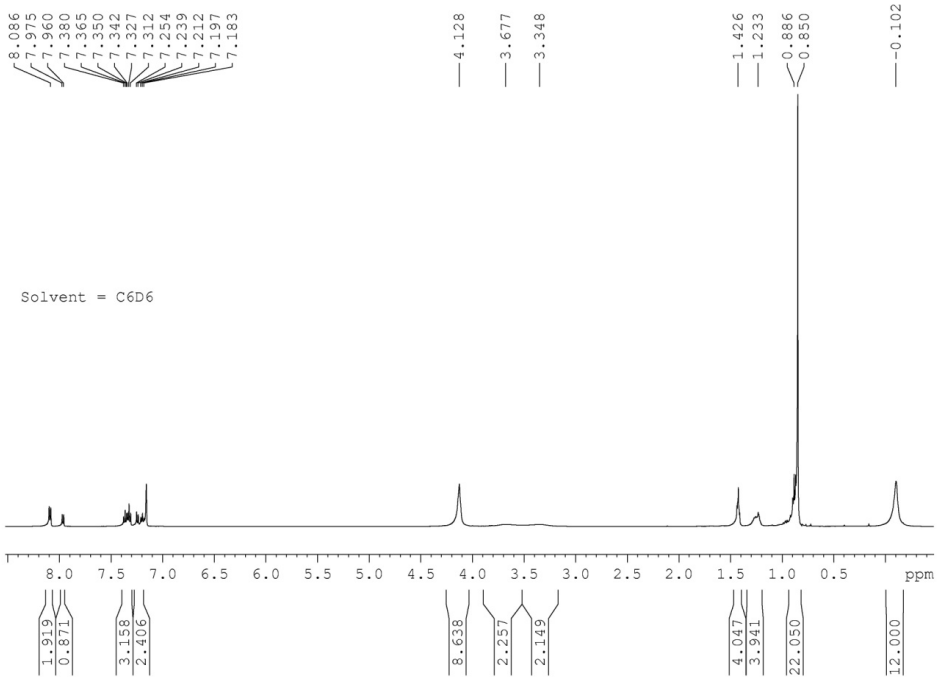
^{1}H NMR (300 MHz, C_6D_6)

Note: n-Hexanes is present at 1.23 and 0.88 ppm. This spectrum is approximately 50% **1^{Lu}-py^{Ph}** and 50% **2^{Lu}-Phpy**. The previously published ^{1}H NMR spectrum of **1^{Lu}-py^{Ph}** has been included for reference.



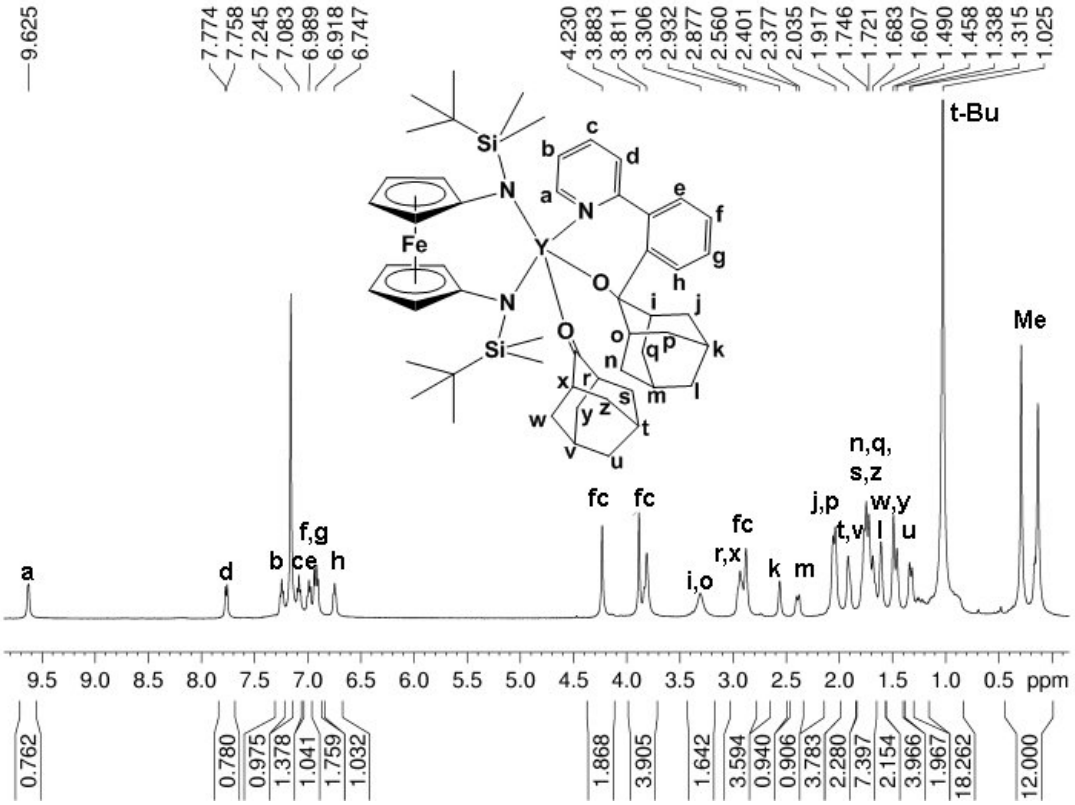
1^{Lu}-py^{Ph}

^{1}H NMR (500 MHz, C_6D_6)

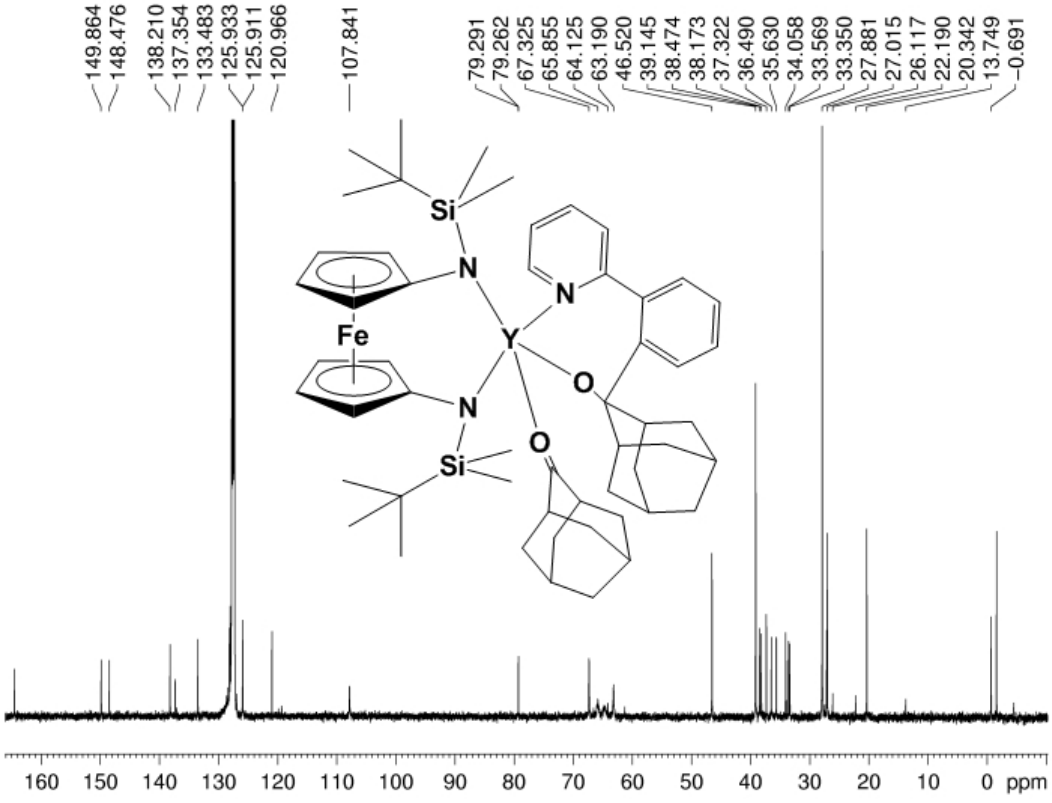


3

^{1}H NMR (500 MHz, C_6D_6)



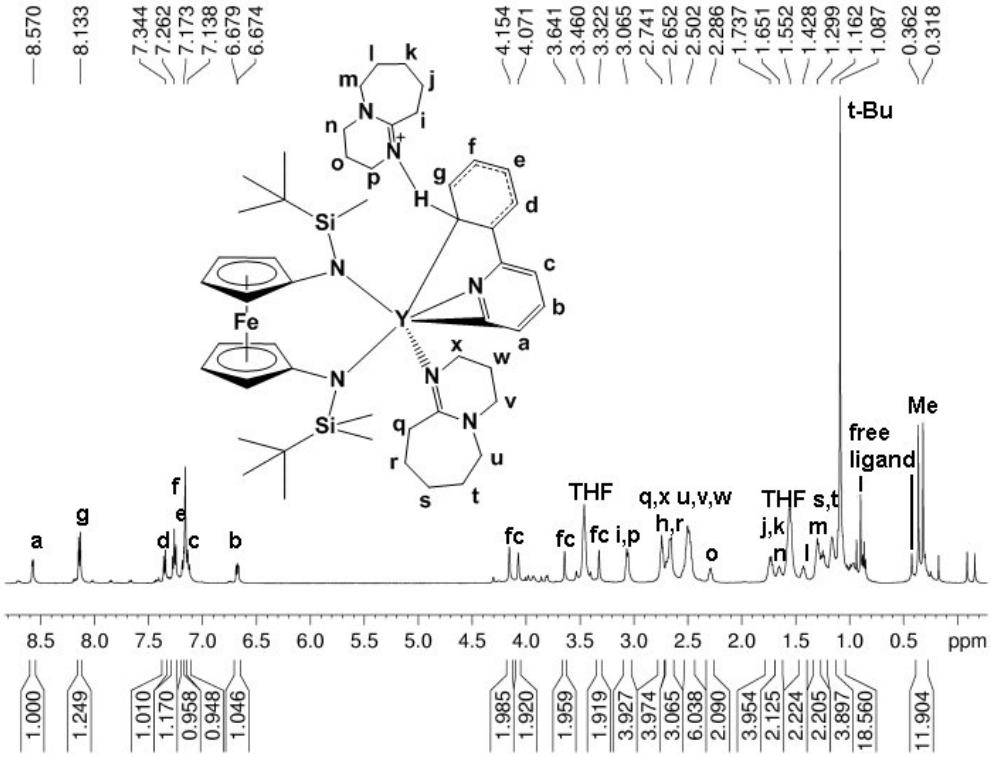
^{13}C NMR (126 MHz, C_6D_6)



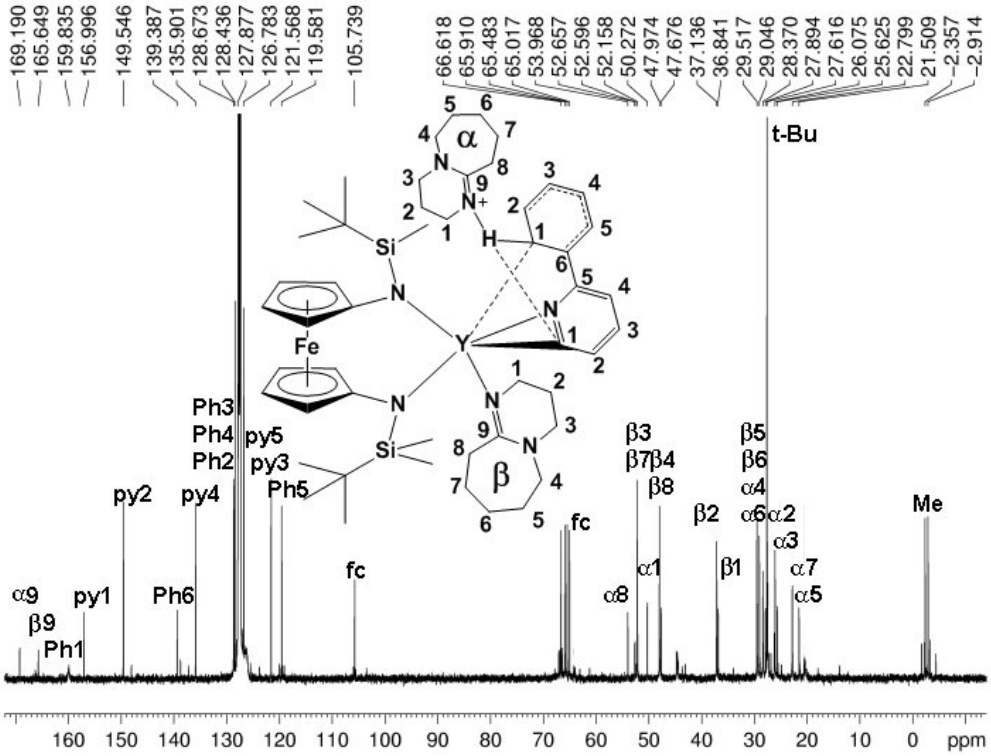
4^{Y}

^{1}H NMR (500 MHz, C_6D_6)

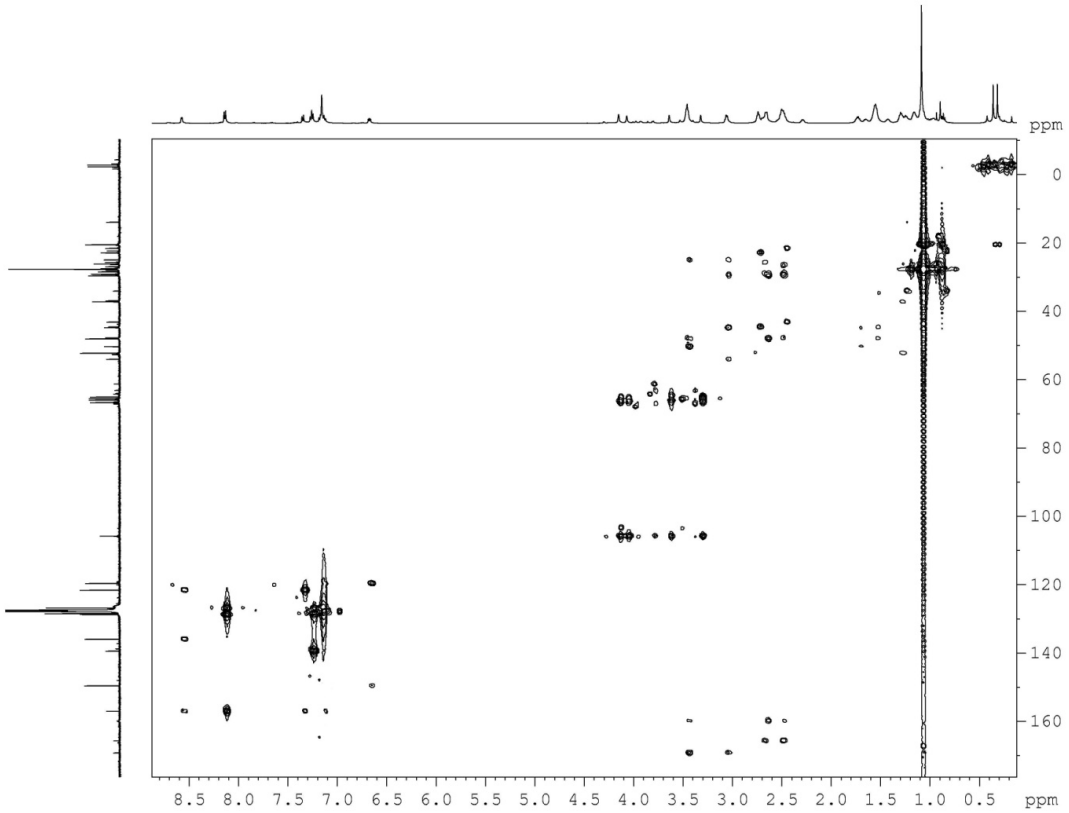
Note: The peaks at 3.46 and 1.55 correspond to THF; all unmarked peaks correspond to a small amount of **2^{Y}-Phpy-DBU**.



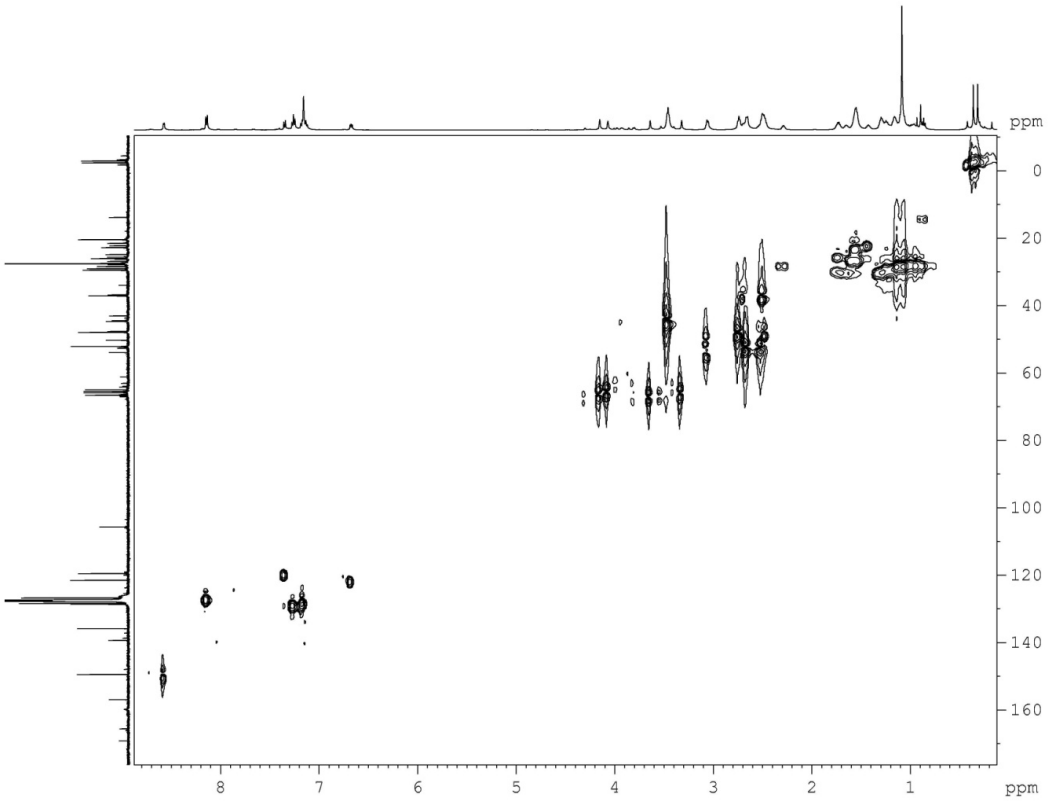
^{13}C NMR (126 MHz, C_6D_6)



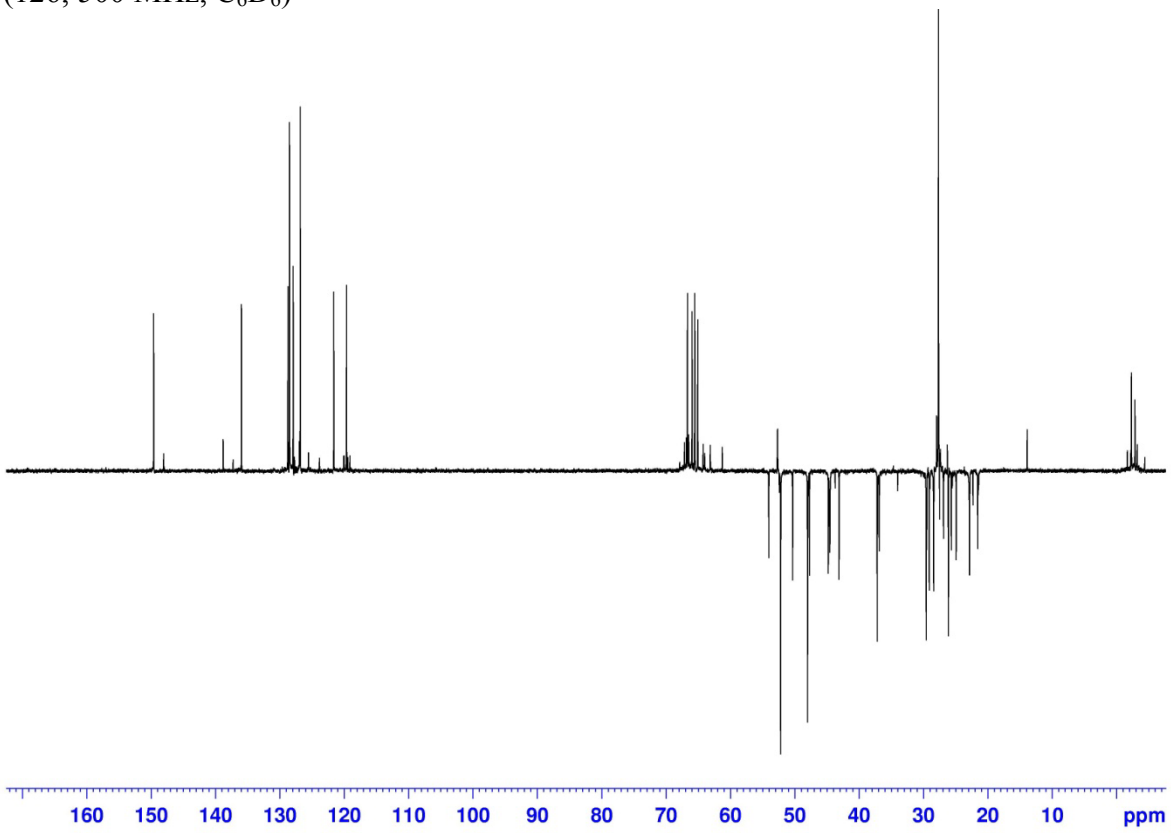
HMBC (126, 500 MHz, C_6D_6)



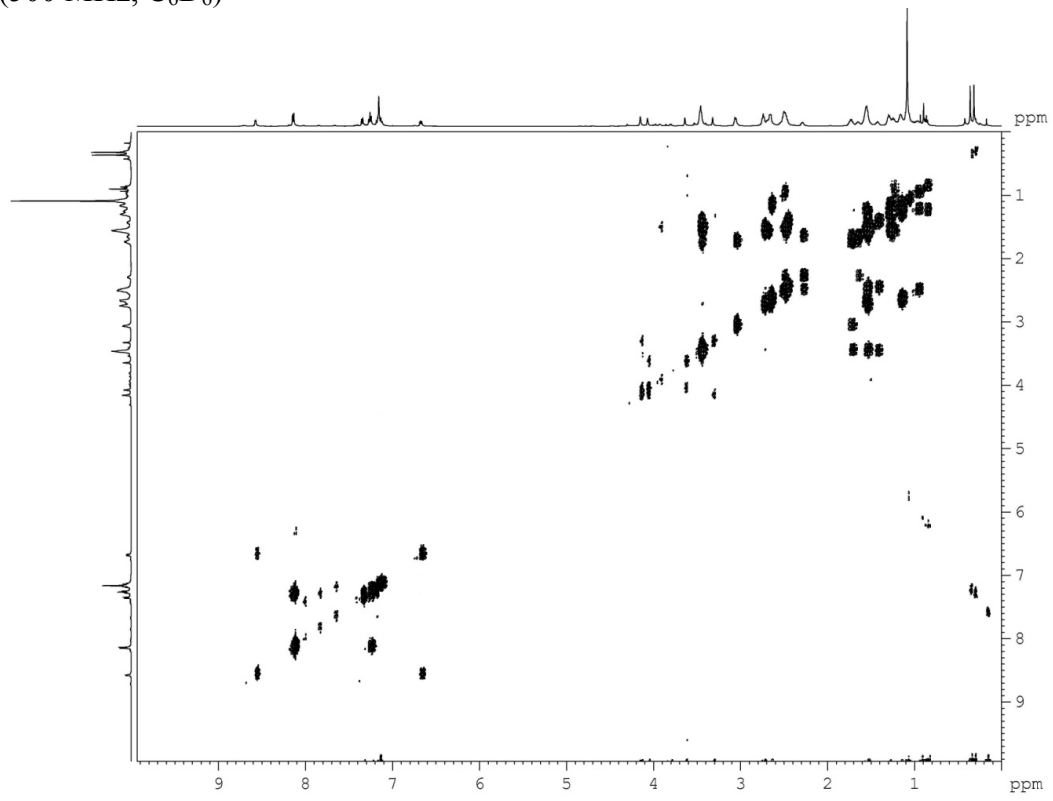
HMQC (126, 500 MHz, C_6D_6)



DEPT (126, 500 MHz, C_6D_6)



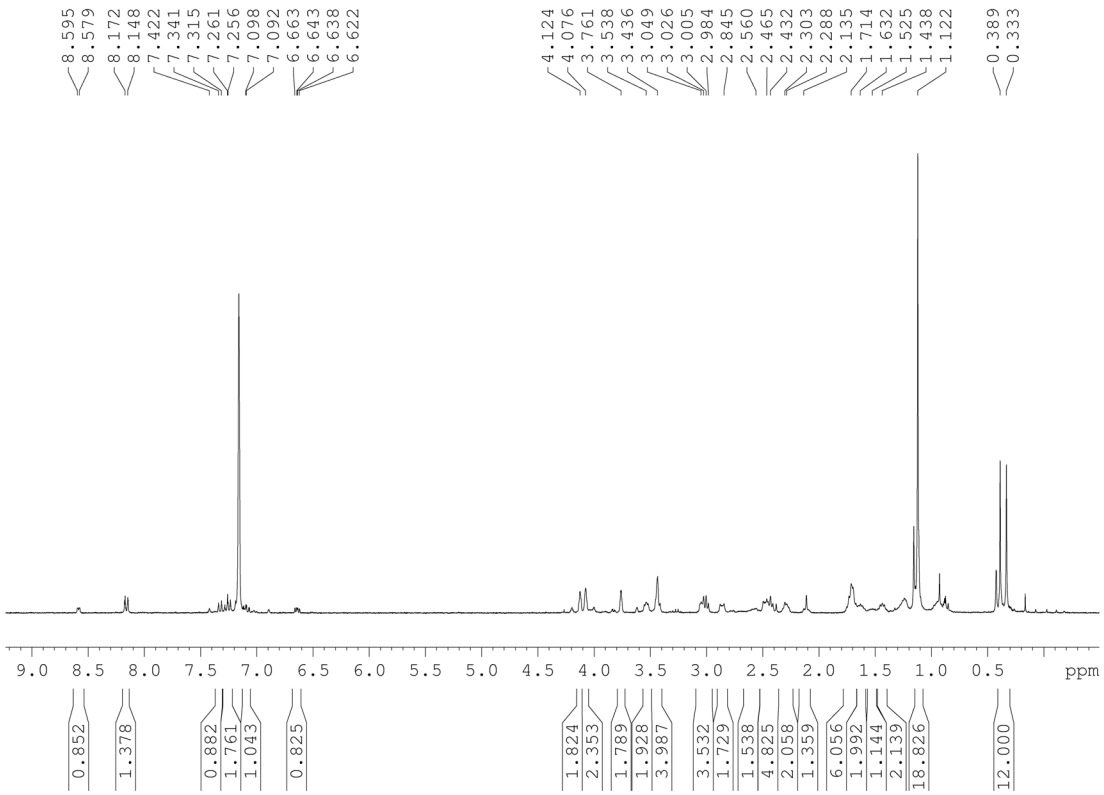
COSY (500 MHz, C_6D_6)



4^{Lu}

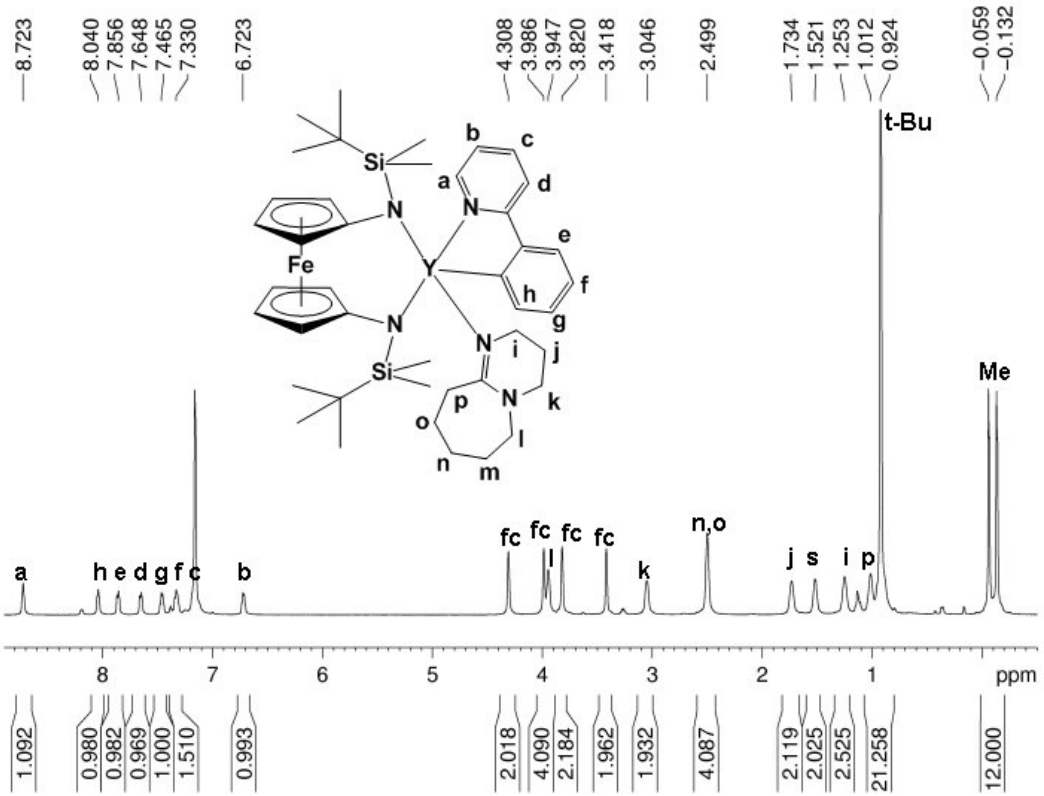
^{1}H NMR (300 MHz, C_6D_6)

Note: Small unmarked peaks correspond to unidentified impurities, which were formed by decomposition while crystallization attempts were being made.

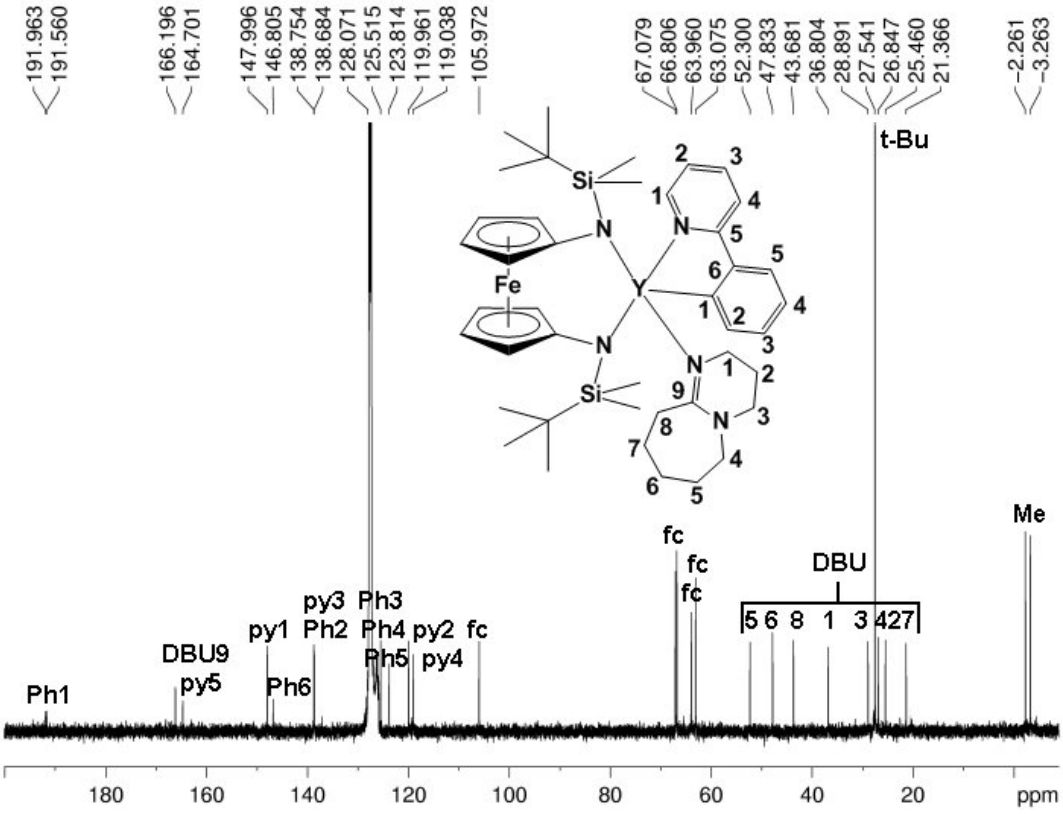


2^{Y}-Phpy-DBU

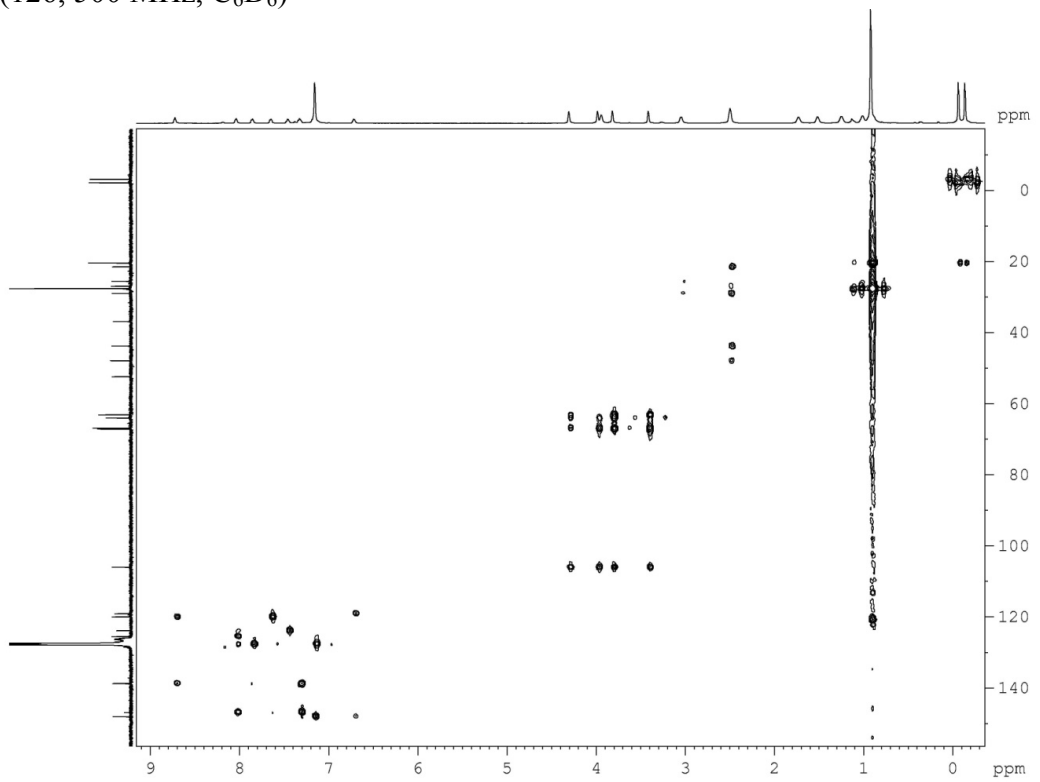
^{1}H NMR (500 MHz, C_6D_6)



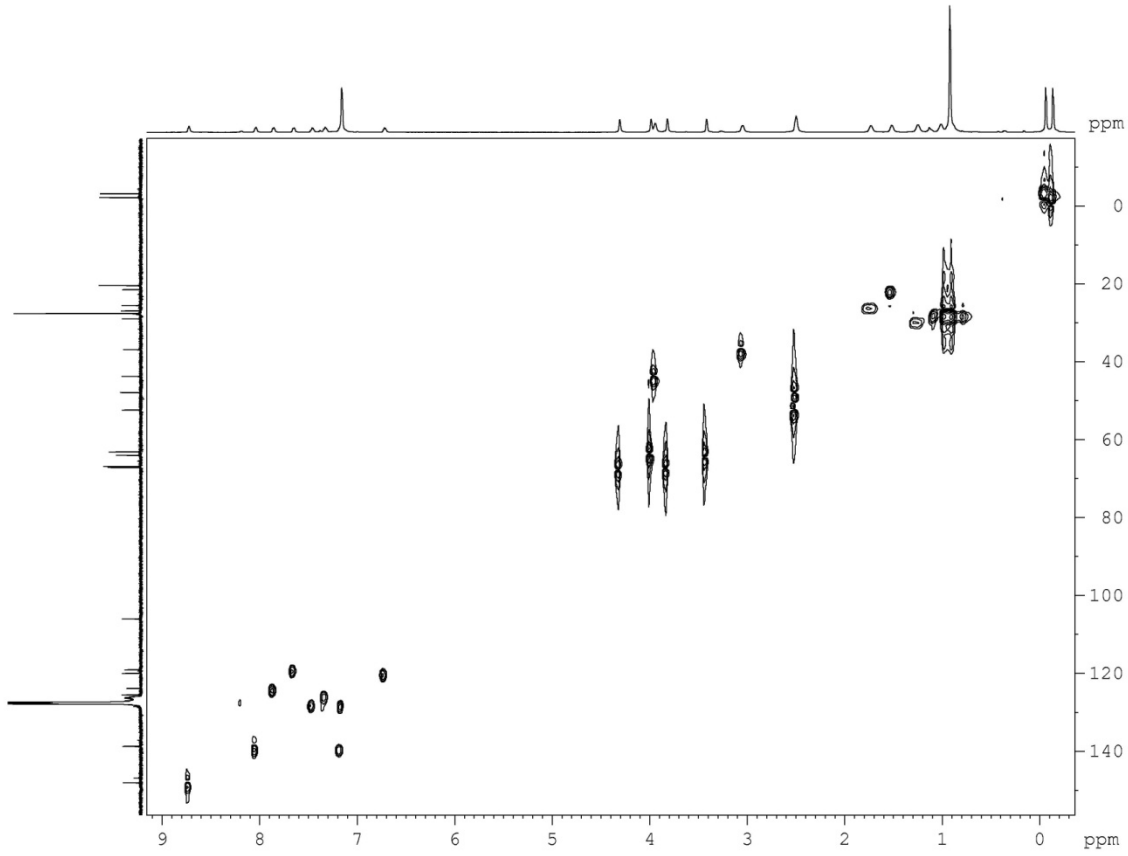
^{13}C NMR (126 MHz, C_6D_6)



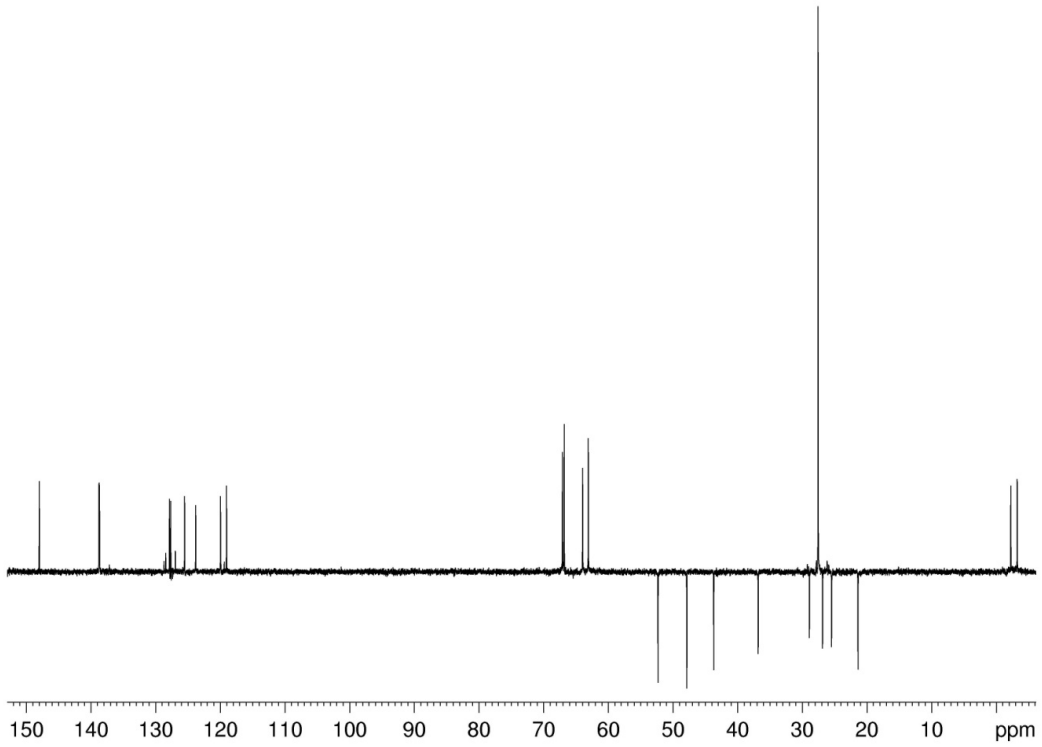
HMBC (126, 500 MHz, C_6D_6)



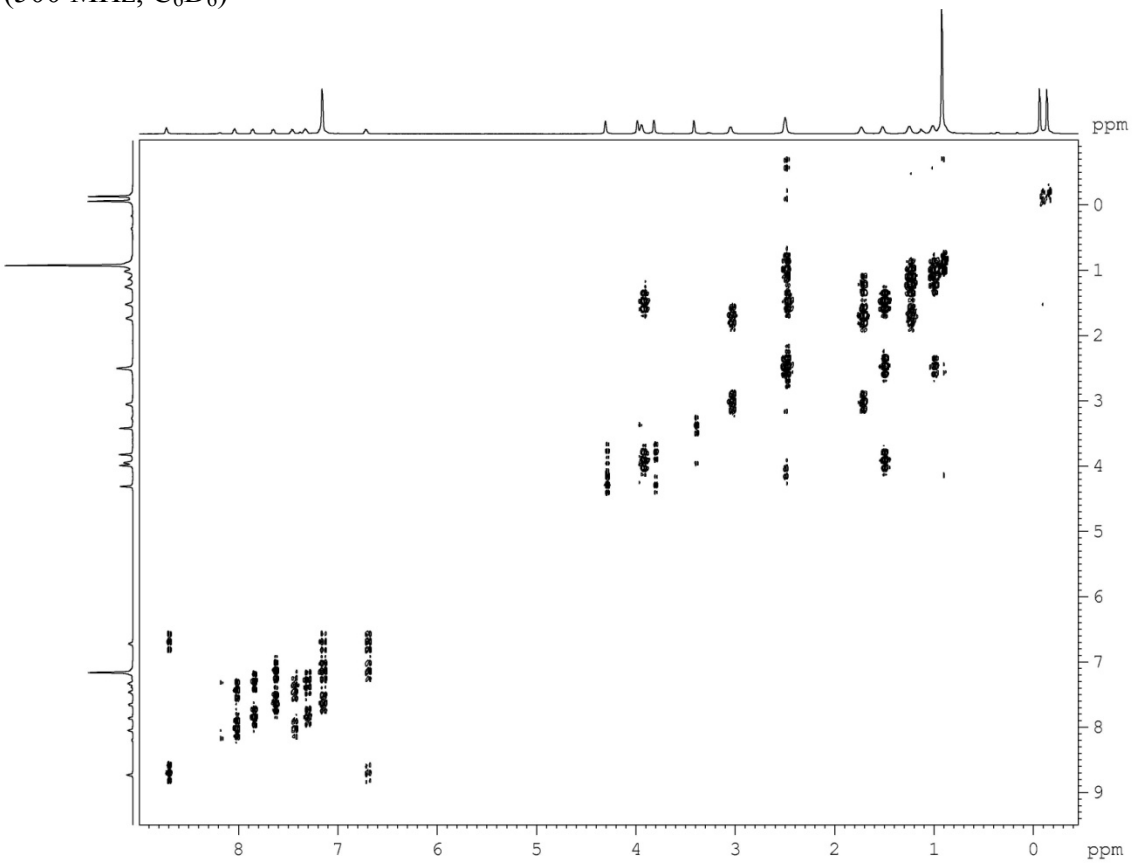
HMQC (126, 500 MHz, C_6D_6)



DEPT (126, 500 MHz, C_6D_6)

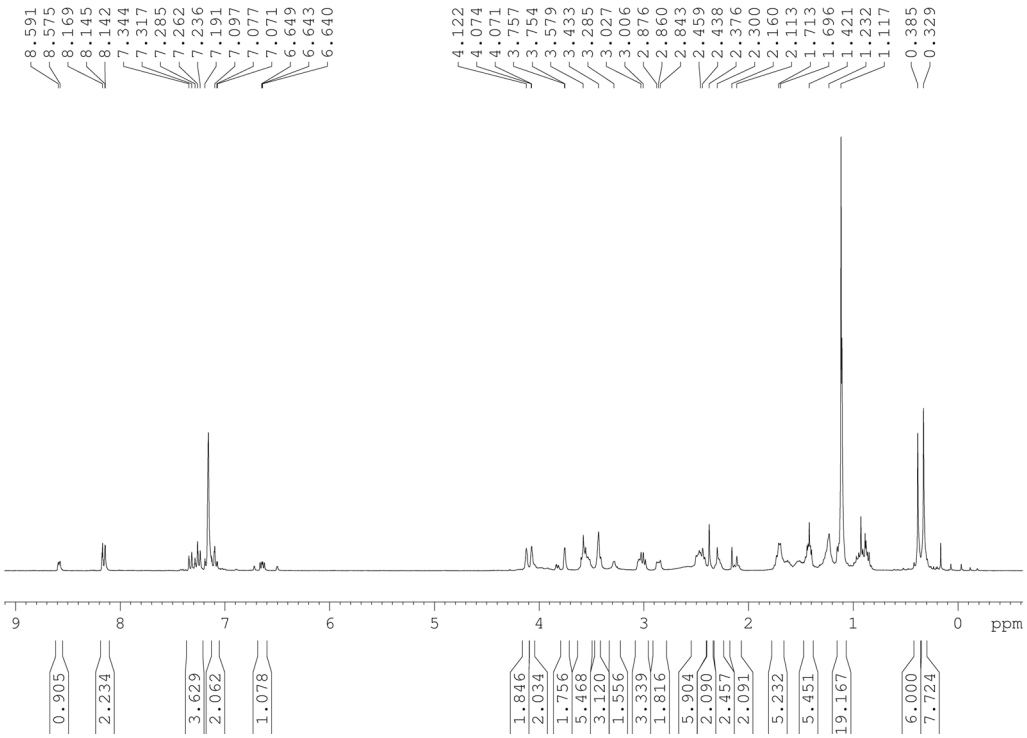


COSY (500 MHz, C_6D_6)

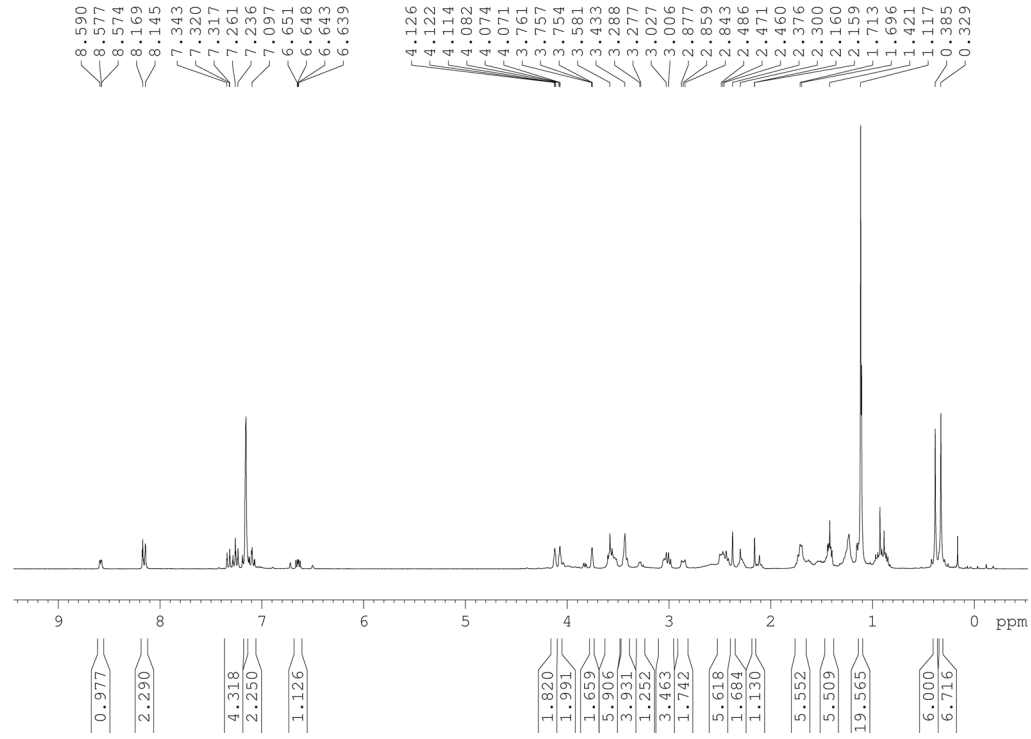


Reaction of 1^{Lu}-py^{Ph} with 2 equiv of DBU

^{1}H NMR (300 MHz, C_6D_6) after 21 hours of heating at 50 ºC. Complete conversion to the product $\mathbf{4}^{Lu}$ is shown, as determined by comparison with the analogous compound $\mathbf{4}^{Y}$.

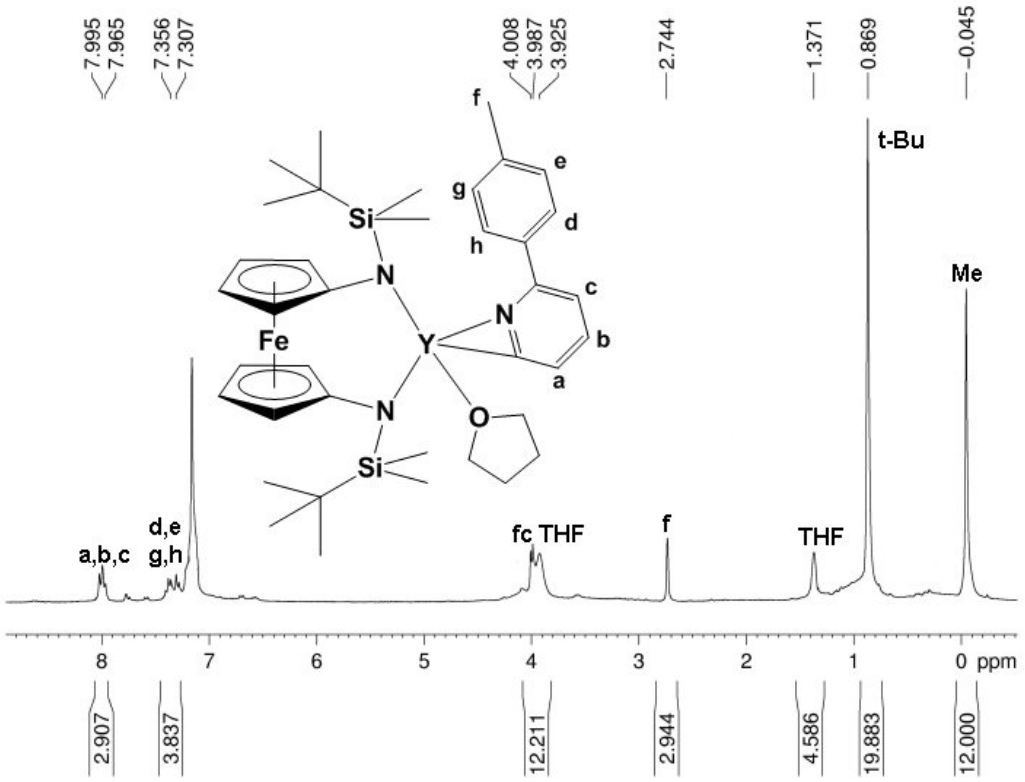


^{1}H NMR (300 MHz, C_6D_6) after 6 days of heating at 50 ºC. No further transformation of $\mathbf{4}^{Lu}$ is observed.

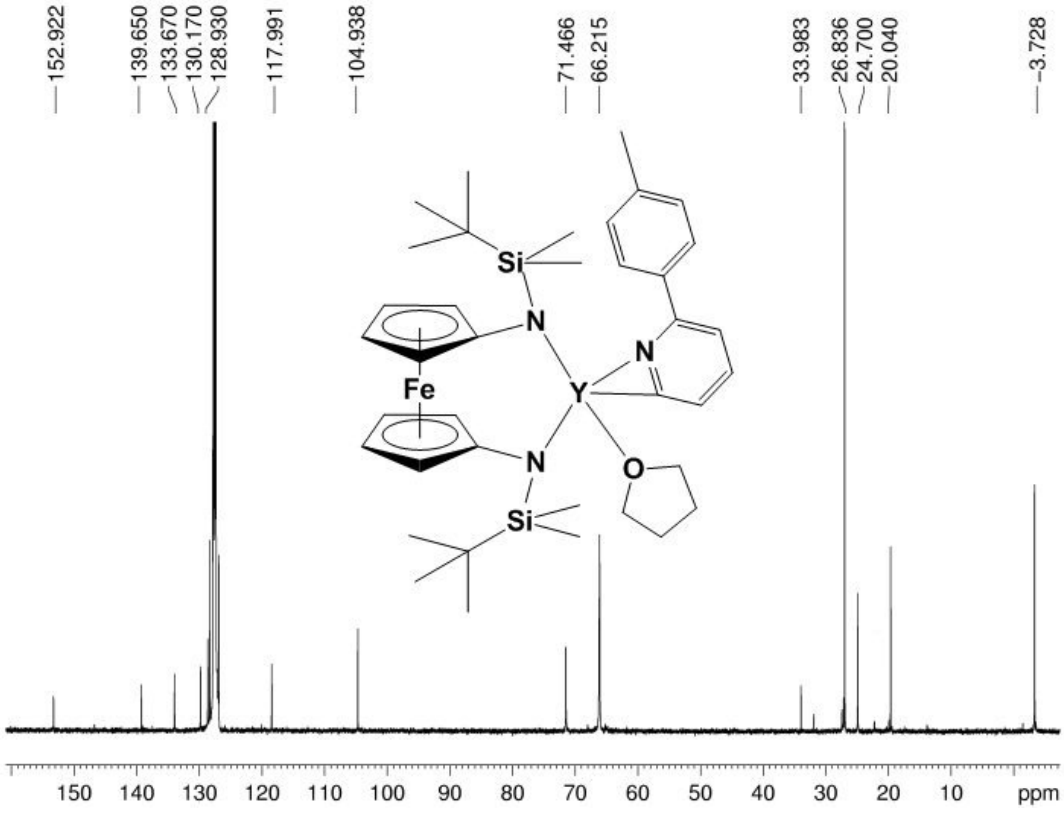


1^{Y}-py^{tol}

^{1}H NMR (500 MHz, C_6D_6)

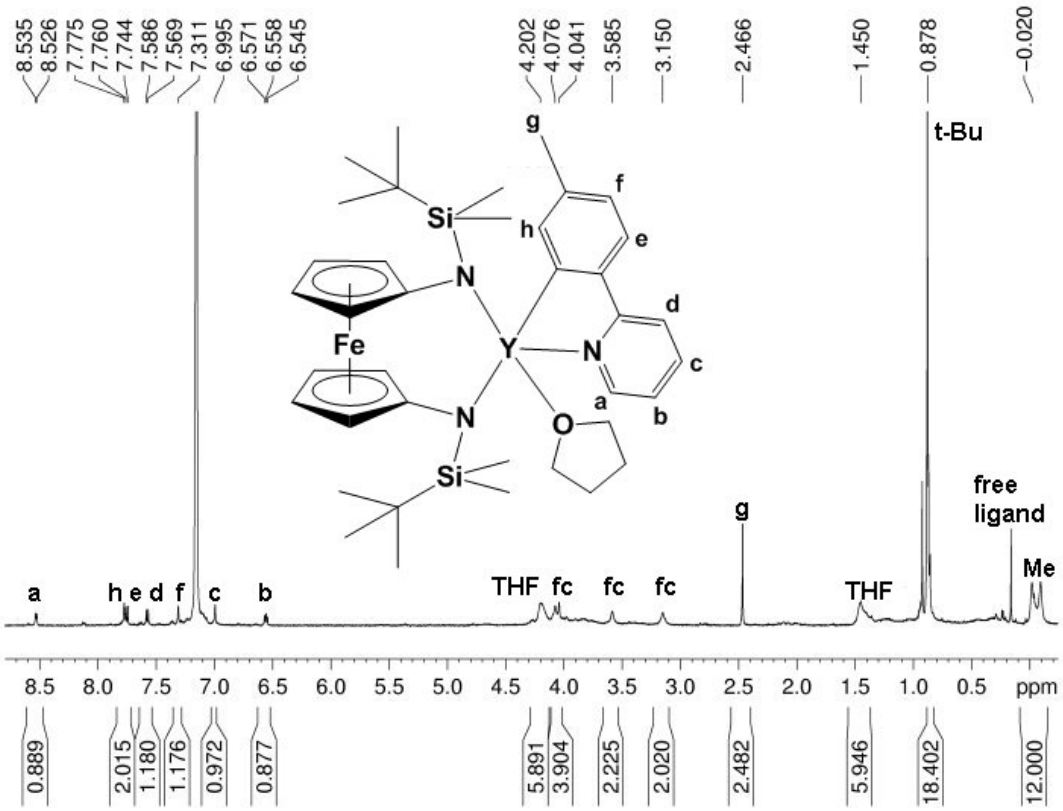


^{13}C NMR (126 MHz, C_6D_6)

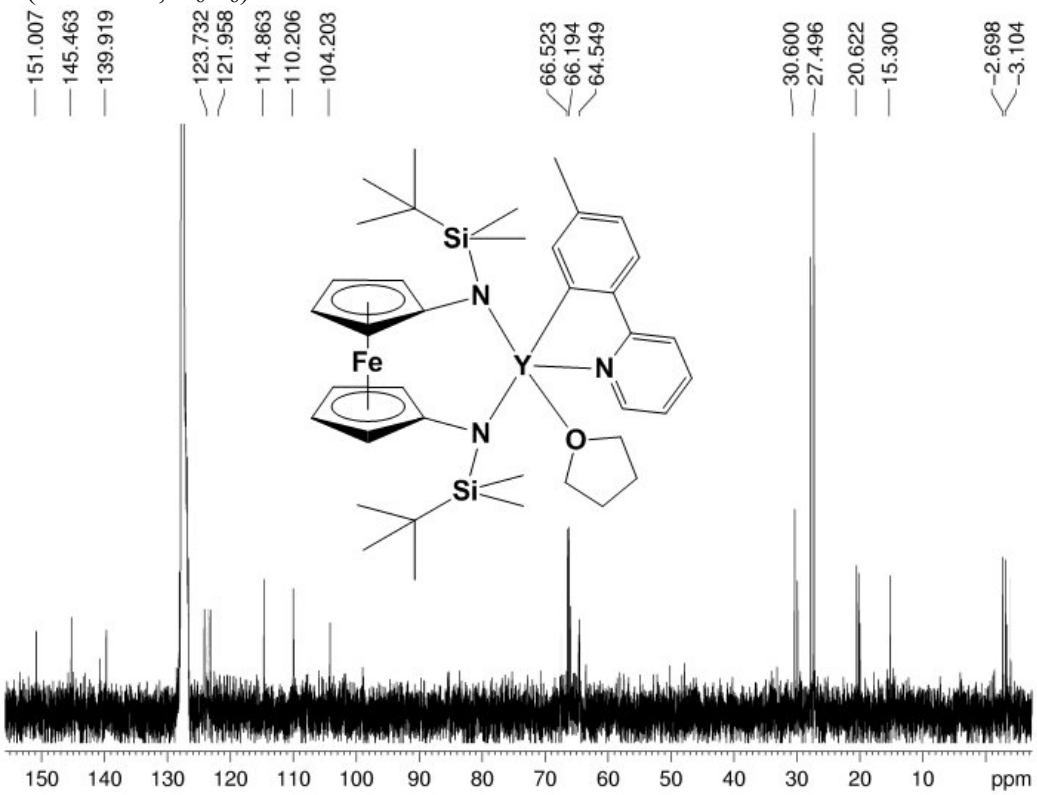


2^{Y}-tolpy

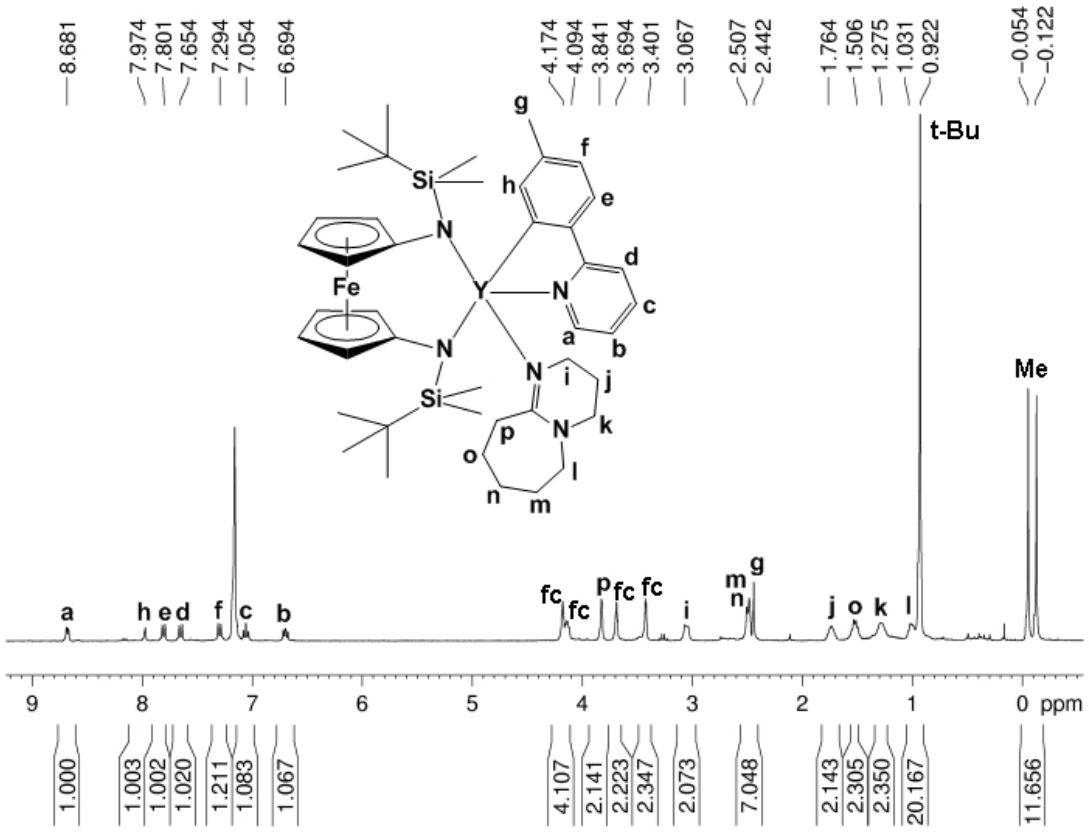
^{1}H NMR (500 MHz, C_6D_6)



^{13}C NMR (126 MHz, C_6D_6)

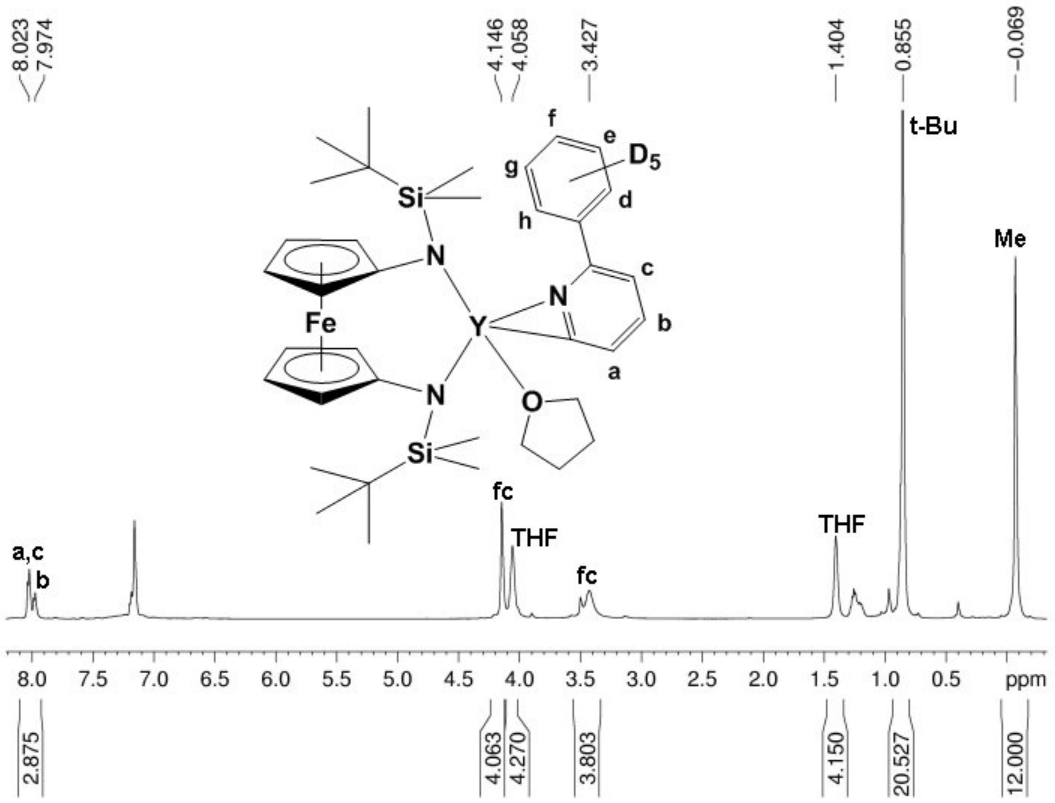


2^{Y}-tolpy-DBU
^{1}H NMR (500 MHz, C_6D_6)

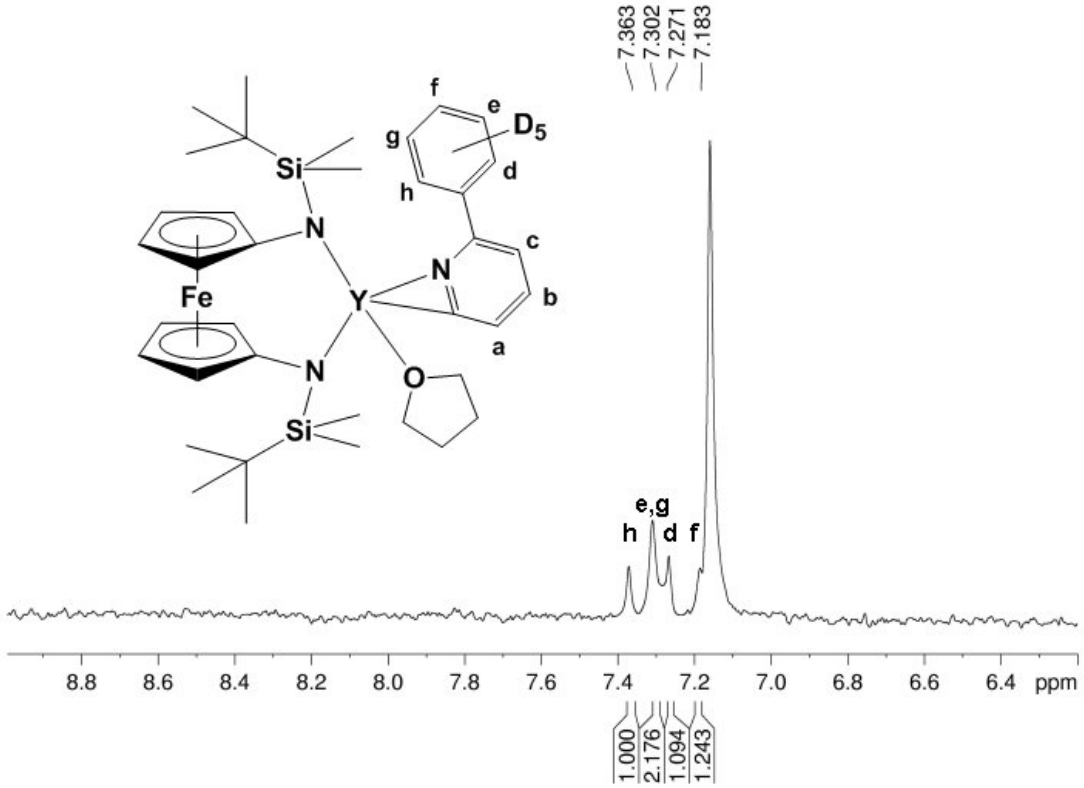


1^{Y}-py^{Ph}-d_5

^{1}H NMR (500 MHz, C_6D_6)

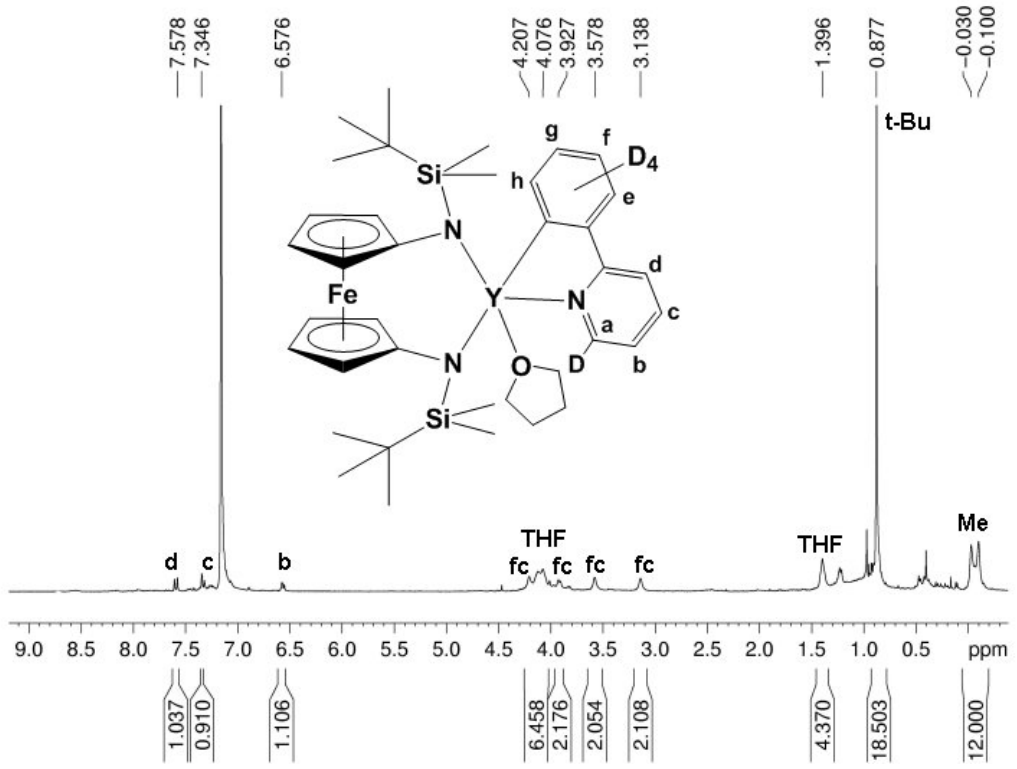


^{2}H NMR (500 MHz, C_6H_6)

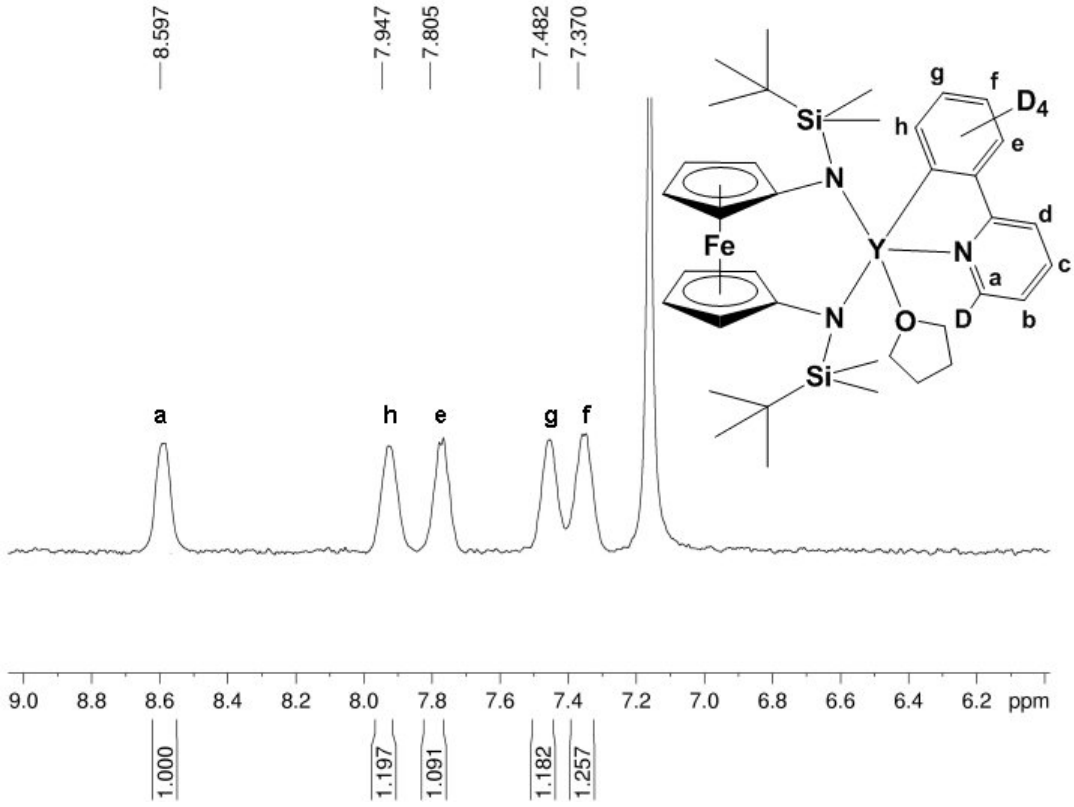


2^{Y}-Phpy-d_5

^{1}H NMR (500 MHz, C_6D_6)

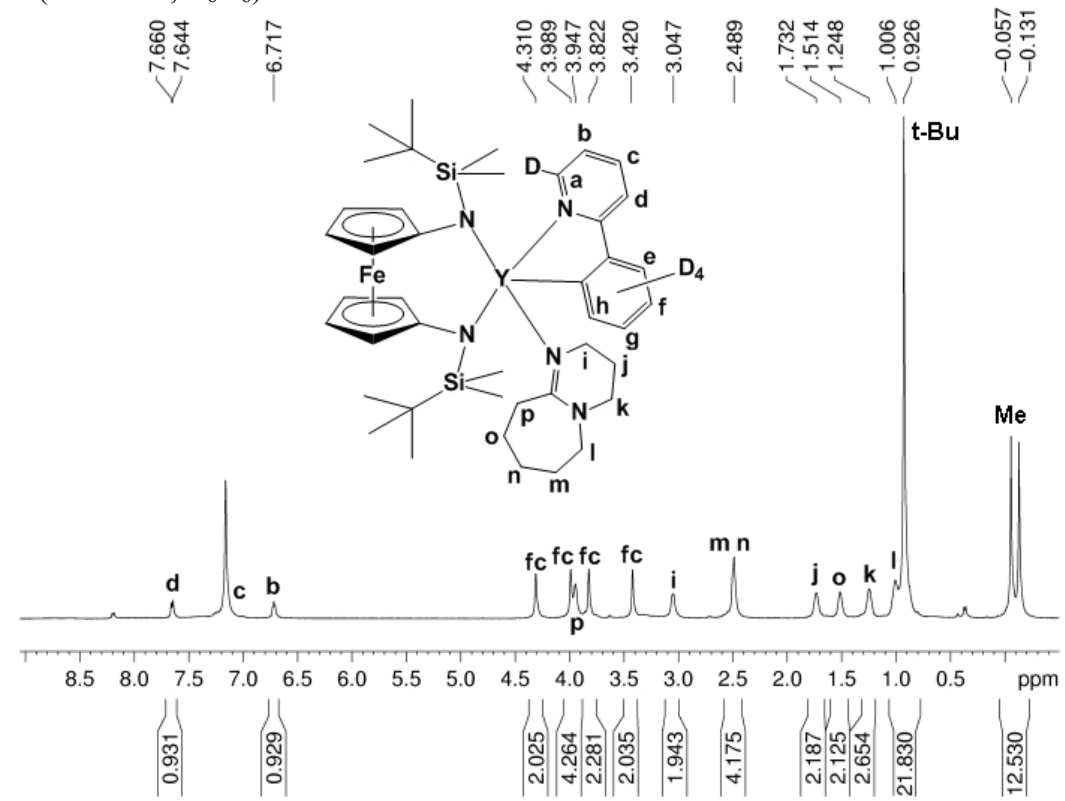


^{2}H NMR (500 MHz, C_6H_6)

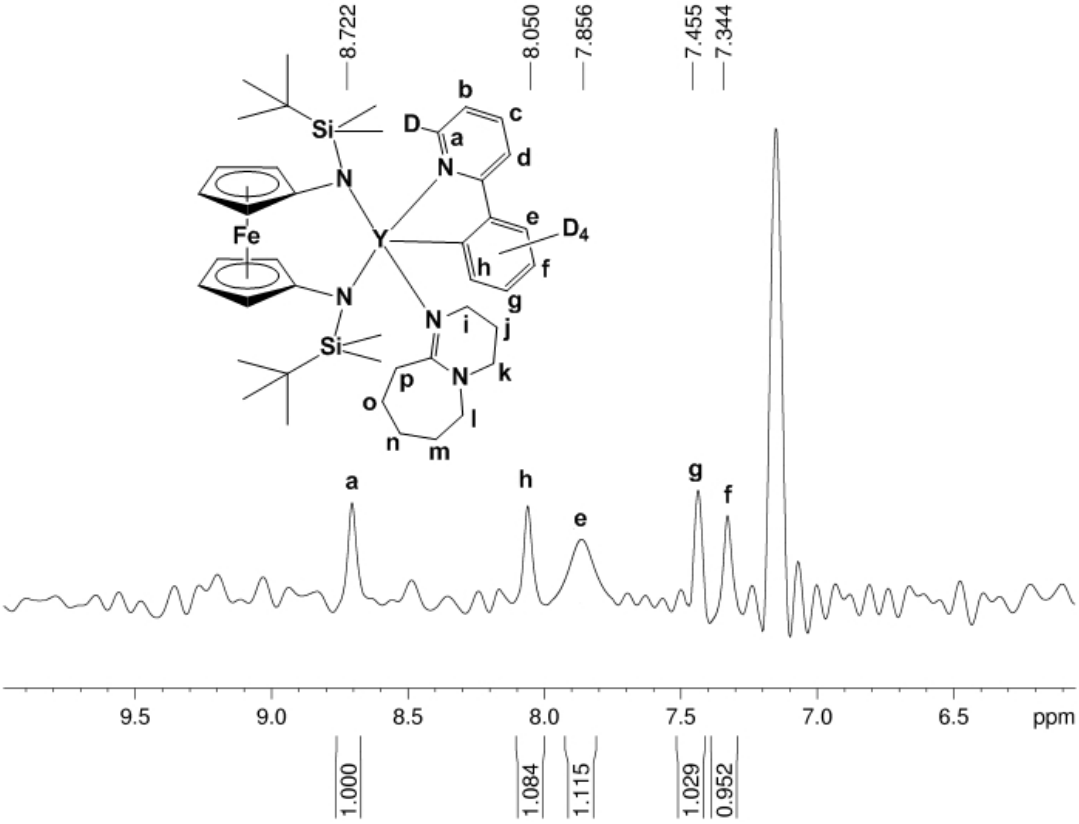


2^{Y}-Phpy-*d*$_5$-DBU

^{1}H NMR (500 MHz, C_6D_6)

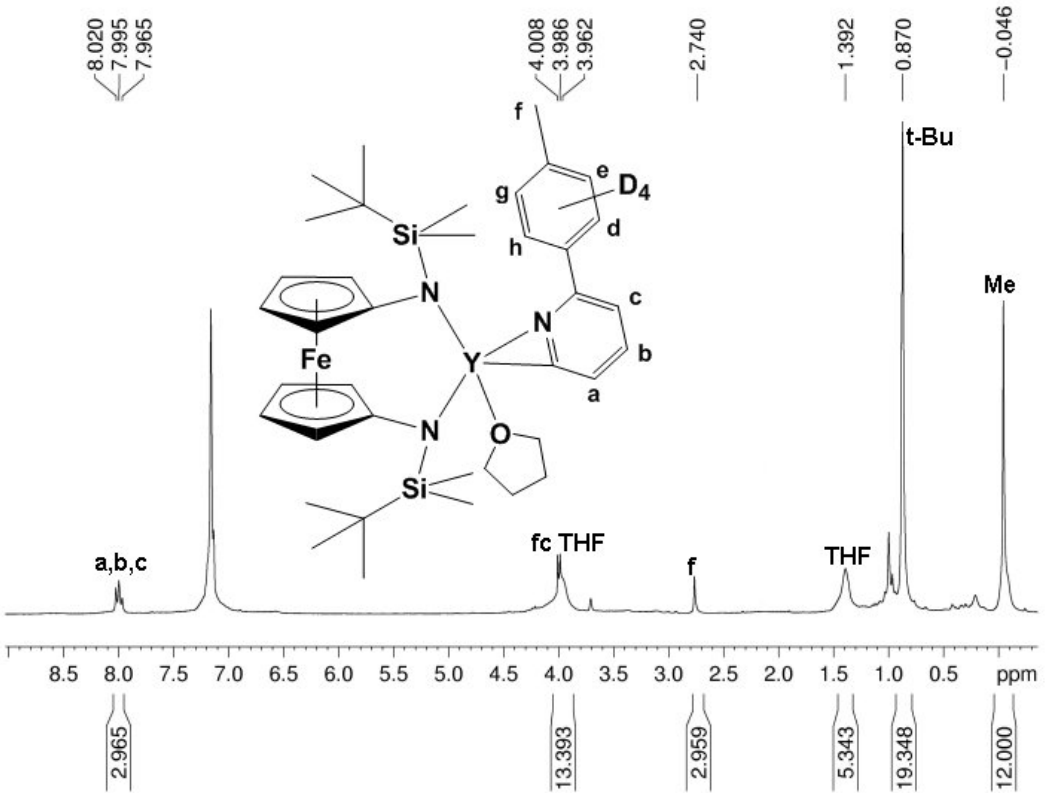


^{2}H NMR (500 MHz, C_6H_6)

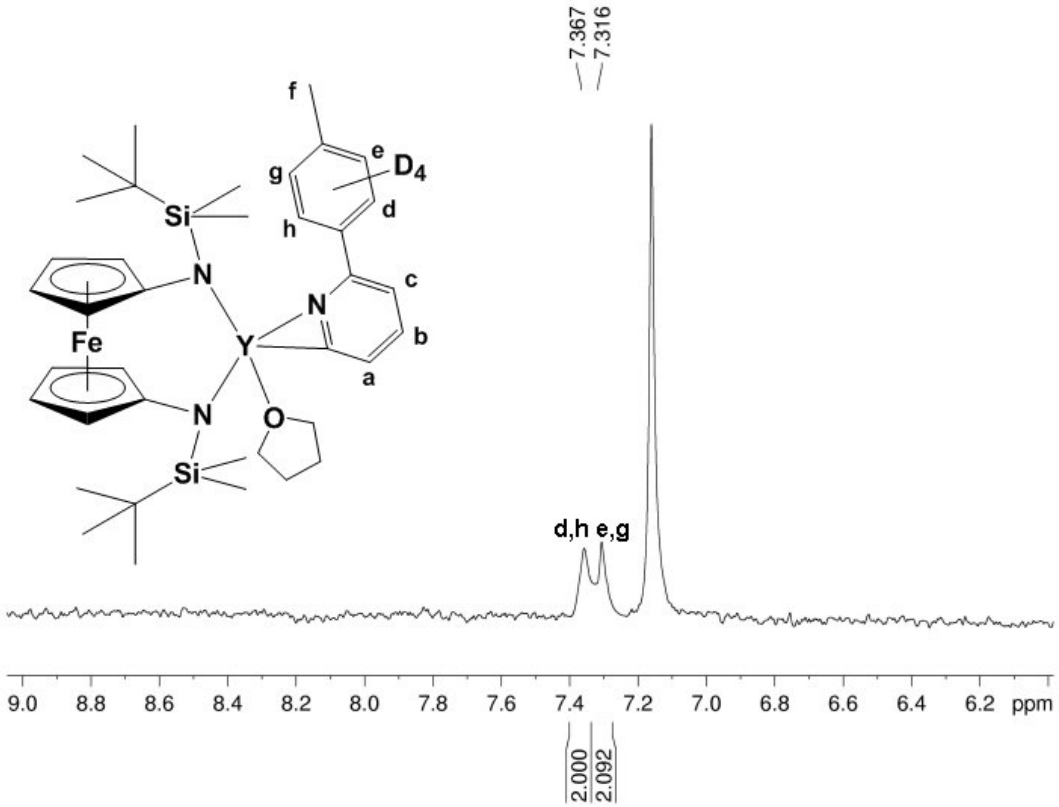


1^{Y}-py^{tol}-*d_4*

^{1}H NMR (500 MHz, C_6D_6)

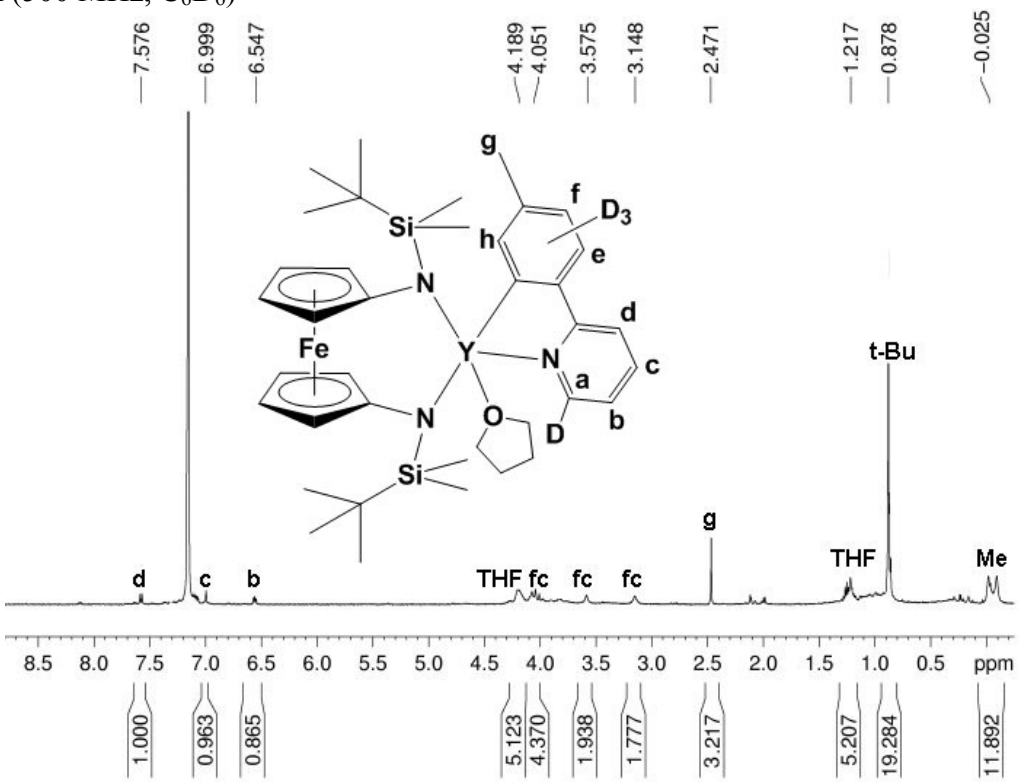


^{2}H NMR (500 MHz, C_6H_6)

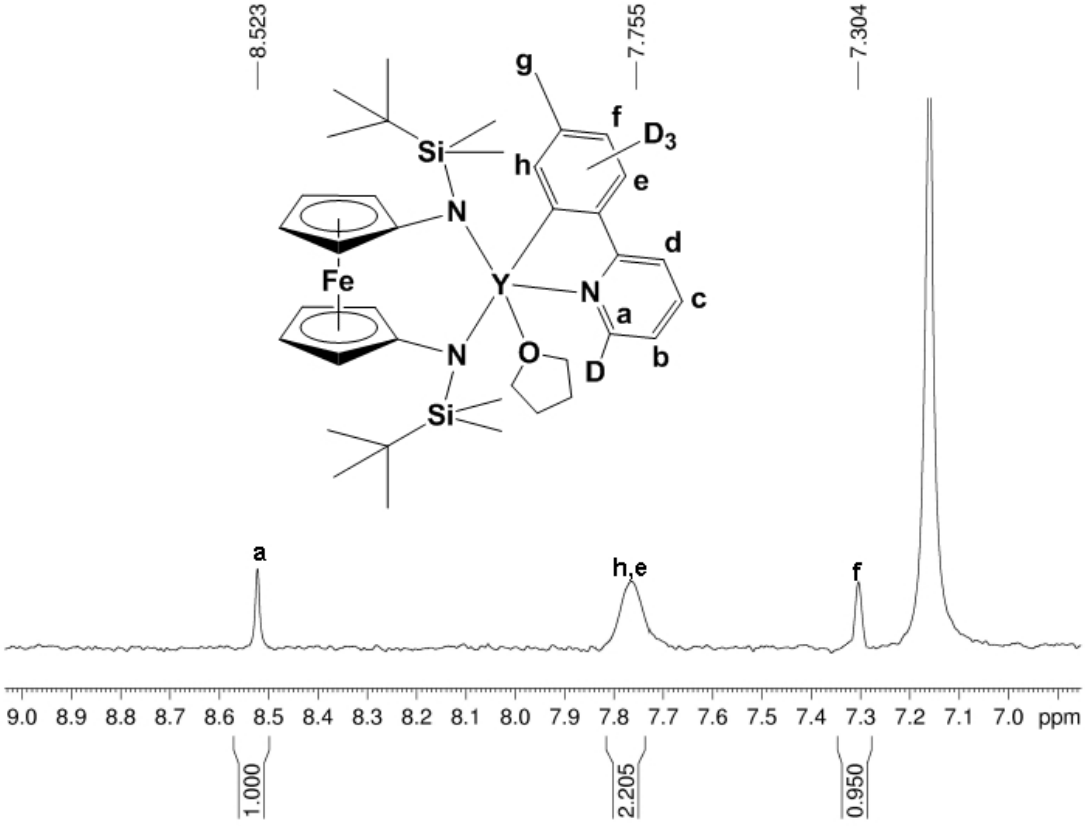


2^{Y}-tolpy-*d*$_4$

^{1}H NMR (500 MHz, C_6D_6)

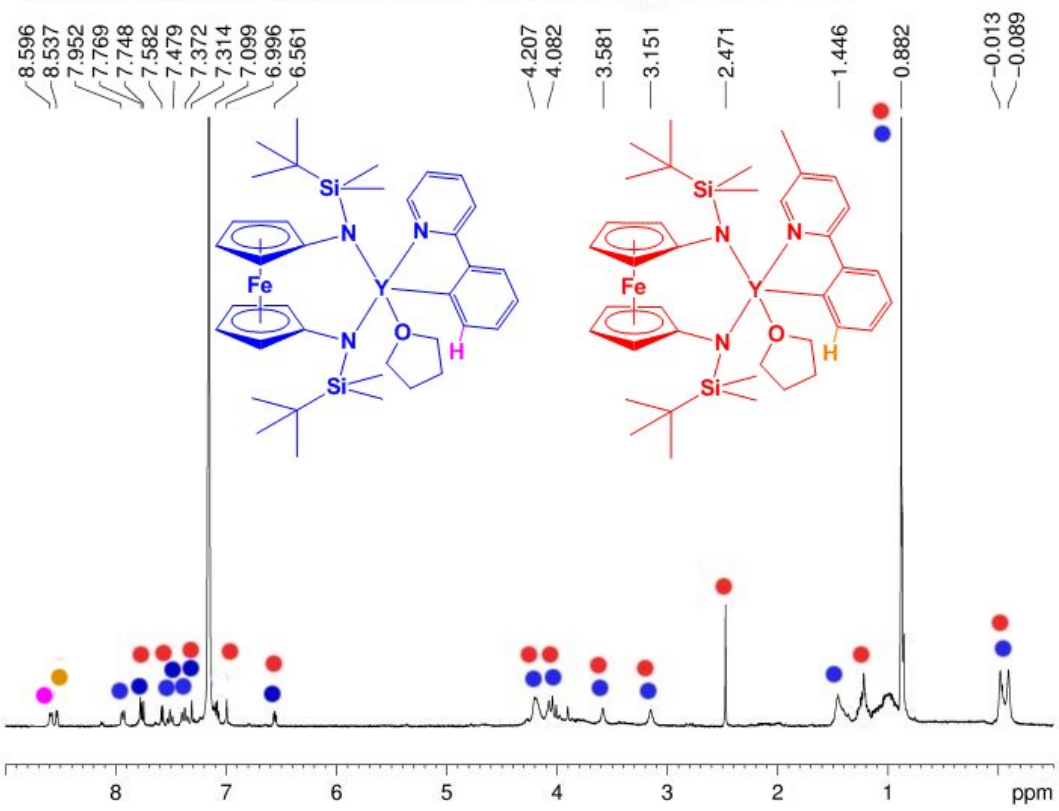


^{2}H NMR (500 MHz, C_6H_6)



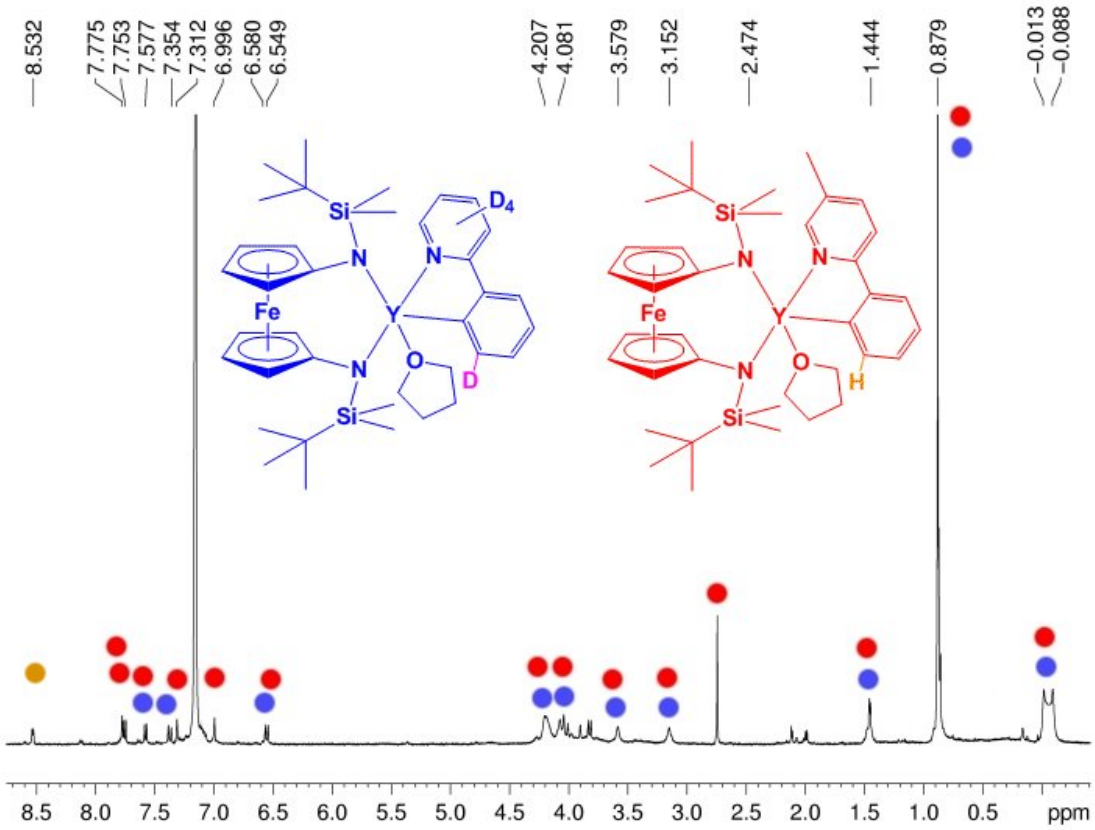
Crossover experiment #1: 1^{Y}-py^{tol} and 1^{Y}-py^{Ph}

^{1}H NMR (500 MHz, C_6D_6)

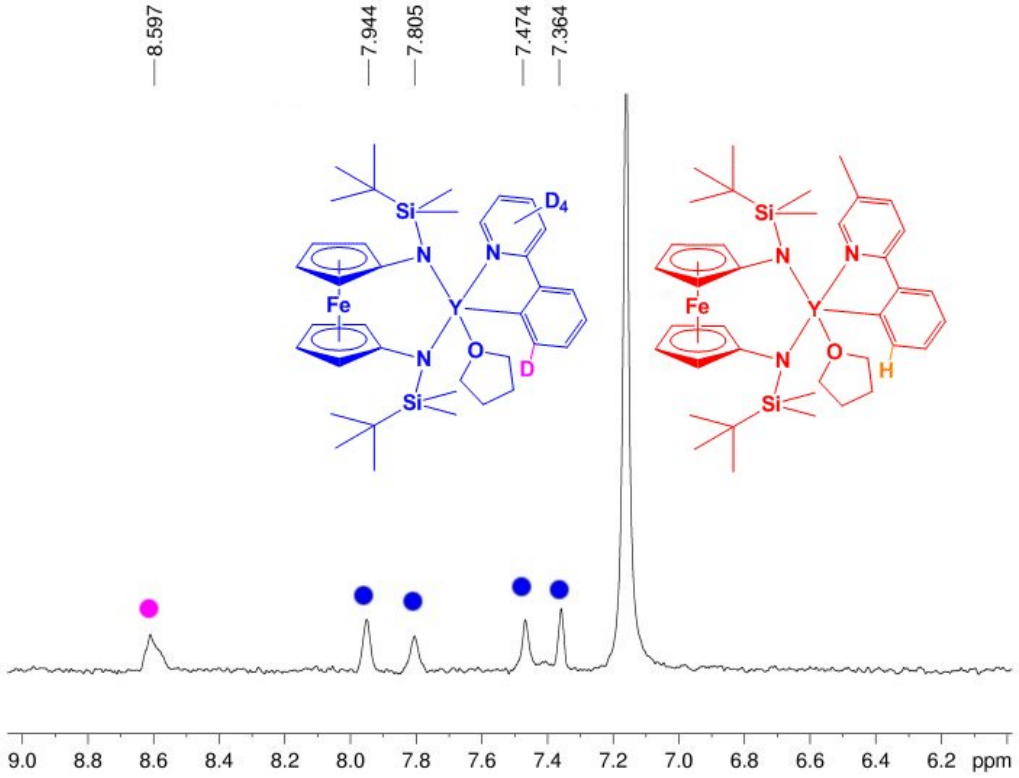


Crossover experiment #2: 1^{Y}-py^{tol} and 1^{Y}-py^{Ph}-d_5

^{1}H NMR (500 MHz, C_6D_6)

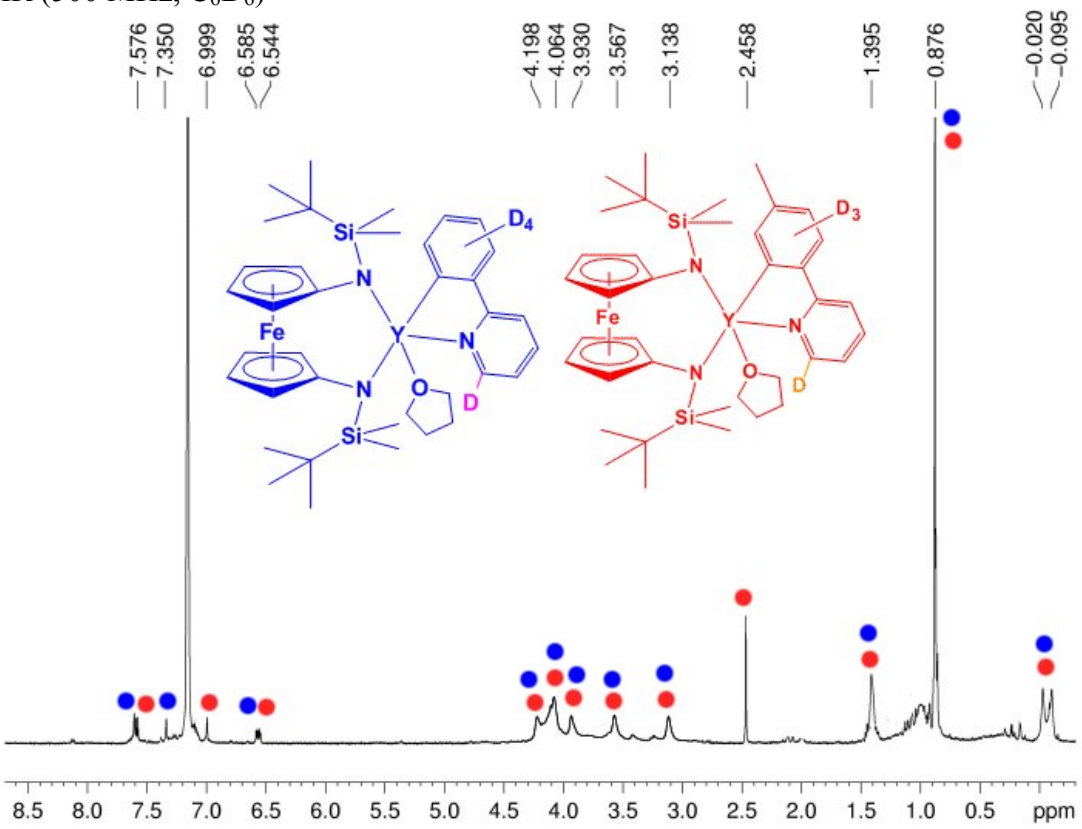


^{2}H NMR (500 MHz, C_6H_6)

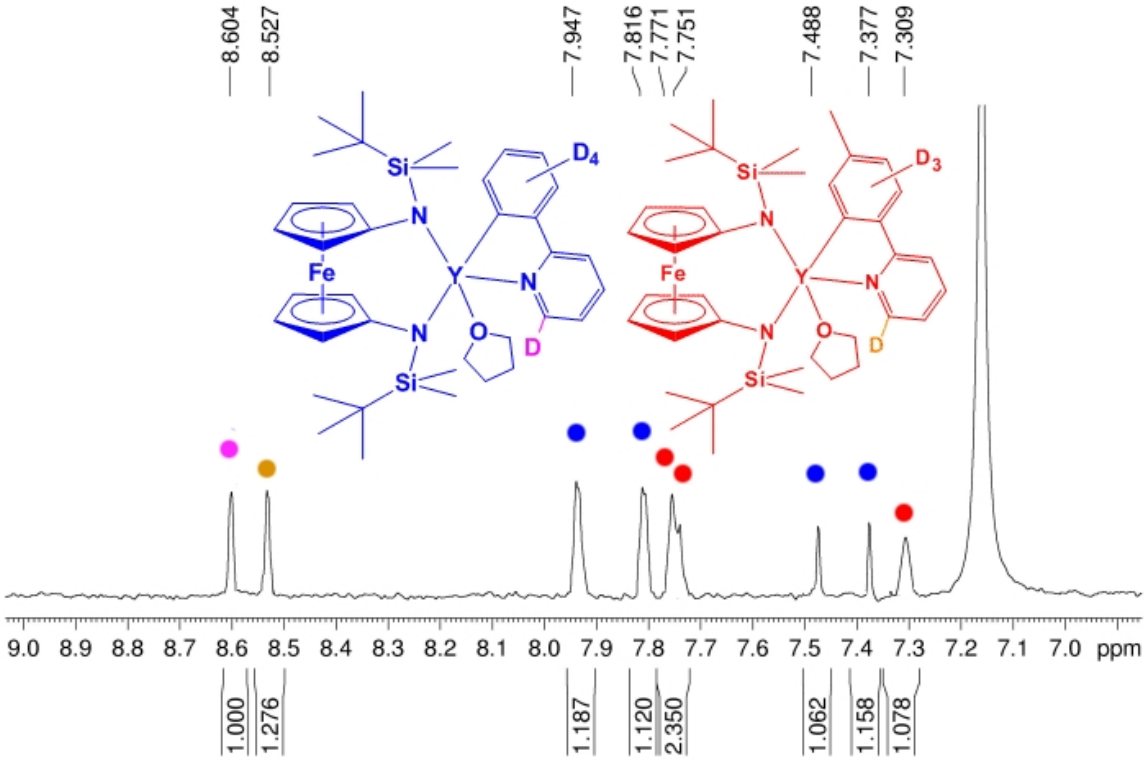


Crossover experiment #3: 1^{Y}-py^{tol}-*d*$_4$ and 1^{Y}-py^{Ph}-*d*$_5$

^{1}H NMR (500 MHz, C_6D_6)

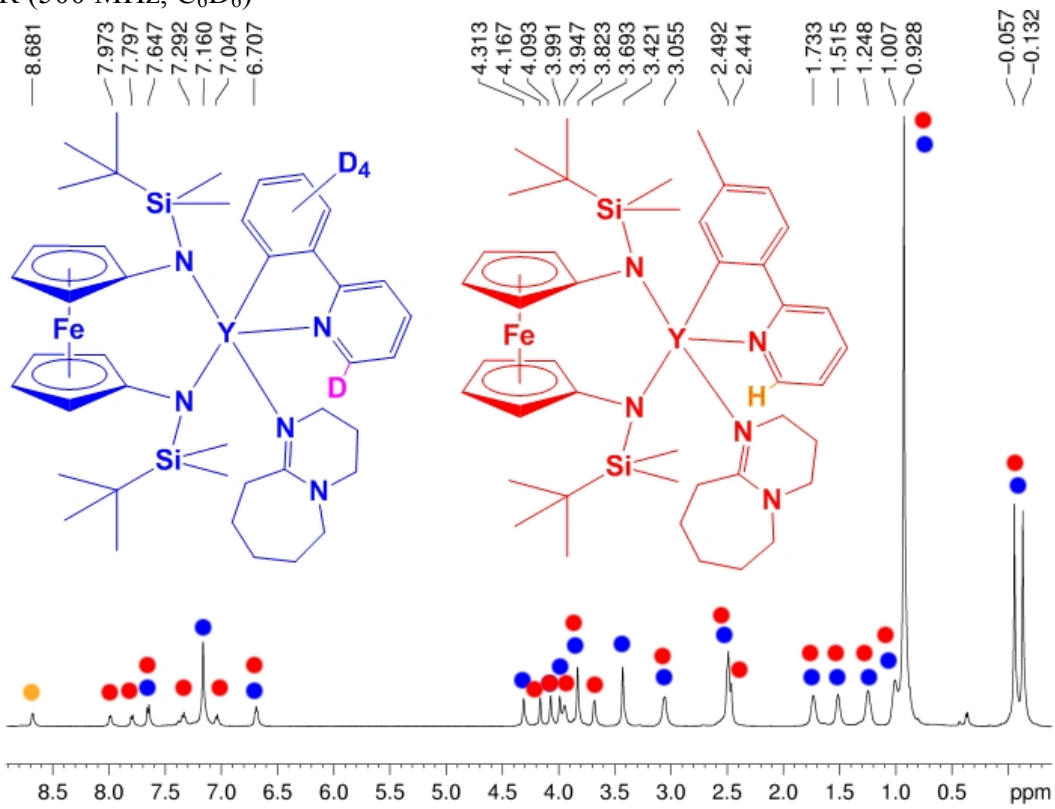


^{2}H NMR (500 MHz, C_6H_6)

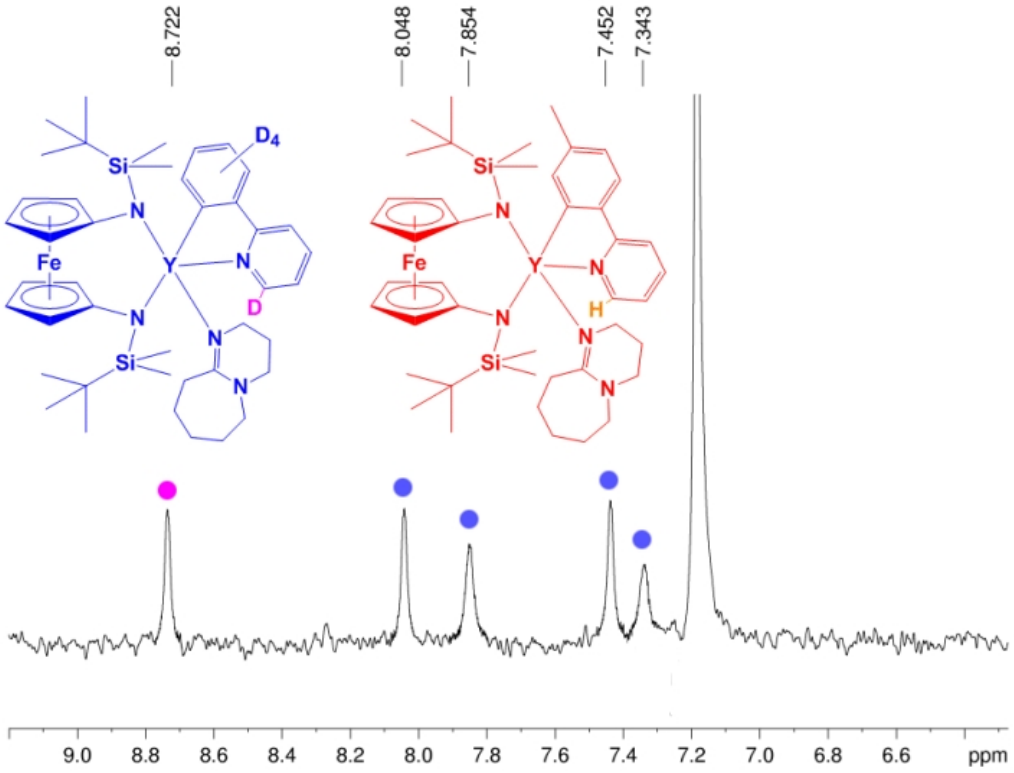


Crossover experiment #4: 1^{Y}-py^{tol} and 1^{Y}-py^{Ph}-d_5 with 4 equiv DBU

^{1}H NMR (500 MHz, C_6D_6)



^{2}H NMR (500 MHz, C_6H_6)



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(1) Pangborn, A.B.; Giardello, M.A.; Grubbs, R.H.; Rosen, R.K.; Timmers, F.J. *Organometallics* **1996**, *15*, 1518.

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(4) Carver, C.T.; Benitez, D.; Miller, K.L.; Williams, B.N.; Tkatchouk, E.; Goddard, W.A.; Diaconescu, P.L. *J. Am. Chem. Soc.* **2009**, *131*, 10269.

X-ray crystal structures. X-ray quality crystals were obtained from various concentrated solutions placed in a -35 °C freezer in the glove box. Inside the glovebox, the crystals were coated with oil (STP Oil Treatment) on a microscope slide, which was brought outside the glove box. The X-ray data collections were carried out on a Bruker AXS single crystal X-ray diffractometer using MoK_α radiation and a SMART APEX CCD detector. The data was reduced by SAINTPLUS and an empirical absorption correction was applied using the package SADABS. The structures were solved and refined using SHELXTL (Brucker 1998, SMART, SAINT, XPREP AND SHELXTL, Brucker AXS Inc., Madison, Wisconsin, USA). All atoms were refined anisotropically and hydrogen atoms were placed in calculated positions unless specified otherwise. Tables with atomic coordinates and equivalent isotropic displacement parameters, with all the bond lengths and angles, and with anisotropic displacement parameters are listed in the cifs.

X-ray crystal structure of 2^{Y}-Phpy-iqn. X-ray quality crystals were obtained from a concentrated hexanes solution. A total of 10980 reflections ($-24 \le h \le 24$, $-16 \le k \le 16$, $-27 \le l \le 27$) was collected at T = 100(2) K with $2\theta_{max}$ = 56.45°, of which 8150 were unique (R_{int} = 0.0531). The residual peak and hole electron density were 0.99 and -0.71 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0429 and GOF = 1.016. Crystal and refinement data for **2^{Y}-Phpy-iqn**: formula $C_{43}H_{55}N_4Si_2FeY \cdot C_5$, space group $P2_1/c$, a = 18.311(2), b = 12.1533(14), c = 20.892(3), β = 103.439(1)°, V = 4522.0(9) $Å^3$, Z = 4, μ = 1.687 mm^{-1}, F(000) = 1856, R_1 = 0.0656 and wR_2 = 0.1061 (based on all 10980 data).

X-ray crystal structure of 3. X-ray quality crystals were obtained from a concentrated hexanes solution. A total of 27285 reflections ($-33 \le h \le 33$, $-22 \le k \le 22$, $-37 \le l \le 37$) was collected at T = 100(2) K with $2\theta_{max}$ = 56.14°, of which 17239 were unique (R_{int} = 0.0800). The residual peak and hole electron density were 1.09 and -0.99 eA^{-3}. One of the silyl group was disordered over two sites and this disorder was modeled. One of the disordered carbon counterparts was only refined isotropically. The solvent molecules were disordered; this disorder was not modeled. The least-squares refinement converged normally with residuals of R_1 = 0.0530 and GOF = 1.008. Crystal and refinement data for **3**: formula $2(C_{53}H_{74}N_3O_2Si_2FeY \cdot (C_4H_9, C_5H_{12}, CH_3)$, space group $P2_1/n$, a = 25.084(2), b = 17.1073(15), c = 28.101(3), β = 110.800(1)°, V = 11272.8(17) $Å^3$, Z = 4, μ = 1.366 mm^{-1}, F(000) = 4512, R_1 = 0.0978 and wR_2 = 0.1284 (based on all 27285 data).

X-ray crystal structure of 5. X-ray quality crystals were obtained from a concentrated toluene solution layered with *n*-pentane. A total of 32436 reflections ($-24 \le h \le 24$, $-28 \le k \le 28$, $-25 \le l \le 25$) was collected at T = 100(2) K with $2\theta_{max}$ = 56.78°, of which 9039 were unique (R_{int} = 0.1152). The residual peak and hole electron density were 2.06 and -2.79 eA^{-3}. Some carbon atoms of the coordinated DBU were disordered over two sites and this disorder was modeled. Two of the disordered carbon counterparts were only refined isotropically. The solvent molecule (*n*-pentane) sits in a special position and was disordered; this disorder was not modeled. The least-squares refinement converged normally with residuals of R_1 = 0.0734 and GOF = 1.128. Crystal and refinement data for **5**: formula $C_{62}H_{104}N_8OSi_4Fe_2Lu_2 \cdot (C_5H_6, 2(H))$, space group $C2/c$, a = 18.664(4), b = 21.774(4), c = 18.892(4), β = 107.578(3)°, V = 7319(3) $Å^3$, Z = 4, μ = 3.173 mm^{-1}, F(000) = 3312, R_1 = 0.1185 and wR_2 = 0.1576 (based on all 9039 data).

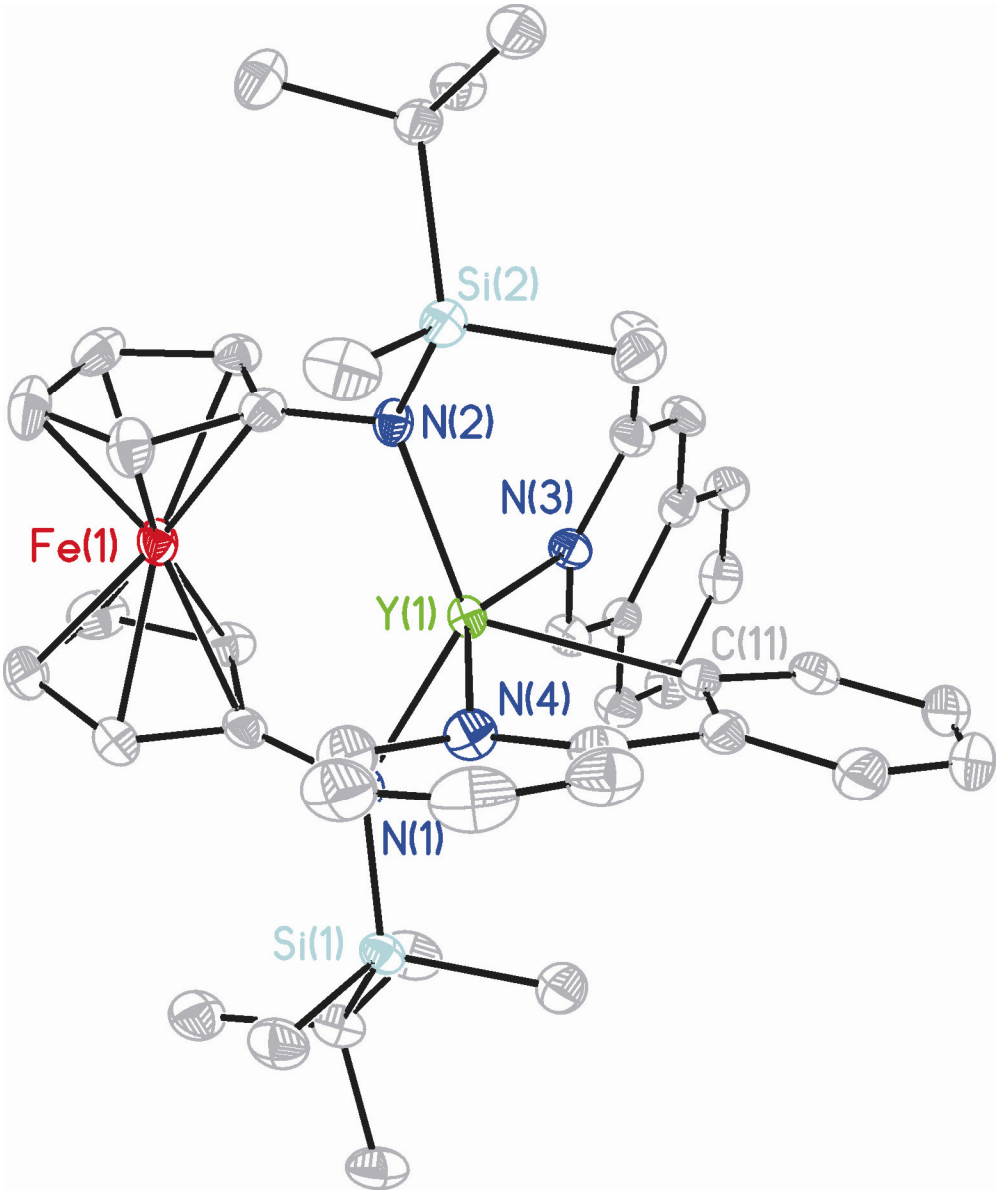

Figure SX1. Thermal-ellipsoid (50% probability) representation of **2^{Y}-Phpy-iqn**; hydrogen and solvent atoms omitted for clarity.

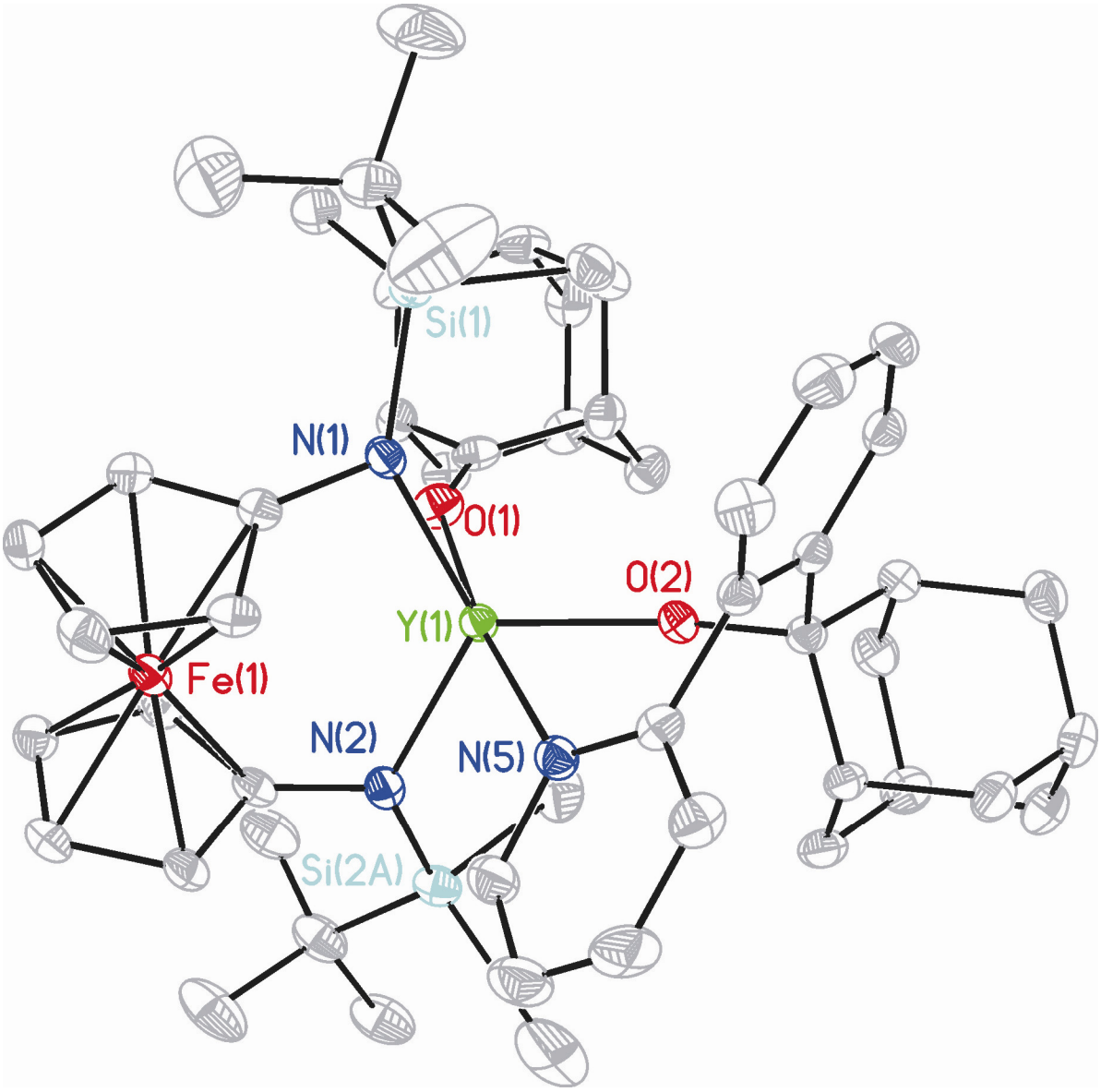

Figure SX2. Thermal-ellipsoid (50% probability) representation of **3**. Only one of the two independent molecules in the unit cell is shown. Hydrogen, disordered counterparts, and solvent atoms were omitted for clarity.

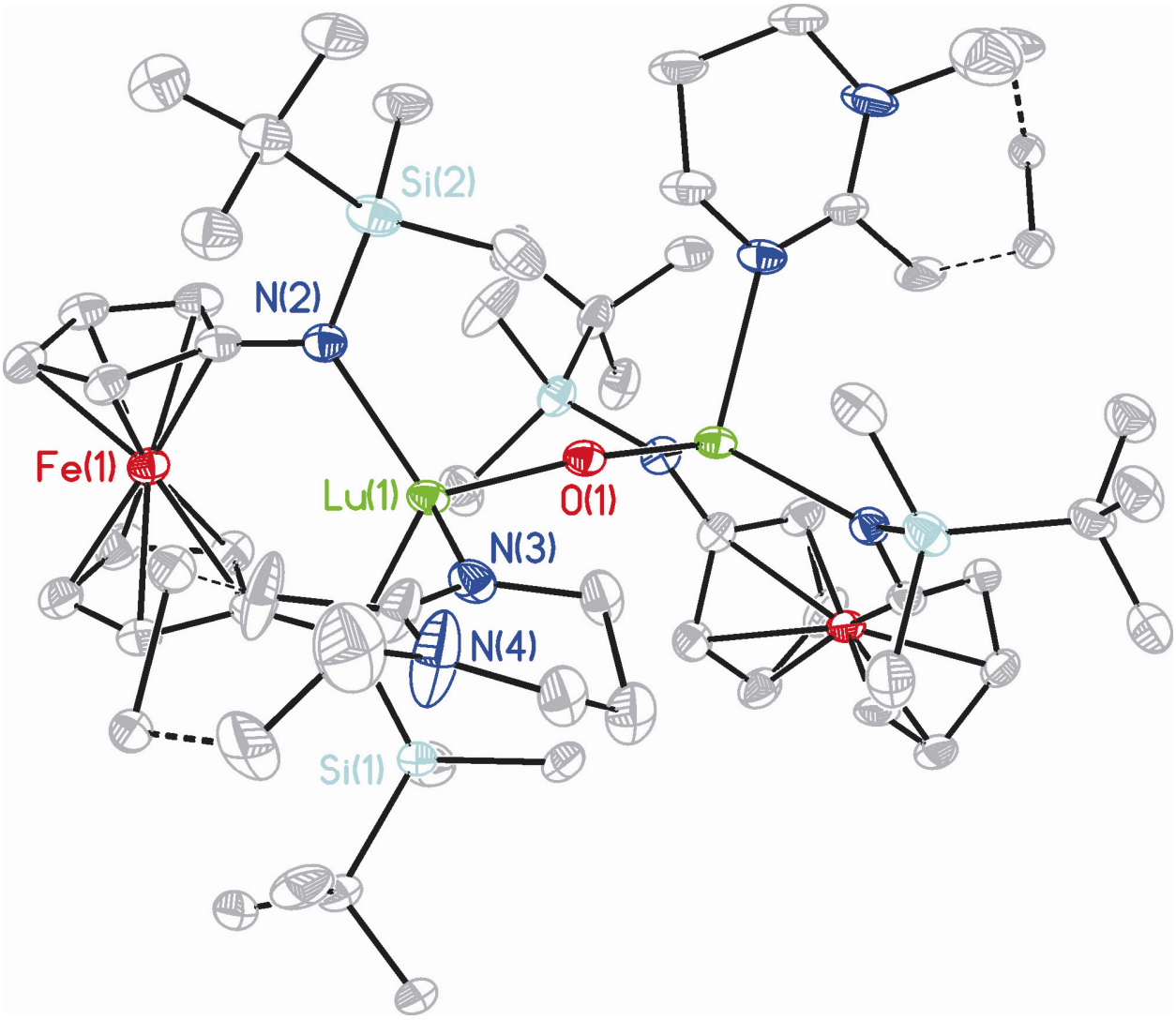

Figure SX3. Thermal-ellipsoid (35% probability) representation of **5**. Hydrogen, disordered counterparts, and solvent atoms were omitted for clarity.

Computational Details

Methods

Calculations were performed using density functional theory (DFT) with the B3LYP functional, as implemented in Jaguar 7.6.[1] All calculations used the Hay and Wadt small core-valence relativistic effective-core-potential[2] (ECP). The LACVP** basis set was used for all geometry optimizations and LACV3P++** for energies. For Y, the LACV3P++**(2f) basis set was employed as implemented in Jaguar with an extra double-ζ f-shell using coefficients reported by Martin and Sundermann.[3] All electrons for all other atoms were described using the 6-31G** or 6-311++G** basis sets.[4,5] Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for benzene (ε =2.284 and R^0=2.60 Å) using the PBF[6] module in Jaguar.

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6. Tannor, D. J. et al. J. Am. Chem. Soc. 1994, 116, 11875–11882.

XYZ coordinates B3LYP/LACVP** geometry optimization

1^{Y}-py^{Ph}

Y1	8.9142850619	9.9710820127	18.2825140802
Fe2	11.5041075432	9.7959166917	19.9593474297
Si3	10.6359460776	8.6626292857	15.3082136065
Si4	9.1111678484	13.5838794514	18.7449999612
N5	9.2271958368	11.9534867771	19.3384379604
N6	7.1671550496	8.5455324168	18.9918250838
N7	10.5281962727	9.1839520785	16.9686770886
C8	5.2920760364	9.1415092892	17.6566140773
H9	4.8595920643	9.7141208653	16.8406430010
C10	6.6555540357	9.2868266398	17.9677245364
C11	6.4252460157	7.6843674429	19.7304142727
C12	4.4998780627	8.2733155806	18.4027568389
H13	3.4421870309	8.1550310579	18.1774122942
C14	5.0661921510	7.5374655305	19.4490685554
H15	4.4695886283	6.8363891501	20.0235945590
C16	9.7326306693	10.2044902245	21.0471256387
H17	8.7607173758	9.7208428855	21.0682715482
C18	10.8314481392	9.8673629324	21.9027941834
H19	10.8664449765	9.0346801844	22.5913855716
C20	11.5374947642	9.0210861689	17.9320699445
C21	10.0470354085	11.4239727758	20.3186589489
C22	12.6475592266	9.8933120953	18.2153356191
H23	12.8562435831	10.8157134603	17.6917242302
C24	11.4016799605	11.7514851463	20.6874698597
H25	11.9753099924	12.5682163550	20.2745632809
C26	13.4041446531	9.3503918926	19.2967236231
H27	14.2920934880	9.7875457726	19.7337694215
C28	12.7549670673	8.1561201579	19.7350387726
H29	13.0661745045	7.5301540157	20.5607061034
C30	11.6063213308	7.9614795534	18.9182440123
H31	10.9124688593	7.1344377124	18.9759975665
C32	11.8478264097	10.8421676348	21.6961722590
H33	12.8149039423	10.8629710101	22.1804167955
C34	8.0155147498	14.6644150027	19.9095549963
C35	8.6905755432	14.7793985208	21.2940512559
H36	8.0630369628	15.3651629692	21.9812956805
H37	9.6629969472	15.2827249698	21.2379404510
H38	8.8487058924	13.7970271857	21.7531356165
C39	10.7857235011	14.4515797259	18.4853270535
H40	11.4611124967	13.8220272244	17.8945174114
H41	11.2905578691	14.6885520619	19.4282414452
H42	10.6572484707	15.3947727314	17.9409085461
C43	6.6334280670	14.0008232293	20.0870072572
H44	6.0088619383	14.5878156709	20.7758377192
H45	6.7251253807	12.9899325476	20.4981453840
H46	6.0890441131	13.9266247409	19.1377599902
C47	7.8258830670	16.0807117393	19.3253744565
H48	7.2021308708	16.6923100890	19.9937850244
H49	7.3275239708	16.0608240365	18.3485937608
H50	8.7796539820	16.6074638847	19.2029446812
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H53	8.0446052316	14.3703886311	16.5945719550
H54	7.3609148565	12.8220627683	17.0916510246
C55	11.1499540817	6.8376462037	15.2075910959
H56	10.3821577456	6.2004969350	15.6613679551
H57	12.0868715520	6.6572769461	15.7464194975
H58	11.2921838114	6.5001209715	14.1744487160
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H60	14.0126120571	9.9990813034	13.9866933161
H61	13.5641040407	8.3362796236	14.3808772047
H62	13.5551952970	9.5746684319	15.6413811627
C63	11.8584165458	9.7195806371	14.2383096891
C64	11.6363128490	9.4159764340	12.7395247745
H65	12.3509537713	9.9813849452	12.1239706236
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H67	11.7822703759	8.3541558933	12.5072441113
C68	8.8824613927	8.8564426924	14.6048545679
H69	8.5688165998	9.9062296322	14.5478672265
H70	8.1504748591	8.3267225994	15.2257759579
H71	8.8111413716	8.4436694333	13.5924052702
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H75	10.5896549407	11.5196086171	14.2148222017
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C77	6.4586133908	6.7021620211	22.0430585217
H78	5.4695334558	7.1165715185	22.2177621726
C79	8.3839563342	6.4011892867	20.6171758164
H80	8.8718553414	6.5489923966	19.6598673037
C81	9.0214619261	5.6832052292	21.6269703380
H82	10.0154352498	5.2786536216	21.4563510240
C83	8.3820700451	5.4777825930	22.8509418400
H84	8.8799753688	4.9216444059	23.6403957168
C85	7.0992395439	5.9889505096	23.0551391657
H86	6.5994693709	5.8393040139	24.0081845156

TS 1

Y1	8.8278268897	9.8768704922	17.9714861206
Fe2	11.0631410108	9.4822420871	20.0194391932
Si3	11.2238025529	8.8476556067	15.2357671877
Si4	9.3215416026	13.5052074991	18.5412212164
N5	9.1539147445	11.8539697774	19.0716388591
N6	6.5417874598	10.0867347785	17.4124549587
N7	10.6317134540	9.1380401591	16.8556913401
C8	5.8381975413	9.1006105489	15.3639920395
H9	6.0447356709	8.5675485866	14.4411640857
C10	6.8682440663	9.4551175440	16.2417201910
C11	5.4367200337	9.5867610894	17.9903447269
C12	4.5049643800	9.2868599908	15.8002357924
H13	3.6664256732	9.1177137562	15.1291447152
C14	4.2920074706	9.3873439267	17.1766793294
H15	3.3347217145	9.1147005914	17.6105004138
C16	9.2069354017	10.0816860255	20.8315965437
H17	8.1954498539	9.7081386416	20.7074451637
C18	10.1203922084	9.6420264001	21.8432808397
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C21	9.7548830512	11.2517566335	20.1605564292
C22	12.5330181235	9.4697230522	18.5515031628
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C24	11.0647614704	11.4394233352	20.7352799463
H25	11.7791199887	12.1839914495	20.4168610430
C26	12.9681563312	8.7639999491	19.7129658328
H27	13.8031129030	9.0349931475	20.3453570124
C28	12.0743043769	7.6714650256	19.9284903365
H29	12.1164701690	6.9661599008	20.7472758531
C30	11.1021826491	7.6968079703	18.8901424287
H31	10.3046211326	6.9818341452	18.7449067338
C32	11.2544654047	10.5009595768	21.7960159589
H33	12.1346738307	10.4235077170	22.4198039283
C34	8.3289674244	14.7105967126	19.6795987598
C35	8.8710563705	14.6406566070	21.1240536251
H36	8.3038711570	15.3161795264	21.7810468418
H37	9.9235652381	14.9421016380	21.1847839006
H38	8.7884033274	13.6317186851	21.5427023817
C39	11.1227047163	14.1204459819	18.4441214665
H40	11.7523549076	13.3999862207	17.9103014257
H41	11.5693288446	14.2874646236	19.4305850468
H42	11.1799497085	15.0704897051	17.8994894223
C43	6.8391862865	14.3094124637	19.6906729653
H44	6.2659000380	14.9678635886	20.3594573996
H45	6.7057648582	13.2797719528	20.0397973198
H46	6.3880449179	14.3846291606	18.6941623852
C47	8.4585844625	16.1627862202	19.1707337258
H48	7.8843539116	16.8480910284	19.8113629184
H49	8.0754541831	16.2788247710	18.1498956636
H50	9.4983434787	16.5098415880	19.1780905979
C51	8.6133666707	13.5207829564	16.7803836225
H52	9.2612054479	12.9556358499	16.0978455062
H53	8.5404542670	14.5370887258	16.3771657316
H54	7.6113443994	13.0780256780	16.7426294340
C55	11.9266605911	7.0880786024	15.1030957778
H56	11.1356885567	6.3478136955	15.2697584789
H57	12.7072348270	6.9087416117	15.8505584402
H58	12.3620654344	6.8914512661	14.1164845545
C59	13.9860156104	9.7120603491	15.1913460046
H60	14.7401757802	10.4438119268	14.8659553263
H61	14.3065647942	8.7314770744	14.8221033042
H62	14.0180302349	9.6759436808	16.2843893814
C63	12.5922453327	10.1000240052	14.6491341527
C64	12.6695969882	10.0915369398	13.1053382318
H65	13.4811478995	10.7486520252	12.7603726514
H66	11.7430540052	10.4492257384	12.6441650835
H67	12.8759276829	9.0903628856	12.7071969725
C68	9.7402976896	8.9901302958	14.0663081938
H69	9.3071586690	9.9963321712	14.0534994124
H70	8.9499669436	8.2984706954	14.3746524269
H71	10.0257728215	8.7380232055	13.0394132061
C72	12.2497483731	11.5305114113	15.1137933705
H73	13.0055656401	12.2470064032	14.7600068537
H74	12.2049707423	11.6058122948	16.2051071167
H75	11.2799556406	11.8655696541	14.7243972776
C76	5.8693207118	8.6364966083	19.0506063693
C77	5.1311616165	8.2240193911	20.1710360550
H78	4.2260632551	8.7558797625	20.4548229358
C79	7.0658515917	7.9540720877	18.6302642506
C80	7.4034675816	6.7920103162	19.3463323682
H81	8.2643631167	6.1993630312	19.0434334411
C82	6.6844715485	6.3939721289	20.4766950265
H83	7.0032401218	5.5213054013	21.0420481038
C84	5.5577119377	7.1159704243	20.8966104695
H85	5.0034507207	6.7951639320	21.7742116347
H86	7.4332985297	8.4147610005	16.9315673347

TS2

Y1	8.9118588340	9.8995991224	18.4285523551
Fe2	11.4731303936	9.8735457198	20.0093254439
Si3	10.5860575017	8.8818452572	15.3364403660
Si4	9.1085327576	13.5524565536	18.5040643727
N5	9.1873733404	11.9786675331	19.2546845709
N6	7.1011492358	8.2345757088	19.1993769263
N7	10.5070948743	9.2651225615	17.0373885562
C8	5.3713881882	8.9432613763	17.7339165593
H9	5.0314314931	9.5635279240	16.9092639969
C10	6.7067944006	9.0344105114	18.1647516174
C11	6.2595110222	7.3619107280	19.8350964807
C12	4.4872343470	8.0780641678	18.3739125911
H13	3.4499243068	8.0127469145	18.0534069062
C14	4.9297428218	7.2835663515	19.4357706371
H15	4.2547259530	6.5977002889	19.9369942435
C16	9.7383675787	10.3949997368	21.1067594772
H17	8.7644518382	9.9247402799	21.2152857052
C18	10.8599283983	10.1308350569	21.9583446092
H19	10.9088956897	9.3662249300	22.7207563733
C20	11.4975392313	9.0359617627	18.0065106218
C21	10.0356271380	11.5407940311	20.2594298538
C22	12.6645288919	9.8278101155	18.3020232814
H23	12.9596488686	10.7193580467	17.7669908010
C24	11.4026610980	11.8891984274	20.5557388739
H25	11.9681292529	12.6594072656	20.0523469210
C26	13.3477016717	9.2526553726	19.4149635102
H27	14.2582647659	9.6277378661	19.8628522351
C28	12.5909967417	8.1298196171	19.8687457127
H29	12.8315488160	7.4994316239	20.7139961118
C30	11.4530299170	8.0013857559	19.0228679006
H31	10.6931337985	7.2329517902	19.0928669760
C32	11.8737712160	11.0747190230	21.6319716336
H33	12.8543675674	11.1343335388	22.0844551345
C34	8.2389312889	14.8288584636	19.6595541210
C35	9.0786005941	15.0394885719	20.9389553329

H36	8.5798450769	15.7514778308	21.6122902260
H37	10.0717141211	15.4481466810	20.7177010612
H38	9.2174747538	14.1063936207	21.4961474435
C39	10.7956588888	14.2500440429	17.9658421333
H40	11.3599696979	13.5043894735	17.3947209505
H41	11.4170301224	14.5638410974	18.8116733018
H42	10.6647465834	15.1262999518	17.3195939566
C43	6.8450566398	14.3030289497	20.0620574392
H44	6.3473026819	15.0100839947	20.7410406590
H45	6.9135722443	13.3384534131	20.5761529700
H46	6.1898269485	14.1718236568	19.1925128025
C47	8.0806156469	16.1854012214	18.9388717376
H48	7.5847508077	16.9140847196	19.5962371036
H49	7.4701695570	16.1024790089	18.0318642154
H50	9.0475624779	16.6153144390	18.6525776334
C51	8.0822577610	13.2644870624	16.9324628637
H52	8.6319283866	12.6334696539	16.2214540837
H53	7.8595741728	14.2019879099	16.4111198426
H54	7.1247113124	12.7776541714	17.1523288755
C55	10.9164076438	7.0303325255	15.0860905761
H56	10.0984857509	6.4386722490	15.5131857956
H57	11.8408302958	6.7196962712	15.5857521082
H58	11.0049340420	6.7590744990	14.0276718621
C59	13.3347240346	9.4073650621	14.6613080523
H60	14.0749165617	9.9977774629	14.1016439960
H61	13.4763710863	8.3585345318	14.3769251454
H62	13.5820803963	9.4969069507	15.7240718323
C63	11.9046900934	9.8992878255	14.3461100223
C64	11.6574730683	9.7241205677	12.8301902591
H65	12.4209696395	10.2658969474	12.2533444610
H66	10.6813772973	10.1157391679	12.5232093009
H67	11.7081094696	8.6730065940	12.5220015740
C68	8.8586178144	9.3065955445	14.6718372946
H69	8.6508792825	10.3829375279	14.7175379478
H70	8.0791498880	8.7909474845	15.2457607865
H71	8.7448511063	9.0016306996	13.6259008362
C72	11.7979319422	11.3997851991	14.6904997001
H73	12.5362349793	11.9821231899	14.1204239660
H74	11.9767977919	11.5890456353	15.7540014479
H75	10.8087626692	11.8069522883	14.4469448854
C76	6.9326328754	6.5612795954	20.8869720277
C77	6.3394945192	5.6630104565	21.7813816228
H78	5.2679688228	5.4763792464	21.7863802404
C79	8.3088294514	6.8061617932	20.8923548263
H80	8.2346990476	7.7592419222	19.8695433294
C81	9.1235124537	6.1539228804	21.8087313767
H82	10.1973237989	6.3309140118	21.8363612222
C83	8.5456433771	5.2469861366	22.7088388913
H84	9.1713592892	4.7223687220	23.4278472798
C85	7.1667825475	5.0055857100	22.6949363004
H86	6.7371183353	4.3027215669	23.4036746193

Intermediate

Y1	8.8752093416	9.8402721939	18.0876876854
Fe2	11.1453237580	9.5132967915	20.0736082528
Si3	11.0899695749	8.4198932129	15.3929061195
Si4	9.2594965547	13.5527387560	18.5473232475
N5	9.2048324318	11.8727822998	19.0341046436
N6	10.5136637068	8.7830952236	17.0098349852
C7	9.4454224467	10.3516140250	21.0228720963
H8	8.4248083476	9.9907432277	21.0534593993
C9	10.4739530273	10.0220370175	21.9568741689
H10	10.3890280918	9.3210891880	22.7760174451
C11	11.2775754670	8.5081154062	18.1548418159
C12	9.9396694227	11.3562202360	20.1000925204
C13	12.5266196764	9.0956432175	18.5759582549
H14	13.0713017233	9.8526529793	18.0312152993
C15	11.3281346236	11.5514828565	20.4481978840
H16	12.0160055584	12.1949715800	19.9197876018
C17	12.9237857979	8.5046885378	19.8108201353
H18	13.8194951537	8.7434977501	20.3686444214
C19	11.9057700894	7.5881589971	20.2140093003
H20	11.8979448559	7.0050840256	21.1252403740
C21	10.8945371595	7.5953089877	19.2124706852
H22	10.0000214444	6.9880255264	19.1977953212
C23	11.6283409541	10.7850794428	21.6140592036
H24	12.5848432600	10.7482671463	22.1174299464
C25	8.4732537464	14.6930148550	19.8980160737
C26	9.2725668066	14.6164937618	21.2173185129
H27	8.8220176962	15.2739299152	21.9750270120
H28	10.3128270889	14.9382534714	21.0898731088
H29	9.2859284702	13.6032596935	21.6317722487
C30	11.0163936357	14.1814427879	18.1590778418
H31	11.5365228422	13.4870227612	17.4887075756
H32	11.6348129844	14.3058194022	19.0547129722
H33	10.9785343803	15.1547590687	17.6552643903
C34	7.0226367044	14.2453276359	20.1757520626
H35	6.5668921494	14.8721223485	20.9556885798
H36	6.9827200556	13.2055703428	20.5183992306
H37	6.3905569980	14.3276122091	19.2835338888
C38	8.4644204058	16.1600212300	19.4141576166
H39	8.0069475660	16.8117783699	20.1726383359
H40	7.8892990528	16.2880091484	18.4898685636
H41	9.4767624922	16.5388542778	19.2326432655
C42	8.2539659656	13.6868838495	16.9465561084
H43	8.6808453456	13.0603641332	16.1552195858
H44	8.2474406600	14.7181739929	16.5761812447
H45	7.2133318688	13.3786786628	17.0896159469
C46	12.4157272881	7.0651295105	15.4918902210
H47	12.0044407354	6.1667536846	15.9655074021
H48	13.2829116978	7.3769798085	16.0837967875
H49	12.7763429301	6.7789267999	14.4979023506
C50	13.0742910476	10.5063449814	15.1604837668
H51	13.5075916112	11.3356625896	14.5827466893
H52	13.8572623827	9.7477032442	15.2754510499
H53	12.8353779072	10.9008150222	16.1541232144
C54	11.8190229576	9.9538304493	14.4533467623
C55	12.2138220715	9.5365532101	13.0182885930
H56	12.6339315964	10.3943079919	12.4732995894
H57	11.3545953871	9.1769591950	12.4415571949
H58	12.9745795913	8.7476892472	13.0118968297
C59	9.6046382723	7.7600871053	14.4160638391
H60	8.7921560637	8.4956695679	14.3955408223
H61	9.2283843512	6.8450041817	14.8904862041
H62	9.8595631453	7.5115001154	13.3799354850
C63	10.7731492133	11.0848490849	14.3703352615
H64	11.1796790830	11.9446164101	13.8180429529
H65	10.4893031420	11.4437847139	15.3672477362
H66	9.8549972499	10.7684550689	13.8636990505
C67	5.9173577671	7.9764587780	18.5861071174
C68	4.9190389759	7.1490894904	19.1270934870
H69	3.9489429767	7.0679949429	18.6404956543
C70	7.2211897470	8.1349027036	19.1588714096
C71	7.4268990029	7.3682002144	20.3263285212
H72	8.3847383712	7.4339576001	20.8411936657
C73	6.4512347311	6.5290321288	20.8745316427
H74	6.6686188266	5.9626586992	21.7780190192
C75	5.1915617778	6.4142200298	20.2756384193
H76	4.4366565999	5.7578010798	20.6990669272
C77	6.0288598864	11.0055790525	15.7214721328
C78	4.7614050493	10.7164022481	16.2402842567
C79	4.5808390244	9.6605636919	17.1461284100
C80	5.6613743742	8.8334480582	17.4211660139
N81	6.7737569569	9.0327069952	16.6358629514
C82	7.1252767441	10.1365035783	15.8984140528
H83	6.1824930185	11.9283797758	15.1705861402
H84	3.9226144039	11.3760469271	16.0275654275
H85	3.6611700864	9.5531476948	17.7108620142
H86	7.4427617207	8.2623853623	16.6878395450

TS3

Y1	9.1093327168	9.6721970668	18.9247452886
Fe2	11.8645501615	9.9402047822	20.0809435332
Si3	10.4275182526	8.4012878910	15.7019499678
Si4	9.0257117329	13.3796895688	18.8088888941
N5	9.3223934140	11.8468772189	19.6012177393
N6	6.5816344456	9.3374342951	18.6849198265
N7	10.5085812853	8.9434979340	17.3549318233
C8	4.7061785564	9.6732045226	17.2332179598
H9	4.0656965260	10.3173417204	16.6386278185
C10	5.8376606691	10.2205832137	17.8643071397
C11	6.2145676183	8.0212609889	18.9720952095
C12	4.4530426227	8.3090771641	17.3267482320
H13	3.6574150540	7.8574214971	16.7374508058
C14	5.1868209463	7.4899602595	18.1997815231
H15	4.9538940514	6.4335405701	18.2741788923
C16	10.3124367246	10.4605173051	21.4330750672
H17	9.4128746496	9.9275086949	21.7197204495
C18	11.5822423993	10.3405335859	22.0819995490
H19	11.8253687921	9.6542930485	22.8815790900
C20	11.6422026701	8.9014150011	18.1820803758
C21	10.3654520345	11.5382379913	20.4573209397
C22	12.7694732662	9.8008305546	18.2127119129
H23	12.9022683676	10.6488504620	17.5565239689
C24	11.7393170405	11.9865045537	20.4659477766
H25	12.1521681654	12.7371535004	19.8105368799
C26	13.6656902816	9.3884906158	19.2433494663
H27	14.5994236353	9.8694535594	19.5024896124
C28	13.0871199263	8.2671425959	19.9116251326
H29	13.5075071639	7.7455202637	20.7606145389
C30	11.8462790328	7.9765447034	19.2797817482
H31	11.1701203888	7.1711454029	19.5308978683
C32	12.4520822940	11.3052637658	21.4992933866
H33	13.4909427910	11.4608853615	21.7570092964
C34	7.8532120256	14.4539753983	19.9054856119
C35	8.5400790840	14.7559233207	21.2543936121
H36	7.8733532346	15.3386853052	21.9062959383
H37	9.4584911923	15.3410442148	21.1271291363
H38	8.8009487699	13.8361266036	21.7897188086
C39	10.5918000957	14.3920018550	18.4215501844
H40	11.3052996782	13.8014409955	17.8353448235
H41	11.1078397132	14.7559196036	19.3157419534
H42	10.3274908481	15.2683159753	17.8178458976
C43	6.5426743357	13.6860307462	20.1797888805
H44	5.8646610971	14.2867890116	20.8036957880
H45	6.7388199569	12.7493480473	20.7146364764
H46	6.0070161455	13.4394223692	19.2556961816
C47	7.5175163415	15.7873171590	19.2026471958
H48	6.8519184581	16.3972528151	19.8308097443
H49	7.0050631666	15.6316652456	18.2460094499
H50	8.4141775932	16.3871783865	19.0072994779
C51	8.2126371921	12.9943766193	17.1418009781
H52	8.9355856423	12.5063961443	16.4755124318
H53	7.8887738730	13.9139458180	16.6399578080
H54	7.3374850594	12.3420510455	17.2367966702
C55	10.9724727332	6.5883066247	15.5600462521
H56	10.2995544024	5.9439240046	16.1372294202
H57	11.9831429989	6.4441849785	15.9577773369
H58	10.9703708229	6.2299451233	14.5240293250
C59	12.9733074844	9.1480833569	14.5842628145
H60	13.5550784591	9.7633367965	13.8822952555
H61	13.1950731333	8.0996692028	14.3550739843
H62	13.3541503770	9.3524133961	15.5898916464
C63	11.4654388485	9.4582296911	14.4490008603
C64	11.0361263100	9.1196036986	13.0030679149
H65	11.6519558305	9.6764913844	12.2821460460
H66	9.9911560668	9.3854593840	12.8096236874
H67	11.1586652478	8.0543830536	12.7735841931
C68	8.5874806451	8.5264740187	15.2456884960
H69	8.2199738886	9.5591891288	15.2786074205
H70	7.9770751333	7.9282586182	15.9339320451
H71	8.3949148542	8.1466743599	14.2366044478
C72	11.2344271524	10.9650933158	14.6877578508
H73	11.8193423090	11.5649859154	13.9752958119
H74	11.5283650222	11.2706118211	15.6973994651
H75	10.1813903183	11.2431311127	14.5552502679
C76	6.9924159897	7.3092063594	19.9941792125
C77	6.4361818112	6.1662973662	20.6073755679
H78	5.4317861577	5.8354210175	20.3528324553
C79	8.2874043904	7.8022501275	20.3264304256
C80	8.9697280341	7.0646599238	21.3151607343
H81	9.9655059827	7.3845397755	21.6208095058

C82	8.4318791071	5.9295532454	21.9283385563
H83	9.0016165620	5.3969616828	22.6870951212
C84	7.1573488685	5.4754539468	21.5729582060
H85	6.7285992457	4.6006592213	22.0534508841
H86	6.3591929182	10.4094712292	19.1276453138

2^{Y}-Phpy

Y1	8.9815627950	10.0346752161	18.1295014112
Fe2	12.0802846358	10.5158807576	19.5145260638
Si3	10.5595539707	7.3422848076	16.1968193164
Si4	7.9803934160	13.0221690915	20.0286523971
N5	9.0757401236	11.7296580598	19.5826780829
N6	7.6996856997	10.8064732797	16.2226727220
N7	10.5813487790	8.7533303410	17.2388761051
C8	7.4893339678	12.1328143860	14.2308295257
H9	7.9326380539	12.8387453919	13.5375152869
C10	8.2005582042	11.6807249701	15.3309948071
C11	6.4367820174	10.3123894161	16.0797925402
C12	6.1930972907	11.6397201645	14.0597990597
H13	5.5915108743	11.9588494303	13.2133321750
C14	5.6721648636	10.7372017951	14.9756099151
H15	4.6681692806	10.3590040653	14.8344078461
C16	10.8123130643	10.7583594643	21.1632604676
H17	10.1978151042	9.9955617723	21.6238669286
C18	12.1627301896	11.0676268955	21.4996326900
H19	12.7718684956	10.5546613032	22.2318935168
C20	11.7698336636	9.1258595233	17.8855679016
C21	10.3612797080	11.6732447912	20.1399868580
C22	12.6436106808	10.2164136749	17.5257344972
H23	12.4695938146	10.9022939199	16.7071862116
C24	11.4971468104	12.4990970366	19.8147067364
H25	11.5006259191	13.2689453490	19.0550940035
C26	13.7787319485	10.2060491957	18.3887348608
H27	14.6058268152	10.9032015483	18.3643179276
C28	13.6078255387	9.1402336795	19.3238041971
H29	14.2808741358	8.8946454754	20.1341890306
C30	12.3689157670	8.4981451212	19.0387435619
H31	11.9424411622	7.6605787662	19.5740204580
C32	12.5828842676	12.1500150479	20.6686712704
H33	13.5691272559	12.5942955942	20.6583831054
C34	7.5297884187	13.0003022372	21.9122874650
C35	8.7338808509	13.4445205465	22.7737447088
H36	8.4696092877	13.4156049576	23.8410895049
H37	9.0427835111	14.4710744902	22.5460647904
H38	9.6046287031	12.7962671708	22.6358143373
C39	8.7132200732	14.7277804795	19.6054430692
H40	8.8876226022	14.8143772750	18.5261550238
H41	9.6718871775	14.8963468431	20.1077016353
H42	8.0411965613	15.5439550635	19.8959437830
C43	7.1065439117	11.5790418464	22.3385676581
H44	6.8199079423	11.5634942865	23.3999720546
H45	7.9206061575	10.8597652094	22.2056990718
H46	6.2471141807	11.2156716619	21.7624654119
C47	6.3576487439	13.9686907294	22.1859446248
H48	6.1238789370	13.9894245353	23.2604325455
H49	5.4435572641	13.6692691478	21.6613344559
H50	6.5925512417	14.9979556297	21.8889754123
C51	6.4044929649	12.7945140327	18.9985007398
H52	6.6210106569	12.8960405559	17.9290843783
H53	5.6606959120	13.5582090281	19.2508981489
H54	5.9419993300	11.8138134006	19.1532125488
C55	10.9569403159	5.7583604104	17.1718909328
H56	10.2014639510	5.5898168837	17.9482797628
H57	11.9314890062	5.8206355526	17.6679466590
H58	10.9704408990	4.8711013400	16.5282617440
C59	13.2689607513	7.3609207148	15.2034713641
H60	13.9607229031	7.4344049367	14.3511500819
H61	13.4598603523	6.3981335174	15.6910161154
H62	13.5368365635	8.1516005163	15.9111191102
C63	11.8068871184	7.4799059147	14.7177861969
C64	11.5398449123	6.3425028545	13.7063262207
H65	12.2576526219	6.3952821787	12.8749376623
H66	10.5357425309	6.4017481177	13.2721716211
H67	11.6486558266	5.3510560993	14.1614011291
C68	8.8017840301	7.1907103950	15.5049805139
H69	8.5457255386	8.0226834474	14.8392082526
H70	8.0595786577	7.1690759929	16.3099474517
H71	8.6900576695	6.2638632020	14.9311364090
C72	11.6283251508	8.8316795005	13.9954298186
H73	12.3120357577	8.9060404115	13.1372343403
H74	11.8399546213	9.6748535478	14.6607526161
H75	10.6090225907	8.9587405326	13.6101955933
C76	5.9455634281	9.3494798217	17.1036718890
C77	4.6399731221	8.8262151797	17.0050817896
H78	3.9729700096	9.1145094937	16.1979744249
C79	6.8133717116	8.9685479444	18.1701380356
C80	6.2909060255	8.0503069314	19.0996996379
H81	6.9087237961	7.7226437385	19.9370812362
C82	4.9982164737	7.5262914335	19.0040552382
H83	4.6360376826	6.8167545774	19.7449787061
C84	4.1696779957	7.9188805937	17.9504216775
H85	3.1623558515	7.5211807432	17.8646130951
H86	9.2166145216	12.0234691762	15.5167436463

1^{Y}-py^{Ph}-DBU

Y1	8.4964555965	9.3451696433	17.9622914858
Fe2	10.1493050943	10.0692867997	20.4860022693
Si3	11.0325262673	6.5391964380	17.3337579522
Si4	10.5990446910	12.0868299134	16.4162944477
N5	9.5787401604	11.3566678916	17.6297721523
N6	6.4875747813	8.3126533324	19.1040120406
N7	10.1833631466	7.7606056283	18.2375297797
C8	4.8743655879	10.0503243697	18.8374415341
H9	4.6106552923	11.0407426387	18.4721658167
C10	6.1735805257	9.5490753524	18.6204538967
C11	5.6014714382	7.5573697074	19.8048741169
C12	3.9347893865	9.2828222345	19.5179554423
H13	2.9218742305	9.6485958853	19.6773846873
C14	4.2971340611	8.0251278483	20.0056541662
H15	3.5678814445	7.4111077468	20.5213769904
C16	8.6716957642	11.4955642432	19.9752461298
H17	7.6236900964	11.3606510911	19.7351794046
C18	9.2001933724	11.7225998181	21.2836971374
H19	8.6348770486	11.7197818634	22.2052192927
C20	10.4464041495	8.1055748217	19.5727222707
C21	9.7367328361	11.6076796929	18.9946961484
C22	11.6427644000	8.6829724928	20.1397776492
H23	12.5379678470	8.9212822961	19.5878296681
C24	10.9360264247	11.8450352200	19.7639074073
H25	11.9324221185	11.9192040913	19.3577578401
C26	11.4559165491	8.8871273889	21.5406203290
H27	12.1885205304	9.2945297013	22.2241434505
C28	10.1158968836	8.5231224705	21.8626407567
H29	9.6491482290	8.5900166704	22.8363096909
C30	9.4906514690	8.0691750648	20.6658573811
H31	8.4828647895	7.6920452894	20.5900094891
C32	10.5967772763	11.9632697650	21.1463278168
H33	11.2927568915	12.1532029529	21.9523476531
C34	10.1790760379	13.9637914571	16.1846838211
C35	10.5759420724	14.7665837190	17.4431856346
H36	10.3196990807	15.8290009936	17.3176926395
H37	11.6531042683	14.7164260764	17.6401612337
H38	10.0575528744	14.4080253043	18.3386529076
C39	12.4751021653	11.9273382844	16.7291355488
H40	12.7331706514	10.9012487034	17.0137276999
H41	12.8486887253	12.5950450501	17.5120764425
H42	13.0318920805	12.1628616658	15.8138634323
C43	8.6624170288	14.1359778910	15.9569014313
H44	8.4052703051	15.1995698989	15.8449553576
H45	8.0855573764	13.7380334705	16.7986162050
H46	8.3224657137	13.6253958811	15.0466152661
C47	10.9428367669	14.5375128715	14.9713982766
H48	10.7148873325	15.6058414224	14.8411441759
H49	10.6724582124	14.0323945095	14.0364719114
H50	12.0293575880	14.4530276203	15.0928410291
C51	10.2952156012	11.1882962527	14.7662275239
H52	10.2415186574	10.1018786721	14.9031500457
H53	11.1259382760	11.3853650962	14.0789693415
H54	9.3792869797	11.5130403904	14.2633268580
C55	10.3729611434	4.8117636604	17.8118036026
H56	9.3099499415	4.7140387716	17.5633508809
H57	10.4678808160	4.6619882495	18.8936622510
H58	10.9022647803	3.9913784080	17.3144492367
C59	13.4273091447	5.9489810166	18.8728648103
H60	14.5224373227	5.8495951570	18.9048672204
H61	13.0084016475	4.9680418850	19.1255180122
H62	13.1379175838	6.6437332653	19.6657579683
C63	12.9724993794	6.4186804206	17.4728807086
C64	13.4623646321	5.3662923791	16.4470940891
H65	14.5574124195	5.2765903221	16.4960501150
H66	13.2067219995	5.6370301069	15.4167820280
H67	13.0511392451	4.3700668116	16.6439968347
C68	10.6706276514	6.8525110223	15.4879051930
H69	11.4228753049	7.5197000274	15.0519454849
H70	9.6986364002	7.3251506004	15.3258475024
H71	10.6899355195	5.9193628275	14.9122872058
C72	13.6605214010	7.7558609053	17.1243971210
H73	14.7537860728	7.6512992529	17.1822349355
H74	13.3750034991	8.5677468123	17.7986706720
H75	13.4229101306	8.0835042691	16.1055037299
C76	6.0420447188	6.2428777650	20.3472790017
C77	5.3914381465	5.6652284013	21.4527832420
H78	4.5834434761	6.1981840896	21.9446545168
C79	7.1240115383	5.5456679269	19.7820299968
C80	7.5229892480	4.3070748547	20.2855685787
H81	8.3619250541	3.7911561077	19.8286464788
C82	6.8549270625	3.7395627902	21.3722960980
H83	7.1673542389	2.7772527068	21.7683010950
C84	5.7906955062	4.4294043130	21.9569112112
H85	5.2754510299	4.0106482027	22.8174334775
N86	7.3837854928	8.8960304535	15.7828820310
C87	6.9128734033	10.1338010104	15.1432978147
H88	5.9010158709	10.3562311355	15.5119367641
H89	7.5527143566	10.9592344178	15.4620410387
C90	6.9229787289	7.7755854161	15.2900750459
N91	6.1542322789	7.6948851016	14.1643205363
C92	7.2063237157	6.4902362622	16.0262749416
H93	7.9526709319	6.6646860848	16.7991844705
H94	6.2987389577	6.1246945770	16.5194599065
C95	5.6010773275	6.4379784007	13.6748828754
H96	6.2750650003	5.9397350869	12.9638567133
H97	4.6584167708	6.6472509388	13.1597715344
C98	5.9801683974	8.8346139427	13.2491879592
H99	4.9273616244	9.1485522852	13.2762841479
H100	6.1882149819	8.4860241520	12.2291072595
C101	6.9020953618	9.9908466335	13.6223178413
H102	6.5552309815	10.9096272198	13.1386161330
H103	7.9212679938	9.7953752281	13.2720159443
H104	7.5792949865	5.7051312496	15.3631663800
H105	5.3842177646	5.7522980624	14.4928706234
H106	7.6648422632	5.9885477446	18.9555297821

TS1-DBU

Y1	8.5206505770	9.1096911038	18.0929325488
Fe2	10.4258885572	10.4767821708	20.0875052815
Si3	11.5278398231	6.8886110728	17.2046392548
Si4	10.0926647625	11.7027785344	15.8204129334
N5	9.2110876414	11.2096862941	17.2457484031
N6	6.9600972384	7.4401943851	18.9715059491
N7	10.4864749854	7.9535413028	18.1150217019
C8	5.2384678989	8.8432416737	19.9152632248
H9	4.9438724245	9.7838048803	20.3724641669
C10	6.6007687407	8.6188773636	19.5716484044
C11	6.2381093010	6.3841751252	19.4501700425
C12	4.3151060679	7.8205923252	19.6998315867
H13	3.2427824927	7.9769188650	19.7964661934
C14	4.8514228110	6.5242997120	19.6094008870
H15	4.2491714553	5.6612993104	19.8785040896
C16	8.6325612793	11.5036595519	19.6651984176
H17	7.6110054933	11.1412362250	19.6307204369

C18	9.2691393047	12.0119664233	20.8413236268
H19	8.8424776705	12.0326710699	21.8343459358
C20	10.9252409530	8.5095179048	19.3286966249
C21	9.5049711928	11.6868009941	18.5147445408
C22	12.0790304334	9.3396220016	19.5783305205
H23	12.7918850650	9.6481526413	18.8282942412
C24	10.7204612690	12.2482371232	19.0587108852
H25	11.6159837097	12.4560867157	18.4940097285
C26	12.1143137196	9.6908256732	20.9617574397
H27	12.8671676894	10.3005095882	21.4426985272
C28	10.9516242247	9.1475767090	21.5854020371
H29	10.6745155642	9.2541668927	22.6256502899
C30	10.2170293879	8.4380007562	20.5913068670
H31	9.3244683136	7.8546308345	20.7661097196
C32	10.5519197756	12.4935989559	20.4565781506
H33	11.2922571149	12.9276353725	21.1148971572
C34	9.7780417973	13.5519524246	15.3147945276
C35	10.1361566234	14.5160683655	16.4654276205
H36	9.9731034258	15.5590848375	16.1561871357
H37	11.1876528472	14.4293522907	16.7626638897
H38	9.5251300245	14.3363312958	17.3554447276
C39	11.9822395853	11.4539417688	15.9426072979
H40	12.1991536464	10.5337969543	16.4942594575
H41	12.5023169989	12.2741613398	16.4498933897
H42	12.4297107472	11.3575657416	14.9460582347
C43	8.2964948937	13.7653656795	14.9453742956
H44	8.1086515518	14.8164251693	14.6804374384
H45	7.6336257568	13.5129682728	15.7810456348
H46	7.9995949421	13.1576348265	14.0819882883
C47	10.6511922449	13.9073350661	14.0901088217
H48	10.4729862082	14.9475780761	13.7801822415
H49	10.4316517508	13.2711714142	13.2243042656
H50	11.7205356404	13.8131130000	14.3086915683
C51	9.5175174079	10.5920341841	14.3898287545
H52	9.7895980496	9.5480091439	14.5805043620
H53	10.0011560413	10.8815520982	13.4497522287
H54	8.4353737478	10.6270049308	14.2371661328
C55	10.7566023762	6.6166901266	15.4885994405
H56	10.5909908180	7.5753476000	14.9849939157
H57	9.8027813610	6.0819967636	15.5262272685
H58	11.4328387548	6.0341714766	14.8527762110
C59	10.3511020032	4.4978440524	18.2343759416
H60	10.4490095632	3.5295334594	18.7468825527
H61	9.8680078562	4.3031825617	17.2685436629
H62	9.6747497455	5.1197427187	18.8297781201
C63	11.7331862203	5.1622569700	18.0618169583
C64	12.6272411637	4.2391522103	17.2035071334
H65	12.7220261474	3.2501414128	17.6754673901
H66	13.6409793046	4.6394643611	17.0879700172
H67	12.2162103795	4.0775342838	16.1997283216
C68	13.2689429388	7.5982352226	16.8942114484
H69	13.8436810542	7.7338201392	17.8162468086
H70	13.2154683300	8.5707902742	16.3923791076
H71	13.8455600136	6.9294694174	16.2440617805
C72	12.3815192460	5.3187010133	19.4540009292
H73	12.5065763779	4.3356384827	19.9315312280
H74	11.7692803150	5.9321266158	20.1227155595
H75	13.3757830465	5.7777583457	19.3962267858
C76	7.0179776747	5.6629974392	20.5162552246
C77	7.2088746028	4.3119231899	20.8007233297
H78	6.8927778475	3.5454280851	20.0972759127
C79	7.3787609956	6.6575678629	21.4462364806
C80	7.9021270354	6.3043814377	22.6831194822
H81	8.1486832809	7.0598143929	23.4250765495
C82	8.1363135496	4.9462112177	22.9560267177
H83	8.5954659393	4.6566395859	23.8981431073
C84	7.7963871855	3.9618915468	22.0227975401
H85	7.9770837218	2.9151650257	22.2522048855
N86	6.7447096601	9.3277686352	16.3033033528
C87	5.9927126930	10.5811758546	16.4885942411
H88	5.1708641514	10.3890113972	17.1927944601
H89	6.6721866514	11.3018475901	16.9529341152
C90	6.4030009245	8.5356188426	15.3252117520
N91	5.4261213978	8.8086299839	14.4050480149
C92	7.1343482969	7.2202684322	15.1911242881
H93	7.8367173243	7.1022429900	16.0145166435
H94	6.4420330333	6.3739159469	15.2407023307
C95	5.0523799833	7.9191367671	13.3144086397
H96	5.2801289654	8.3811764818	12.3443104863
H97	3.9747545841	7.7135068977	13.3463057597
C98	4.6609644183	10.0604568035	14.4508094868
H99	3.6924683726	9.8795169836	14.9402833999
H100	4.4486476818	10.3620241603	13.4179801115
C101	5.4477992325	11.1431436052	15.1777865731
H102	4.8059835201	12.0096572091	15.3670566915
H103	6.2772424881	11.4830756755	14.5492172921
H104	7.6917041439	7.1560792409	14.2516073051
H105	5.5771316188	6.9685576450	13.3685940296
H106	7.1008938485	8.0033365709	20.8448262099

TS4

Y1	8.6888358824	9.4018966919	17.8610002224
Fe2	10.1238592871	10.3221915654	20.3972328325
Si3	11.1222452732	6.6091796780	17.4466772269
Si4	10.6718929757	12.0880489989	16.2761537652
N5	9.5433649904	11.5084347035	17.4806018570
N6	6.4799306872	7.5619596623	19.4275219733
N7	10.3537673358	7.9478642346	18.2639038712
C8	5.4038059488	9.6551694314	19.3331557196
H9	5.3814714784	10.7015460967	19.0306193125
C10	6.5363683815	8.8604464519	19.0287284231
C11	5.4375669748	7.0225320992	20.1132504325
C12	4.3157959937	9.1318508774	20.0328092024
H13	3.4595657265	9.7611084977	20.2691258109
C14	4.3266011435	7.7961662754	20.4417583921
H15	3.4973276726	7.3694576677	20.9970417846
C16	8.5466261538	11.5962522584	19.7798163340
H17	7.5218513352	11.3706760545	19.5143661383
C18	8.9940214618	11.8980681751	21.1043968394
H19	8.3914385996	11.8618496261	22.0008501059
C20	10.5877666627	8.3592775190	19.5895872002
C21	9.6345223312	11.7979720413	18.8395207987
C22	11.7348947753	9.0573988799	20.1175983171
H23	12.6055584627	9.3413500279	19.5458579893
C24	10.7743866707	12.1522491197	19.6526304402
H25	11.7750628845	12.3165217495	19.2848806403
C26	11.5295329132	9.3110279129	21.5068320135
H27	12.2210025657	9.8161762681	22.1674719067
C28	10.2267651362	8.8424010826	21.8528897242
H29	9.7583887585	8.9157870692	22.8250893229
C30	9.6445308007	8.2709856754	20.6867938206
H31	8.6763728359	7.7945645209	20.6285865274
C32	10.3658533207	12.2666349188	21.0170583478
H33	11.0055772096	12.5386597758	21.8456217058
C34	10.3638474356	13.9522761777	15.8586886003
C35	10.6781330367	14.8395617067	17.0827536419
H36	10.4901778719	15.8976146219	16.8488740334
H37	11.7275155338	14.7592447433	17.3891015589
H38	10.0583692527	14.5794669454	17.9475276549
C39	12.5145240222	11.8573133968	16.7100663370
H40	12.6897317271	10.8611141180	17.1305650724
H41	12.8944117474	12.5929648554	17.4265467811
H42	13.1294049151	11.9436609368	15.8060721881
C43	8.8871073326	14.1635175207	15.4654849935
H44	8.6926673386	15.2218822211	15.2391587933
H45	8.2128679397	13.8658827650	16.2759943168
H46	8.6151973423	13.5882674119	14.5715149160
C47	11.2682242616	14.3879667502	14.6851197319
H48	11.1051666856	15.4487083978	14.4444781646
H49	11.0658176899	13.8145094513	13.7728306246
H50	12.3323267783	14.2713576617	14.9221600825
C51	10.3911198447	11.0517243168	14.7063296512
H52	10.4501065304	9.9774511137	14.9170102387
H53	11.1689802854	11.2726494136	13.9669281145
H54	9.4259214298	11.2467656308	14.2293426946
C55	10.2939875354	4.9719526412	17.9406781301
H56	9.2050076166	5.0379991655	17.8465014611
H57	10.4972101442	4.7387605427	18.9921551703
H58	10.6380574624	4.1233453371	17.3378923394
C59	13.3792222925	6.0480987857	19.1699993048
H60	14.4603609382	5.8758218278	19.2765074579
H61	12.8736175481	5.1359892661	19.5064159151
H62	13.1059978340	6.8511230638	19.8601897326
C63	13.0349523581	6.3883568663	17.7027325502
C64	13.5091405695	5.2097053630	16.8178231836
H65	14.5927584513	5.0629563639	16.9349604459
H66	13.3213659405	5.3871626058	15.7525759133
H67	13.0248939761	4.2660419851	17.0916237987
C68	10.8394110163	6.9081110475	15.5848810070
H69	11.5292634575	7.6663269723	15.1978897106
H70	9.8241095365	7.2552576590	15.3625465882
H71	10.9990658282	5.9914811691	15.0054318775
C72	13.8196339709	7.6454734449	17.2726537399
H73	14.8991098077	7.4901969518	17.4132988483
H74	13.5401515888	8.5307189443	17.8509786392
H75	13.6641244751	7.8835624636	16.2140368838
C76	5.6878777418	5.5874983233	20.4191557156
C77	4.8726906695	4.7324776530	21.1671383423
H78	3.9311233949	5.0686635310	21.5982344218
C79	6.9123320587	5.1774903851	19.8648763634
C80	7.3220667880	3.8620421046	20.0777278186
H81	8.2660215991	3.4980647042	19.6747721593
C82	6.5189925996	2.9880245513	20.8267953474
H83	6.8440793278	1.9629048718	20.9969065566
C84	5.3018871024	3.4182268574	21.3681918039
H85	4.6941780831	2.7309454360	21.9513670859
N86	7.3133165568	9.1491275585	15.8418712918
C87	6.8065280086	10.4123691604	15.2821820520
H88	5.8645901921	10.6719840105	15.7897288172
H89	7.5209881647	11.2055642921	15.5125414761
C90	6.7750758513	8.0411202315	15.3932038711
N91	5.8718980178	7.9923797134	14.3751108542
C92	7.1388230904	6.7361311925	16.0589191676
H93	7.9648400837	6.8710902206	16.7561006274
H94	6.2983481970	6.3478384163	16.6435384947
C95	5.2382518524	6.7542937070	13.9344466367
H96	5.7879139517	6.2869411321	13.1060761379
H97	4.2267024523	6.9835124877	13.5859268545
C98	5.5715011814	9.1630535117	13.5342952109
H99	4.5454610290	9.4946742966	13.7456105172
H100	5.5988967127	8.8410584879	12.4857861943
C101	6.5679171103	10.2907683170	13.7787181290
H102	6.1788429353	11.2251571646	13.3622626860
H103	7.5184134626	10.0734189505	13.2785326970
H104	7.4388761730	5.9738276848	15.3343906290
H105	5.1520693898	6.0380919288	14.7495943972
H106	7.1918314789	6.4192245416	19.3607562334

TS5

Y1	9.3244778261	7.7790510663	18.3670506499
Fe2	11.5712152043	8.6990788643	20.5813469039
Si3	12.3316879249	6.6887411236	16.2583216626
Si4	9.4175668171	11.4431515450	17.7863656715
N5	9.1974362401	10.0939163930	18.9404290523
N6	7.1161284860	8.6979693546	19.3102312187
N7	11.4685549122	7.3030532503	17.6541477621
C8	5.1881923306	10.0670698061	19.0912398832
H9	4.7100740958	10.9630664024	18.7001156957
C10	6.5468055931	9.8253702712	18.7911907250
C11	6.4194876300	7.7822041535	20.0861536813
C12	4.4613694463	9.1815599890	19.8718533987
H13	3.4127803051	9.3670482094	20.1009255943
C14	5.0761325885	8.0261212150	20.3667913235
H15	4.4975798081	7.3103902890	20.9388861244
C16	9.5984852272	9.0648244744	21.2232153062
H17	8.7735808211	8.3716987554	21.2531304177
C18	10.5329095176	9.2506279592	22.2853254050
H19	10.5486007996	8.6950372100	23.2126533572
C20	12.1501066382	7.4842806675	18.8787740308
C21	9.9041710216	9.9987425239	20.1589886010
C22	13.1116929653	8.5045135144	19.2218375207
H23	13.4283981339	9.3034017626	18.5692396027

C24	11.0750674445	10.7155949198	20.5874350272
H25	11.6033270119	11.4584925549	20.0139770193
C26	13.5808421184	8.2822655794	20.5512830111
H27	14.3093825618	8.8856453494	21.0755051300
C28	12.8685813130	7.1688620393	21.0877660022
H29	12.9633949417	6.7716072502	22.0893719028
C30	11.9881806115	6.6892567267	20.0765668913
H31	11.3174454574	5.8494238082	20.1756824269
C32	11.4363133835	10.2781980870	21.8966836278
H33	12.2784063982	10.6414530895	22.4696973129
C34	8.5173066149	13.0814215300	18.3079434427
C35	8.3120989405	13.1226586962	19.8373187225
H36	7.8175550385	14.0609794675	20.1272015041
H37	9.2595887974	13.0702041913	20.3860061773
H38	7.6835209794	12.2939487464	20.1771004060
C39	11.2657577017	11.7939662586	17.4770405850
H40	11.8306363982	10.8580136156	17.4272500776
H41	11.7452250318	12.4398196243	18.2178510084
H42	11.3718383732	12.2944861892	16.5071276543
C43	7.1364271911	13.1817509378	17.6220469990
H44	6.6059720472	14.0795774457	17.9713418687
H45	6.5197065137	12.3079416745	17.8463658273
H46	7.2267080699	13.2623476085	16.5321212477
C47	9.3547079867	14.3090477907	17.8821941015
H48	8.8138959460	15.2347187036	18.1244836403
H49	9.5524429163	14.3262073958	16.8030872949
H50	10.3208000507	14.3534686569	18.3958743091
C51	8.7893381228	10.8720758714	16.0895643124
H52	9.2744542566	9.9421966678	15.7641983754
H53	9.0388251714	11.6330386192	15.3396027737
H54	7.7075133144	10.7312625721	16.0783242450
C55	12.7340923851	4.8431290560	16.5262080694
H56	11.8211023471	4.2471800279	16.6329339044
H57	13.3117607987	4.7098282646	17.4482104736
H58	13.3171756907	4.4081803588	15.7063870255
C59	15.1613659894	7.2274653908	16.7145158424
H60	16.0959824398	7.6867735205	16.3601348285
H61	15.3445274655	6.1502280498	16.7980177357
H62	14.9699168536	7.6084461744	17.7209323213
C63	14.0098320992	7.5360643273	15.7314486151
C64	14.4197312961	6.9675828934	14.3491417495
H65	15.3855944050	7.3940954812	14.0416681887
H66	13.6954897449	7.2127728580	13.5651320812
H67	14.5419010107	5.8785873577	14.3644252377
C68	11.1865040340	6.8792561175	14.7488693899
H69	11.2180738156	7.9047219731	14.3622334979
H70	10.1432435502	6.6566161412	14.9804813807
H71	11.4978355812	6.2148389186	13.9348504289
C72	13.8622657897	9.0641381710	15.5762984407
H73	14.8030010237	9.5055135390	15.2161890891
H74	13.6107817295	9.5599181338	16.5173653316
H75	13.0842743536	9.3301867781	14.8507993038
C76	7.1184342744	6.5458895064	20.5335564300
C77	6.5527059952	5.7751298804	21.5711708701
H78	5.6711587291	6.1252010042	22.1008728617
C79	8.3264513302	6.1439293924	19.8900921460
C80	8.8452030975	4.8977972480	20.2960766571
H81	9.7490085335	4.5128874011	19.8202713097
C82	8.2698173810	4.1111210748	21.2985597561
H83	8.7201528668	3.1608497744	21.5788741448
C84	7.1257740879	4.5669136467	21.9566227045
H85	6.6834796985	3.9881036846	22.7632450153
N86	7.8720836726	6.9561530551	16.5292064693
C87	6.7793042536	7.8225163559	16.0568604805
H88	5.8332567441	7.4616962756	16.4871902228
H89	6.9260722143	8.8295704760	16.4458292726
C90	7.9338457882	5.7725055859	15.9686022549
N91	7.1554923426	5.3962221656	14.9135134735
C92	8.8856180833	4.7429893419	16.5252796230
C93	7.1756310176	4.0449946766	14.3646094494
H94	7.9341574387	3.9307091598	13.5776520721
H95	6.1961406519	3.8337251743	13.9251206164
C96	6.4106122316	6.3691882209	14.0933712325
H97	5.3389297061	6.1432666853	14.1766320480
H98	6.6945764183	6.2149485384	13.0438174038
C99	6.6987832902	7.8009063107	14.5322181942
H100	5.9116941897	8.4664070543	14.1640221649
H101	7.6500448456	8.1491208768	14.1143754738
H102	7.3567570926	3.3027397884	15.1410328081
H103	7.9333791023	9.7104839208	19.0644229556
H104	9.4189436803	4.2064271658	15.7368293744
H105	9.6270971810	5.2190651075	17.1663861371
H106	8.3412803616	4.0171389963	17.1396546271

Intermediate-DBU

Y1	8.9631994249	8.7955502927	17.9763473297
Fe2	10.1156211655	9.9478772005	20.4904637329
Si3	11.7518531198	6.2189108636	17.9474550665
Si4	10.7539988729	11.4357840797	16.2694265968
N5	9.6232294401	10.9841844418	17.5098069731
N6	5.8304273796	8.9426014772	20.4447302226
N7	10.8029221295	7.5964042631	18.4553676155
C8	4.1004937835	10.3837725196	20.9184999295
H9	3.6901454253	11.2546147526	21.4257870823
C10	5.4698288421	10.0640923631	21.1503360298
C11	5.0998060856	8.1654867024	19.5794089245
C12	3.2714241324	9.6363425676	20.0934205732
H13	2.2263206991	9.9145431634	19.9606284208
C14	3.7712470891	8.5204322554	19.3997543538
H15	3.1443529927	7.9482814803	18.7249027705
C16	8.4711932683	11.0256709354	19.7134750964
H17	7.4754229841	10.7443533352	19.3952011308
C18	8.7755057944	11.4177163772	21.0547152995
H19	8.0814827292	11.3449676923	21.8795650155
C20	10.8810668527	8.0693981198	19.7842936511
C21	9.5983550565	11.3325929250	18.8414672453
C22	11.8937662475	8.9054447747	20.3792086173
H23	12.7599723054	9.2903058391	19.8609310925
C24	10.6296971463	11.8203603720	19.7259044596
H25	11.6341396965	12.0785916344	19.4254139222
C26	11.5525732801	9.1575074476	21.7414367841
H27	12.1199910264	9.7636996338	22.4345595564
C28	10.2986850196	8.5306430758	22.0096491557
H29	9.7538201172	8.5674323713	22.9433767362
C30	9.8817810002	7.8682231407	20.8216767231
H31	8.9927645666	7.2643179474	20.7005625050
C32	10.1035135798	11.9268695285	21.0526694134
H33	10.6462217948	12.2891845889	21.9155676736
C34	10.1852971807	13.0249351830	15.3286604611
C35	10.0587527132	14.1984750465	16.3229820932
H36	9.7171319239	15.1083315216	15.8084645880
H37	11.0163393596	14.4386863887	16.7999538849
H38	9.3373165162	13.9780609666	17.1178023080
C39	12.5459577418	11.7120383625	16.8530091381
H40	12.8671910061	10.9079455527	17.5228345710
H41	12.6778916277	12.6618650475	17.3830614507
H42	13.2324204586	11.7197099312	15.9981794289
C43	8.8146573933	12.7958254081	14.6601620752
H44	8.4910986531	13.6982197325	14.1211058524
H45	8.0450020127	12.5606884685	15.4020242835
H46	8.8438964574	11.9750121522	13.9332540131
C47	11.2123003042	13.3955108411	14.2369211304
H48	10.8872108919	14.2923920759	13.6899571948
H49	11.3341949308	12.5946887432	13.4973723001
H50	12.2005085606	13.6127396862	14.6570478034
C51	10.7751162004	9.9632403324	15.0639043640
H52	11.2474643766	9.0932495297	15.5381033590
H53	11.3504487931	10.1784778207	14.1564063396
H54	9.7614319032	9.6848608429	14.7516079364
C55	11.4407407938	4.7405863151	19.1027561990
H56	10.3987997540	4.4060302571	19.0554566289
H57	11.6447229244	5.0143083998	20.1440598988
H58	12.0775396058	3.8825145678	18.8579317342
C59	14.3116697558	6.4645310888	19.2714170109
H60	15.3968589241	6.6291636864	19.2002282215
H61	14.1636864548	5.4980210396	19.7659649201
H62	13.9071698667	7.2367087391	19.9323448464
C63	13.6738268575	6.4927213130	17.8637354421
C64	14.3134585011	5.3518623066	17.0382926107
H65	15.4082212689	5.4546013163	17.0349064025
H66	13.9840921847	5.3603834051	15.9938520577
H67	14.0862965451	4.3622420262	17.4530444609
C68	11.1494630812	5.7894945146	16.1950345787
H69	11.3598947308	6.5961378066	15.4827026398
H70	10.0705306615	5.5986275656	16.1784202773
H71	11.6386336903	4.8852470364	15.8180616300
C72	14.0089774837	7.8351486519	17.1828745341
H73	15.0977702586	7.9736064885	17.1115088175
H74	13.6033341323	8.6867916352	17.7374715603
H75	13.6082494950	7.8900687071	16.1631452065
C76	5.7883768375	7.0115457081	18.9555854228
C77	5.0299021495	5.8439267896	18.7433846181
H78	3.9806967524	5.8212763990	19.0275085094
C79	7.1820035028	7.0820020236	18.6587193658
C80	7.7325884258	5.8667305762	18.1873699483
H81	8.8015134691	5.8150499104	17.9908095978
C82	6.9905705671	4.6987287885	17.9585734603
H83	7.4827785641	3.7990257402	17.5936249045
C84	5.6220704542	4.6908427450	18.2294820016
H85	5.0304537971	3.7908093896	18.0832908066
N86	7.1653790333	9.2505196517	16.2774884100
C87	6.4099597961	10.4367375632	16.7172400498
H88	5.8558753610	10.1954081180	17.6358918613
H89	7.1420456912	11.2107982791	16.9616732435
C90	6.5820716849	8.4214591286	15.4542845054
N91	5.3122099879	8.5663833569	14.9751136217
C92	7.3598648611	7.2109982756	14.9944361574
H93	8.4122549019	7.3326638782	15.2537370972
H94	6.9964097235	6.2996794777	15.4795299075
C95	4.6537640053	7.5722851075	14.1377349170
H96	4.7222333404	7.8212594978	13.0694234948
H97	3.5938637520	7.5301982145	14.4093685319
C98	4.5187954532	9.7704050038	15.2582073633
H99	3.7976569723	9.5525618724	16.0591937886
H100	3.9448987653	10.0156158021	14.3565020886
C101	5.4312093025	10.9244376856	15.6521513522
H102	4.8354786988	11.7613398524	16.0300648567
H103	5.9865480199	11.2788249411	14.7762957122
H104	7.3021321801	7.0798017738	13.9099004059
H105	5.0693814956	6.5783317377	14.2961235530
H106	6.7922750466	8.6262462780	20.5519739554

2^{Y}-Phpy-DBU

Y1	9.3403011751	7.8929256257	18.4834695068
Fe2	11.4537785908	9.0647311496	20.6350407353
Si3	12.3652833005	6.6484524998	16.5719687747
Si4	9.6268397524	11.4399516350	17.3539812647
N5	9.2955444598	10.2559599563	18.5959542492
N6	6.9733790044	8.0778238071	19.5940627826
N7	11.5040609705	7.3859252842	17.8988174635
C8	5.0457003010	9.3857627695	20.1960158150
H9	4.5350462327	10.3428791774	20.1736239413
C10	6.2894232736	9.2352025808	19.5964489376
C11	6.4646573031	6.9869402408	20.2233612515
C12	4.4995622404	8.2725211192	20.8375086849
H13	3.5343051687	8.3372370957	21.3331458008
C14	5.2088761463	7.0795522963	20.8558145077
H15	4.7970700471	6.2244392974	21.3762284800
C16	9.4390484399	9.5151048674	21.0081468075
H17	8.5824933346	8.8597730800	21.0404156707
C18	10.2642444631	9.8127579300	22.1378574695
H19	10.1734591057	9.3713572143	23.1204685756
C20	12.1258742531	7.6710280253	19.1353753812
C21	9.8428680130	10.3367716042	19.8758520586
C22	13.0832069876	8.7109287414	19.4258189907
H23	13.4473973932	9.4346348507	18.7132297213
C24	10.9935827523	11.0722188725	20.3469763342
H25	11.5948793589	11.7376864504	19.7486414450
C26	13.4584815315	8.6401708449	20.8012177213
H27	14.1597076026	9.2942683909	21.3023700485
C28	12.6975505033	7.5978958501	21.4094340536
H29	12.7202868235	7.3156975234	22.4536702737

C30	11.8765111030	7.0134538132	20.4041804465
H31	11.1840838344	6.1990883378	20.5545732163
C32	11.2136818524	10.7891733948	21.7293990532
H33	11.9973815795	11.2136211359	22.3423363187
C34	8.6334037948	13.0892398396	17.6029705555
C35	9.0864980715	13.8153612021	18.8877374299
H36	8.5115788649	14.7427776907	19.0286665694
H37	10.1450960452	14.0962092344	18.8500163581
H38	8.9397483262	13.1976500787	19.7796848451
C39	11.4668346781	11.8959788822	17.1214220331
H40	12.0942564294	11.0046446583	17.2230608370
H41	11.8343640698	12.6446797414	17.8307901431
H42	11.6299389898	12.3003172252	16.1154559271
C43	7.1222438599	12.8061546428	17.7182291247
H44	6.5569718446	13.7455117450	17.8097995616
H45	6.8973374380	12.2027620812	18.6035783043
H46	6.7287259657	12.2787377040	16.8404712492
C47	8.8704061347	14.0233642793	16.3949907743
H48	8.3253913066	14.9699302518	16.5268029149
H49	8.5220551963	13.5789967848	15.4551857795
H50	9.9296679266	14.2756753648	16.2710976947
C51	9.1042233546	10.7090842566	15.6732703145
H52	9.4235925728	9.6663719093	15.5602119754
H53	9.5848425388	11.2759623175	14.8677393938
H54	8.0253317807	10.7560500640	15.4964128115
C55	12.5142610987	4.7673933206	16.8671955574
H56	11.5288849662	4.3049723597	16.9921957364
H57	13.0751545160	4.5717419634	17.7888607642
H58	13.0242477690	4.2404870880	16.0524578719
C59	15.1743032233	6.9307692758	17.2770832374
H60	16.1864239824	7.2489502229	16.9861659887
H61	15.2192673871	5.8523166325	17.4677515147
H62	14.9339378433	7.4238539083	18.2225347424
C63	14.1648822774	7.2713814708	16.1581035931
C64	14.6331016968	6.5508097481	14.8688213989
H65	15.6437408359	6.8886182900	14.5965585475
H66	13.9819178130	6.7608824767	14.0126611241
H67	14.6820012099	5.4635857589	14.9947493783
C68	11.3366861486	6.9639716577	14.9961182165
H69	11.6405403143	7.9015675215	14.5182094774
H70	10.2671810509	7.0496488356	15.2042139944
H71	11.4711506448	6.1635918812	14.2593518592
C72	14.2035228831	8.7884284263	15.8770895558
H73	15.2225212178	9.1004692272	15.6053139033
H74	13.9013825436	9.3848421115	16.7413089141
H75	13.5492852529	9.0691902058	15.0435253269
C76	7.2996544298	5.7564136733	20.2278389087
C77	6.7914868084	4.5646507644	20.7860713277
H78	5.7887084481	4.5207886706	21.2027718433
C79	8.6078330748	5.8227057970	19.6700255118
C80	9.3424362261	4.6176272385	19.7155645219
H81	10.3494038826	4.5923986125	19.2980209092
C82	8.8512220696	3.4332854938	20.2740369656
H83	9.4671212451	2.5356155079	20.2898862491
C84	7.5631006515	3.4067066991	20.8130753475
H85	7.1633036721	2.4957627786	21.2511767562
N86	7.8001022579	7.2975232392	16.5835000352
C87	6.7186938088	8.2661405509	16.3456061956
H88	5.8347130960	7.9632444735	16.9249094702
H89	7.0298035330	9.2388529568	16.7285612282
C90	7.7184925133	6.1711426796	15.9185361096
N91	6.7730056042	5.9128263698	14.9672608089
C92	8.6962108746	5.0667919447	16.2259518370
C93	6.6684875716	4.6260921665	14.2886655508
H94	7.2654348707	4.5978522578	13.3663140733
H95	5.6208459371	4.4568719465	14.0209091115
C96	5.9141071738	6.9655924181	14.4015292143
H97	4.8743280567	6.7710084007	14.6999364031
H98	5.9569822123	6.8874331212	13.3074527745
C99	6.3635340380	8.3466312246	14.8624545237
H100	5.5650043615	9.0743265294	14.6847205079
H101	7.2427748536	8.6732470897	14.2970691020
H102	6.9805882402	3.8072735399	14.9351602918
H103	6.7994018985	10.0641586971	19.1125635472
H104	9.1563021977	4.6655181492	15.3191360124
H105	9.4843465368	5.4335891255	16.8779600567
H106	8.1984810807	4.2503112918	16.7596859783

TS5-DBU

Y1	8.6782914978	7.5884419069	17.6735176495
Fe2	11.0701174628	9.1191168269	19.8755037995
Si3	11.8109123668	5.8209776471	16.4670100913
Si4	6.6471367125	10.5255718036	18.7562405399
N5	8.0425735905	9.4610305205	18.7719931881
N6	8.1054191920	5.6762071380	19.4792802441
N7	10.8627791986	6.9639314632	17.4058560202
C8	8.3105787733	5.1087631736	21.8041183137
H9	8.9168432629	4.8033413889	22.6552356688
C10	8.9450834822	5.3787446670	20.5704654083
C11	6.7129687592	5.6247489411	19.5665668020
C12	6.9376605573	5.2773981838	21.9484604035
H13	6.4652872610	5.2027000354	22.9279152258
C14	6.1324994367	5.5084275390	20.8265060487
H15	5.0527757144	5.6095020406	20.9323593280
C16	9.2945997066	9.1413457721	20.9771220559
H17	8.7726061282	8.2667817565	21.3392805596
C18	10.3281369826	9.8448193149	21.6621670655
H19	10.7410963363	9.5865971973	22.6290805969
C20	11.6054843002	7.6499913421	18.4016033277
C21	9.0475533275	9.7875923336	19.7093058758
C22	12.3518192124	8.8820547135	18.2545360720
H23	12.3520906529	9.5070340125	17.3675482362
C24	9.9939025082	10.8716672277	19.6214329881
H25	10.0939280511	11.5405362435	18.7760350557
C26	13.0912345989	9.1233609922	19.4560804257
H27	13.7365077526	9.9736436107	19.6513673417
C28	12.7797772003	8.0717122225	20.3807076210
H29	13.1455437840	7.9927362632	21.3997484665
C30	11.8571009738	7.1862253016	19.7476190771
H31	11.3755919408	6.3189571591	20.1843962814
C32	10.7560218276	10.9207792546	20.8253977496
H33	11.5512231911	11.6202844252	21.0478976242
C34	5.5570405697	10.4638458418	20.3632945118
C35	6.2508787492	11.1937119878	21.5332574380
H36	5.6309082262	11.1279481067	22.4379750448
H37	6.4029419343	12.2583449466	21.3252234285
H38	7.2281168003	10.7627268403	21.7690036461
C39	7.1527057024	12.3488762414	18.5237382875
H40	7.6562891267	12.5042308108	17.5598645279
H41	7.8321152302	12.6875216273	19.3132289369
H42	6.2648604269	13.0094840561	18.5481376983
C43	5.2803028851	9.0067635195	20.7738985473
H44	4.6193919740	8.9758075645	21.6475740238
H45	6.2037866669	8.4863433340	21.0356113089
H46	4.7894902169	8.4347444085	19.9780560407
C47	4.2030966618	11.1570025762	20.0953955574
H48	3.5912974316	11.1640278920	21.0032323987
H49	3.6210511897	10.6482188050	19.3208768541
H50	4.3287265380	12.2021316674	19.7923565198
C51	5.5757678014	10.0563255469	17.2735939050
H52	6.1727417718	10.0068730914	16.3519742368
H53	4.8056886576	10.8071018055	17.1257534453
H54	5.0925858158	9.0878479099	17.3908069448
C55	12.9761395691	4.8068161980	17.5646989937
H56	12.4115111719	4.2534993827	18.3156411006
H57	13.6983786798	5.4469012948	18.0859974477
H58	13.5378450621	4.0921198933	16.9720185653
C59	14.2758013986	7.1354310334	15.7182163081
H60	14.9232783537	7.5644155007	14.9293742285
H61	14.8332723170	6.3267634253	16.2013989914
H62	14.1042211571	7.9270138626	16.4684905138
C63	12.9659930233	6.6170893554	15.1044192463
C64	13.3355333356	5.5497935299	14.0533255301
H65	14.0251179530	5.9647858334	13.3113822741
H66	12.4687566703	5.1886291685	13.5138348653
H67	13.8314332918	4.6824708846	14.5002890948
C68	10.6276067958	4.5919560957	15.6319793086
H69	10.1752023505	4.9571377725	14.7204324610
H70	9.8174368301	4.3312844213	16.3417433188
H71	11.1612694341	3.6693164566	15.3805945154
C72	12.2661641218	7.7886581874	14.3940786169
H73	12.9009987173	8.1946531212	13.5901736276
H74	12.0422916361	8.5988420512	15.0906689883
H75	11.3208520720	7.4798787696	13.9393613196
C76	5.9214500011	5.7637046219	18.3207348549
C77	4.6120544825	5.2301843026	18.2926794699
H78	4.2368278215	4.6624750089	19.1399607010
C79	6.4884877250	6.4710489588	17.2132110424
C80	5.6045162653	6.6290792338	16.1195766232
H81	5.9236238785	7.1993302806	15.2629071850
C82	4.2982496724	6.1144911327	16.0836811501
H83	3.6636519711	6.2726005410	15.2111800424
C84	3.8042883401	5.3940374009	17.1702440345
H85	2.7972575683	4.9663666041	17.1431934365
N86	8.6175236931	8.3538450261	15.2440160526
C87	8.3890781389	7.2572168901	14.2794100195
H88	9.3809903318	6.8312015734	13.9840637686
H89	7.8257552731	6.4408166916	14.7838630364
C90	8.9325017799	9.5216615315	14.7456923299
N91	8.9408125613	9.8168242952	13.4065731286
C92	9.3143360904	10.6278606175	15.6810099790
H93	9.1057062265	10.3495967391	16.6998399560
H94	10.3744760752	10.8420287651	15.6037620103
C95	9.5599701077	10.9985781180	12.8459453457
H96	9.7480983800	11.7509269406	13.5874115150
H97	8.9004231713	11.4352344545	12.0800286845
C98	8.5261811002	8.8404304878	12.3929600514
H99	9.4126113547	8.4061171657	11.9144435901
H100	7.9718486934	9.3767126939	11.6109968878
C101	7.6793820640	7.7425434744	13.0203352217
H102	7.5485723575	6.9170700714	12.3046347158
H103	6.6837099798	8.1281002695	13.2785564858
H104	8.7574447824	11.5455736485	15.4590386512
H105	10.5062863180	10.7391395704	12.3825933723
H106	9.0514304623	4.8030004978	19.2987250404
N107	9.7920699426	0.6373513573	18.0238918327
C108	9.2582647396	1.9093868469	18.0928141841
N109	9.6653128172	2.8361207501	18.8930642602
C110	10.7123427554	2.5367290781	19.8717158758
C111	11.6747343690	1.4517903451	19.3895301099
C112	10.8606343855	0.2369765629	18.9506722594
C113	9.1268958447	-0.4546629317	17.3362616451
C114	8.1335916558	2.2480614271	17.1308713543
H115	11.2421045247	3.4696436379	20.0899201354
H116	10.2383643743	2.2295433338	20.8192049264
H117	12.2592623414	1.8293951134	18.5412949786
H118	12.3845565591	1.1685440753	20.1779086446
H119	10.4315499167	-0.2768540781	19.8308123852
H120	11.5018882677	-0.4917316356	18.4356827084
H121	9.8883370500	-1.1399393324	16.9377414665
H122	8.4639457137	-1.0314220585	18.0091708877
H123	8.5275733792	-0.0936225761	16.4922422273
H124	7.8616350916	3.2884938345	17.2717607772
H125	8.4366967281	2.1058145031	16.0858613361
H126	7.2412931079	1.6339949448	17.3115133710