Chemical Communications

Supporting Information for:

Ambiphilic Geometrically Constrained Phosphenium Cation

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General experimental considerations

All preparations were carried out under an anhydrous N_2 atmosphere using standard Schlenk and glovebox techniques. All glassware was oven dried and cooled under vacuum before use. Commercial reagents were purchased from Sigma Aldrich, Strem or Apollo Scientific and used without further purification unless indicated otherwise. All solvents were dried using a Vac. Atm. solvent purification system. Compound **2** was prepared as previously reported.[1] NMR spectra were recorded at room temperature using a Bruker AvanceIII-400 MHz spectrometer. Data for 1H NMR are reported as follows: chemical shift (δ ppm), integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, m = multiplet, br = broad), coupling constant (Hz), assignment.

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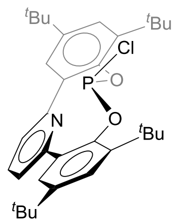
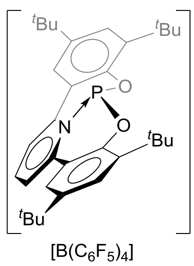


To a stirred 0.59 mL PCl_3 (6.76 mmol, 1.13 eq.) in 30 mL of THF held at -78^0 C was added dropwise 3.30 gr (5.98 mmol, 1 eq.) 6,6'-(pyridine-2,6-diyl)bis(2,4-di-tert-butylphenol), dissolved in THF. When the addition was complete, triethylamine (1.13 mL, 0.012 mol, 2 eq.) was also added dropwise to the reaction flask with the aid of 20 mL THF. The reaction was left to stir overnight at -78 °C and slowly warmed to room temperature. The $[Et_3NH][Cl]$ was separated from the red solution, which was evaporated under reduced atmosphere to give **3** in 78% yield as a pink solid, which was used in the next step without purification.

^{1}H NMR (400 MHz; $CDCl_3$), δ 1.27 (18H, s, t-Bu), 1.36 (18H, s, t-Bu), 7.60 (2H, d, *J* = 1.8, Ar-H), 7.77 (2H, d, *J* = 1.8 Hz, Ar-H), 8.49 (2H, d, *J* = 8.24 Hz, Ar-H), 9.21 (1H, t, *J* = 8.16 Hz, Ar-H) ^{13}C NMR (100 MHz; $CDCl_3$), δ 29.6 (C(**C**H_3)$_3$), 31.2 (C(**C**H_3)$_3$), 35.0 (**C**(CH_3)$_3$), 35.18(**C**(CH_3)$_3$), 120.2 (Ar), 120.3 (Ar), 131.5 (Ar), 139.9 (Ar), 142.2 (Ar), 145.7 (Ar), 145.8 (Ar), 150.4 (Ar), 150.6 (Ar) ^{31}P NMR (162 MHz; C_6H_5Br) δ 90.91. ^{31}P NMR (162 MHz; THF) δ 92.68. ^{31}P NMR (162 MHz CH_2Cl_2) δ 119.37. ^{31}P NMR (162 MHz; MeCN) δ 127.79.

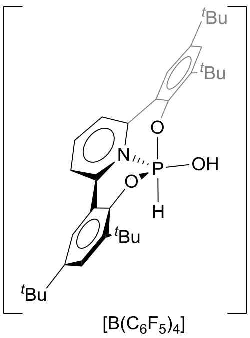
[1][B(C_6F_5)$_4$]



To a stirred dark red solution of **3** (0.48 gr, 0.087 mmol, 1 eq.) in DCM was added an equimolar amount of $KB(C_6F_5)_4$ (1.07 gr, 0.087 mmol, 1 eq.) at r.t under inert atmosphere, which caused an immediate change in color to yellow/green. The mixture was filtered and evaporated under reduced atmosphere to give a pale yellow solid. A recrystallization of the solid in a 10:1 Hexane/DCM solution afforded clean **[1][B(C_6F_5)$_4$]** in 93% yield as pale yellow needles.

^{1}H NMR (400 MHz; DCM with [D_6] DMSO capillary), δ 1.86 (18H, s, t-Bu), 1.97 (18H, s, t-Bu), 8.15 (2H, d, *J* = 1.88Hz, Ar-H), 8.31 (2H, d, *J* = 2.04 Hz, Ar-H), 8.55 (2H, d, *J* = 8.04 Hz, Ar-H), 8.93 (1H, t, *J* = 8.12 Hz, Ar-H) ^{13}C NMR (100 MHz; DCM with [D_6] DMSO capillary), δ 29.7 (C(**C**H_3)$_3$), 31.2 (C(**C**H_3)$_3$), 35.5 (**C**(CH_3)$_3$), 35.6 (**C**(CH_3)$_3$), 120.3 (Ar), 120.4 (Ar), 123.4 (Ar), 133.2 (Ar), 140.0 (Ar), 140.1 (Ar), 143.5 (Ar), 148.1 (Ar), 151.8 (Ar); ^{31}P NMR (162 MHz, DCM with [D_6] DMSO capillary) δ 128.24. MS (ESI) calc'd for $C_{33}H_{43}NO_2P$ (M^+) 516.3026, found 516.3031

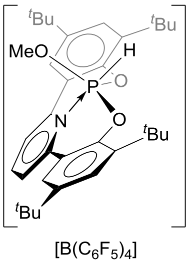
Reaction with H_2O ([4][B(C_6F_5)$_4$)



An equimolar amount of H_2O (2 mg, 0.011 mmol) was added to **[1][B(C_6F_5)$_4$]** (0.13 gr, 0.011 mmol) dissolved in DCM, resulting in an immediate reaction between the two. The DCM was evaporated under reduced pressure, giving **[4][B(C_6F_5)$_4$** in 93% yield.

^{1}H NMR (400 MHz; DCM with [D_6] DMSO capillary), δ 1.76 (9H, s, t-Bu), 1.77 (9H, s, t-Bu), 1.87 (9H, s, t-Bu), 1.88 (9H, s, t-Bu), 7.28 (1H, d, *J* = 724 Hz, P-H), 7.78 (1H, d, *J* = 2.4 Hz, Ar-H), 7.87 (1H, d, *J* = 2.32 Hz, Ar-H), 8.09 (1H, d, *J* = 2.32 Hz, Ar-H), 8.22 (1H, d, *J* = 2.16 Hz, Ar-H), 8.30 (1H, d, *J* = 7.92 Hz, Ar-H), 8.87 (1H, d, *J* = 8.08 Hz, Ar-H); ^{13}C NMR (100 MHz; DCM with [D_6] DMSO capillary), δ 29.2 (C(**C**H_3)$_3$), 30.1 (C(**C**H_3)$_3$), 30.3 (C(**C**H_3)$_3$), 30.4 (C(**C**H_3)$_3$), 34.1 (**C**(CH_3)$_3$), 34.4 (**C**(CH_3)$_3$), 34.6 (**C**(CH_3)$_3$), 35.0 (**C**(CH_3)$_3$), 118.5 (Ar), 124.1(Ar) (Ar), 124.9 (Ar), 125.1 (Ar), 125.4 (Ar), 125.9 (Ar), 129.4 (Ar), 129.6 (Ar), 139.6 (Ar), 142.5 (Ar), 143.0 (Ar), 145.3 (Ar), 145.9 (Ar), 149.3 (Ar), 150.1 (Ar), 150.7 (Ar), 152.5 (Ar); ^{31}P NMR (162 MHz, DCM with [D_6] DMSO capillary) δ 3.07 (d, *J* = 725 Hz). MS (ESI) calc'd for $C_{33}H_{45}NO_3P$ (M^+) 534.3132, found 534.3137

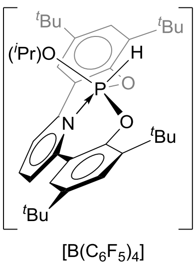
Reaction with MeOH ([5][B(C_6F_5)$_4$)



An equimolar amount of MeOH (4 mg, 0.013 mmol) was added to **[1][B(C_6F_5)$_4$]** (0.15 mg. 0.013 mmol) dissolved in DCM, resulting in an immediate reaction between the two. The DCM was evaporated under reduced pressure, giving **[5][B(C_6F_5)$_4$** in 90% yield as a yellow oil.

^{1}H NMR (400 MHz, CD_2Cl_2), δ 1.41 (s, 18H, t-Bu), 1.57 (s, 18H, t-Bu), 3.32 (s, 3H, P-OMe), 6.68(d, *J* = 708 Hz, 1H, P-H) 7.65 (d, *J*=2.20Hz, 2H, Ar-H), 7.74 (d, *J*=2.24 Hz, 2H, Ar-H), 8.13 (dd, *J* = 8.12 Hz, Ar-H), 8.49 (t, *J*= 8.20 Hz, 1H, Ar-H); ^{13}C NMR (100 MHz, CD_2Cl_2), δ 29.9 (C(**C**H_3)$_3$), 30.8 (C(**C**H_3)$_3$), 34.2 (**C**(CH_3)$_3$), 34.6 (**C**(CH_3)$_3$), 73.0 (**C**H_3O), 117.4 (Ar), 123.6 (Ar), 125.0 (Ar), 129.9 (Ar), 137.0 (Ar), 145.7 (Ar), 145.8 (Ar), 150.3 (Ar), 150.8 (Ar); ^{31}P NMR (162 MHz, CD_2Cl_2) δ 11.69 (d, *J* = 708 Hz) MS (ESI) calc'd for $C_{34}H_{47}NO_3P$ (M^+ +H_2O) 566.3395, found 566.3399

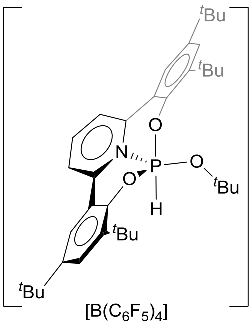
Reaction with i-PrOH ([6][B(C_6F_5)$_4$])



A tenfold excess of i-PrOH (102 mg, 1.70 mmol, 10 eq.) was added to **[1][B(C_6F_5)$_4$]** (0.2 gr, 0.17 mmol, 1 eq.) dissolved in DCM, and stirred overnight. The reaction proceeds with 99% conversion to give **[6][B(C6F5)$_4$]**. Upon an attempt to remove the excess of i-PrOH under vacuum and heating to 50 ºC, **[6][B(C6F5)$_4$]** reacted further giving a complex mixture of products.

^{1}H NMR (400 MHz, DCM with [D_6] DMSO capillary), 1.78 (6H, d, J = 6.40 Hz, POC(C_2H_6)) 1.81 (18H, s, t-Bu), 1.92 (18H, s, t-Bu), 5.09 (1H, sept, *J* = 6.40 Hz, POCH), 7.23 (1H, d, J = 689 Hz, P-H), 7.89 (2H, d, *J*= 2.20 Hz), 7.99 (2H, d, *J* = 2.16 Hz), 8.15 (2H, d, *J* = 8.00 Hz), 8.43 (1H, t, *J*= 7.84 Hz), ^{13}C NMR (400 MHz, DCM with [D_6] DMSO capillary), δ 28.7 (C(**C**H_3)$_3$), 30.7 (C(**C**H_3)$_3$), 33.7 (**C**(CH_3)$_3$), 34.6 (**C**(CH_3)$_3$), 119.7 (Ar), 120.6 (Ar), 122.3 (Ar), 125.5 (Ar), 136.4 (Ar), 139.3 (Ar), 140.9 (Ar), 152.4 (Ar), 156.6 (Ar); ^{31}P NMR (162 MHz, DCM with [D_6] DMSO capillary) δ 3.92 (d, *J* = 690 Hz) calc'd for $C_{36}H_{53}NO_4P$ (M^+ +H_2O) 594.3716, found 594.3712.

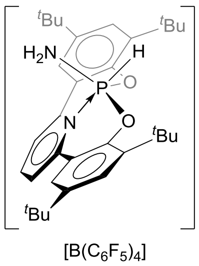
Reaction with t-BuOH ([7][B(C_6F_5)$_4$])



A fivefold excess of t-BuOH (40 mg, 0.11 mmol, 5 eq.) was added to **[1][B(C_6F_5)$_4$]** (0.13 gr, 0.022 mmol, 1 eq.) dissolved in DCM. The reaction proceeded slowly, over the period of 4 days. The DCM was evaporated under reduced pressure to give **([7][B(C_6F_5)$_4$]** as a yellow solid in 90% yield

^{1}H NMR (400 MHz, CD_3CN), δ 0.90 (9H, s, t-Bu), 1.34 (9H, s, t-Bu), 1.37 (9H, s, t-Bu), 1.45 (9H, s, t-Bu), 1.47 (9H, s, t-Bu) 6.98 (1H, d, *J* = 737 Hz, P-H), 7.35 (1H, d, J = 2.45 Hz, Ar-H), 7.50 (1H,d, *J* = 2.50 Hz, Ar-H), 7.62 (1H, d, *J* = 2.50 Hz, Ar-H), 7.80 (1H d, *J* = 1.90 Hz, Ar-H), 8.05 (1H, d, *J* = 8.0 Hz, Ar-H), 8.11 (1H, d, *J* = 8.10 Hz, Ar-H), 8.62 (1H, t, *J* = 8.00, Ar-H), ^{13}C NMR (100 MHz, DCM with [D_6] DMSO capillary), 25.5 (C(**C**H_3)$_3$), 28.7(C(**C**H_3)$_3$), 29.7 (C(**C**H_3)$_3$), 30.2 (C(**C**H_3)$_3$), 30.3 (C(**C**H_3)$_3$), 33.7 (**C**(CH_3)$_3$), 34.2 (**C**(CH_3)$_3$) , 34.7 (**C**(CH_3)$_3$), 34.8 (**C**(CH_3)$_3$), 69.9 (**C**(CH_3)$_3$), 118.5 (Ar), 123.5 (Ar), 125.1 (Ar), 126.6 (Ar), 126.9 (Ar), 127.5 (Ar), 127.6 (Ar), 128.2 (Ar), 128.3 (Ar), 129.0 (Ar), 138.4 (Ar), 141.9 (Ar), 143.3 (Ar), 145.6 (Ar), 150.5 (Ar), 151.3 (Ar), 153.0 (Ar) ^{31}P NMR (162 MHz, DCM with [D_6] DMSO capillary) δ 4.95 (d, *J* = 731 Hz) (ESI) calc'd for $C_{33}H_{45}NO_3P$ (M^+) 590.3768, found 590.3763.

Reaction with NH_3 ([8][B(C_6F_5)$_4$])



Ammonia gas was introduced to **[1][B(C_6F_5)$_4$]** (60 mg, 0.050 mmol) dissolved in toluene at r.t. The yellow color of the solution became less pronounced over the following minutes leading to an oxidative addition product **[8][B(C_6F_5)$_4$]** with 99% conversion. Mild heating with concurrent evacuation of the headspace lead to the regeneration of **[1][B(C_6F_5)$_4$]**.

^{1}H NMR (400 MHz, C_7D_8), δ 1.26 (18H, s, t-Bu), 1.41 (18H, s, t-Bu), 3.06 (2H, brs, P-NH_2), 7.16-7.63 (7H, m, Ar-H), 7.62 (1H, d, *J* = 757 Hz, P-H) ^{13}C NMR (100 MHz, toludene-d8), 29.5 (C(**C**H_3)$_3$), 31.4 (C(**C**H_3)$_3$), 34.2 (**C**(CH_3)$_3$), 35.3 (**C**(CH_3)$_3$), 119.5 (Ar), 121.1 (Ar), 122.7 (Ar), 126.1 (Ar), 139.2 (Ar), 141.0 (Ar), 153.7 (Ar), 157.3 (Ar) ^{31}P NMR (162 MHz, toluene-d8) δ -10.64 (d, *J* = 755 Hz). MS (ESI) calc'd for $C_{33}H_{45}NO_3P$ (M^++H_2O) 534.3405, found 534.3403

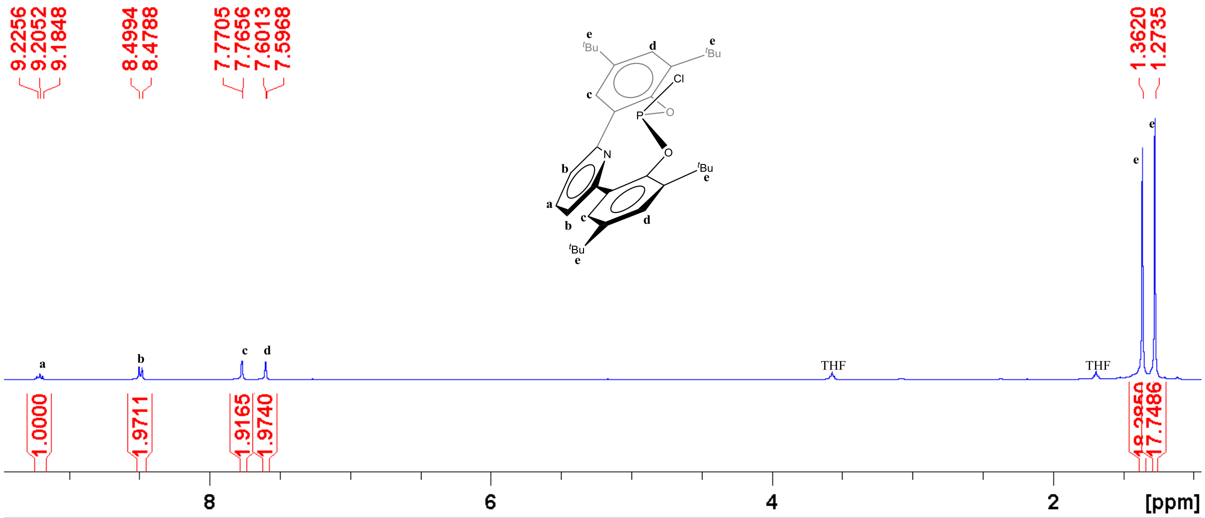


Figure S1. ^{1}H NMR of **3**

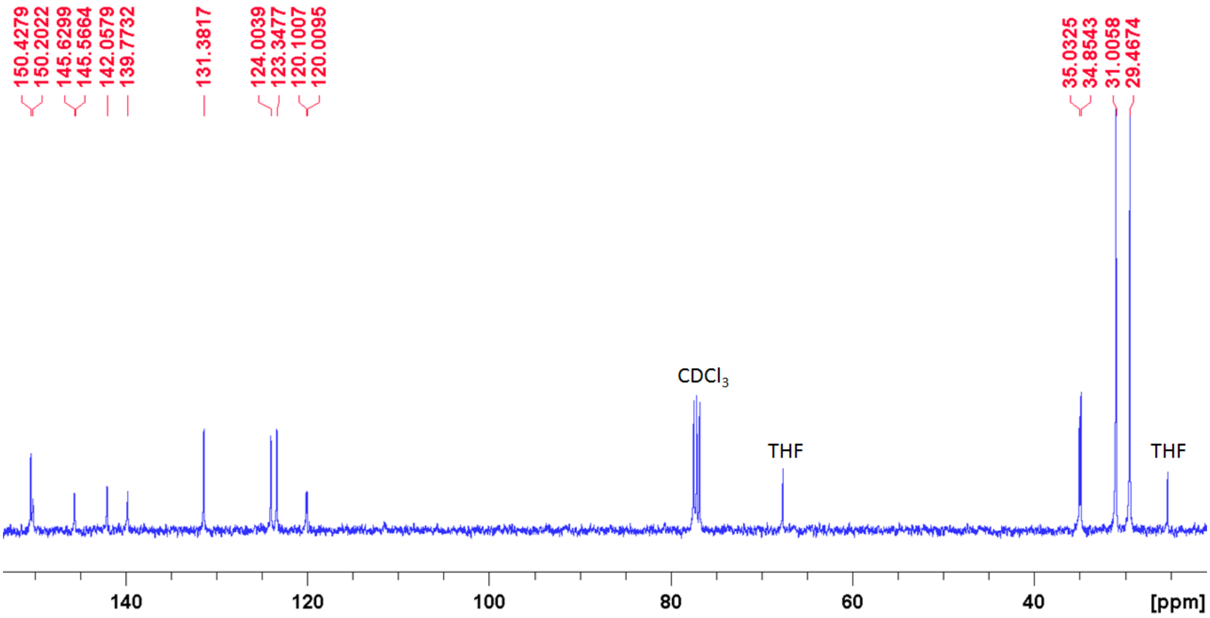


Figure S2. ^{13}C NMR of **3**

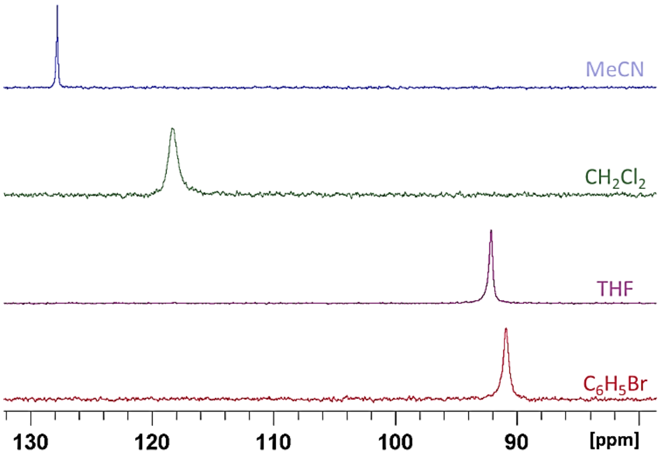


Figure S3. ^{31}P NMR of **3**

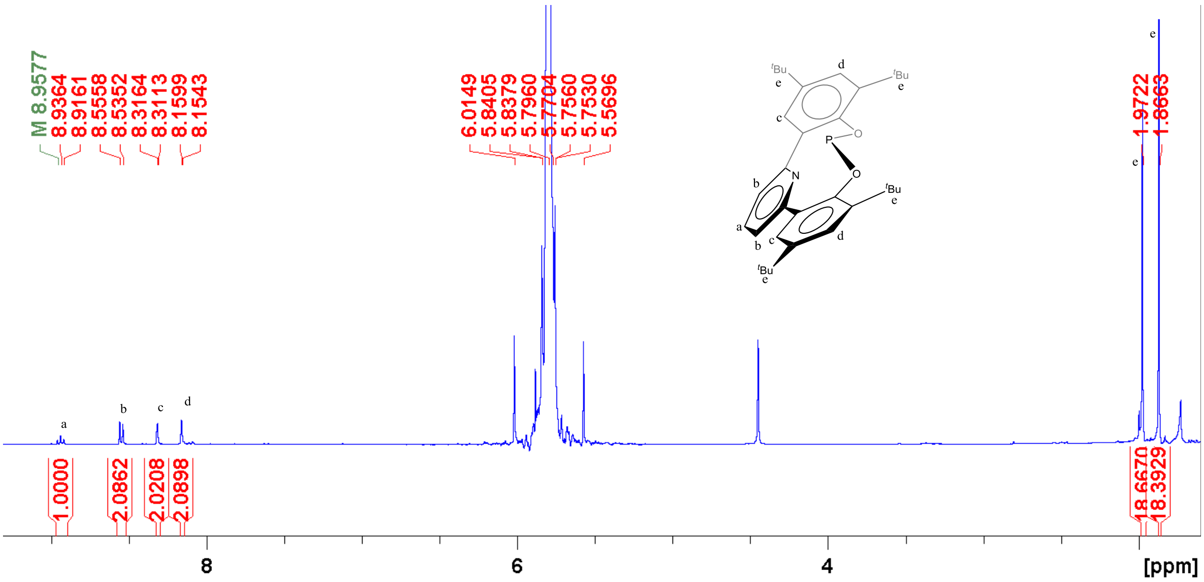


Figure S4. ^{1}H NMR of **[1][B(C$_6$F$_5$)$_4$]**

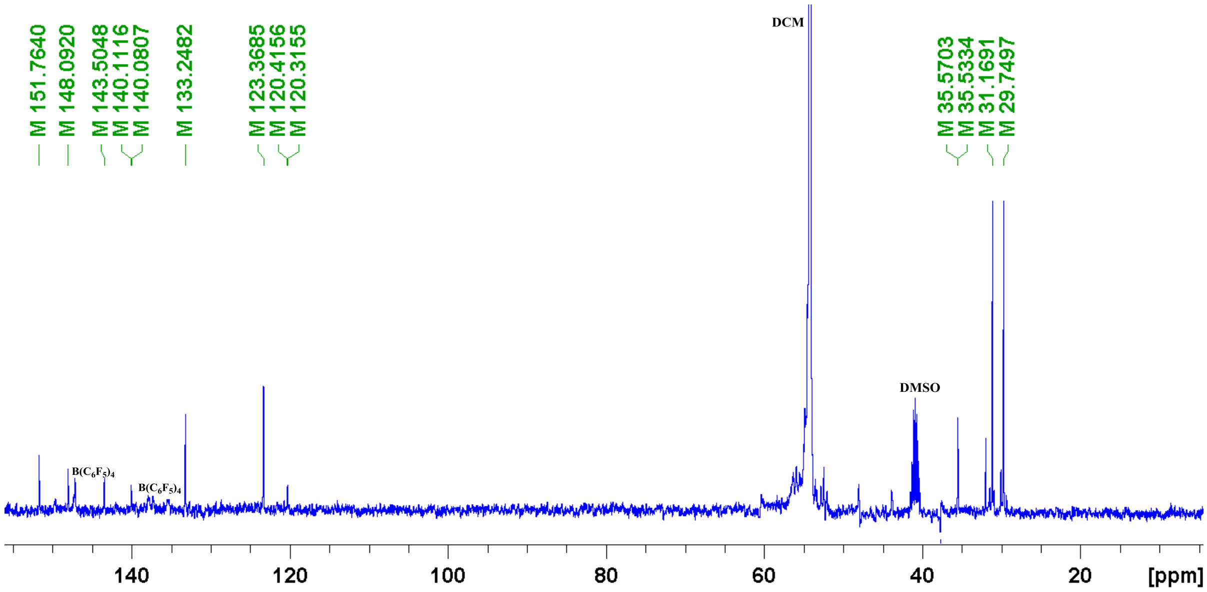


Figure S5. ^{13}C NMR of **[1][B(C$_6$F$_5$)$_4$]**

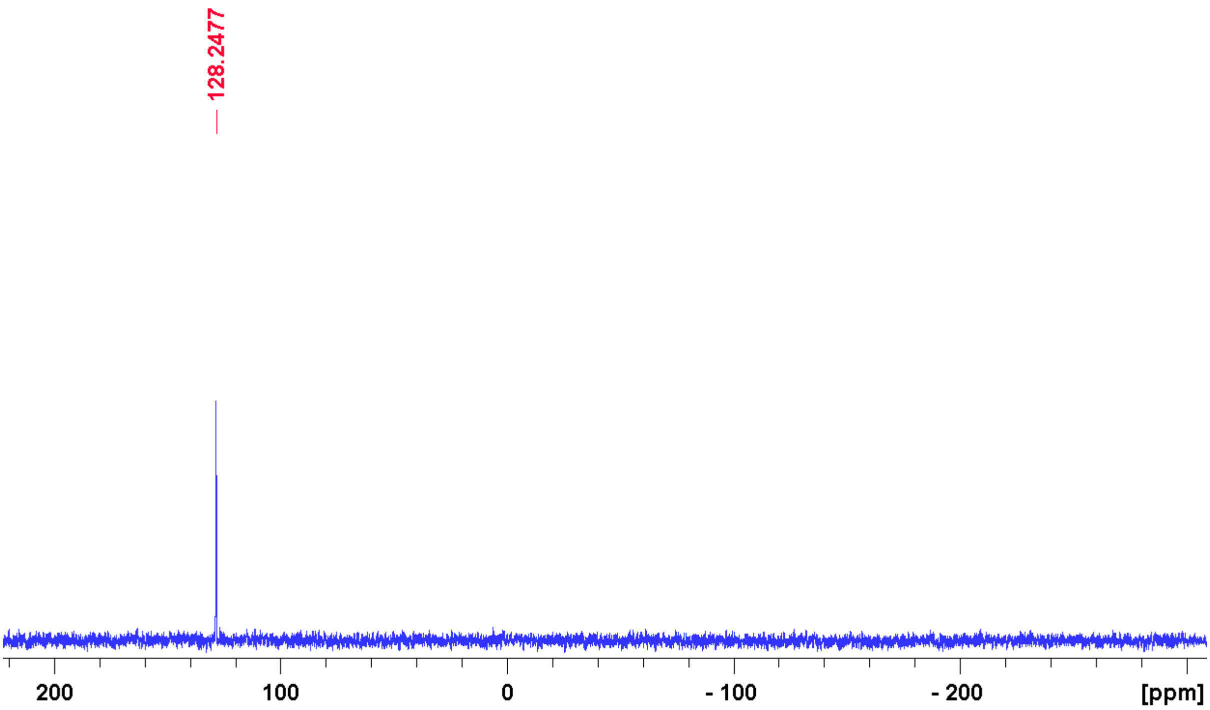


Figure S6. ^{31}P NMR of **[1][B(C$_6$F$_5$)$_4$]**

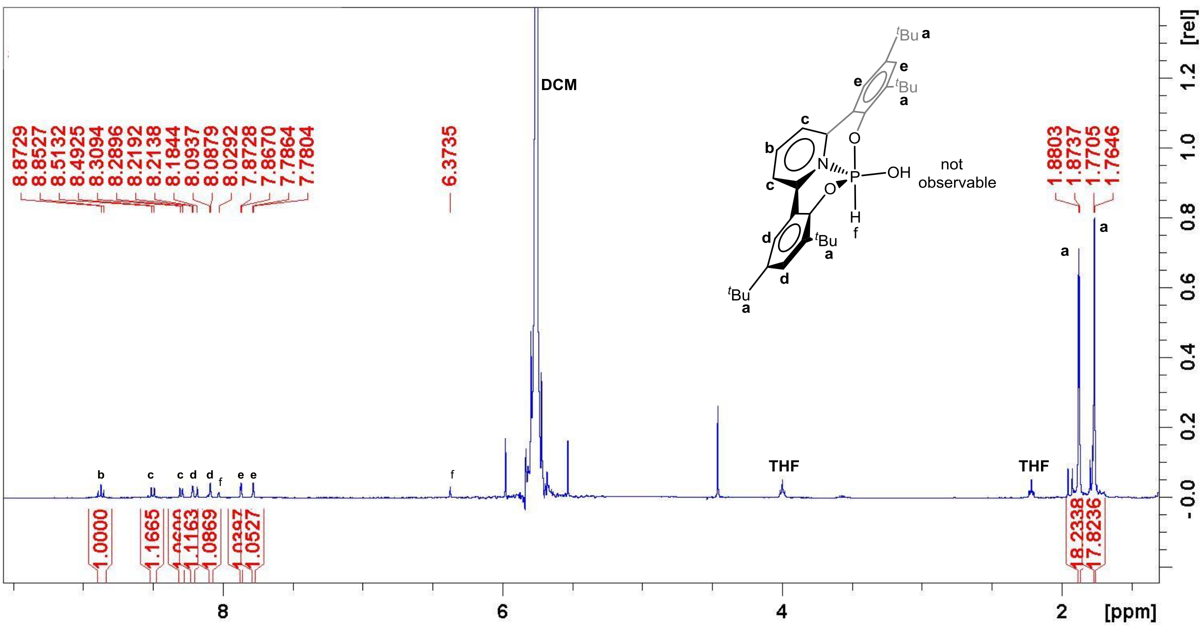


Figure S7. ^{1}H NMR of **[4][B(C6F5)4]**

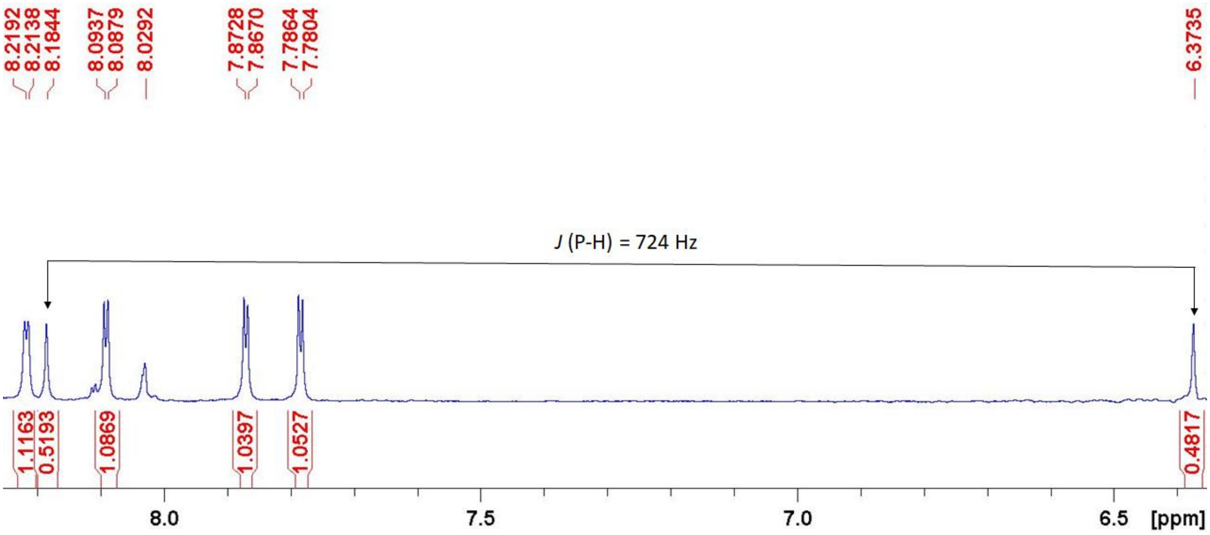
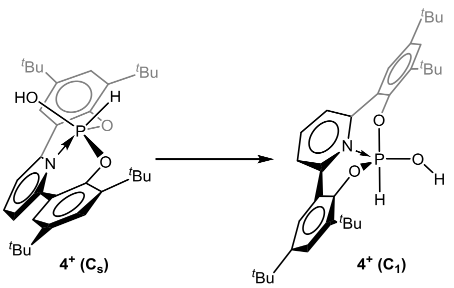


Figure S8. ^{1}H NMR of **[4][B(C6F5)4]**, P-H coupling emphasized

Noteworthy, the symmetry of **[4][B(C6F5)4]**, is not of a C_s type, likely due to formation of a geometrical isomer in which the C_s symmetry is lost.



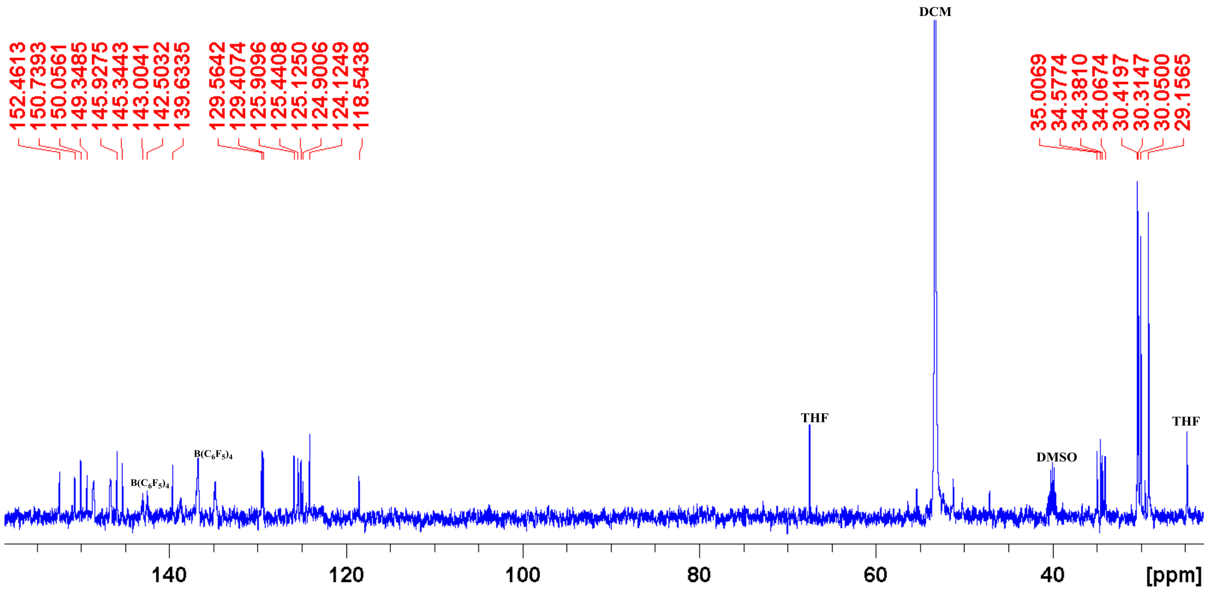


Figure S9. ^{13}C NMR of **[4][B(C_6F_5)$_4$]**

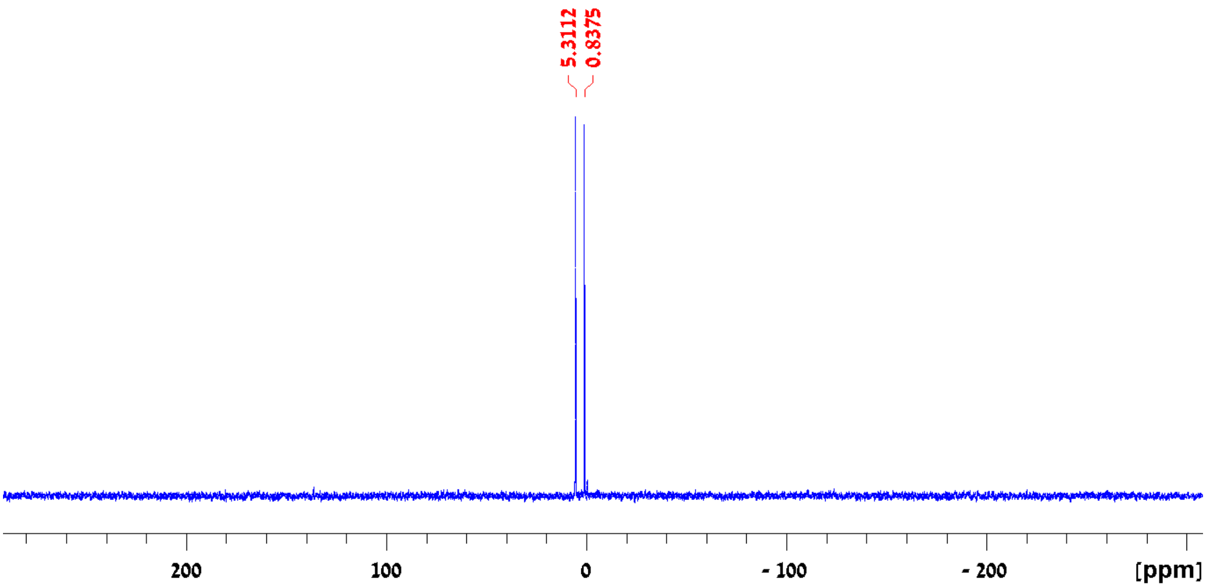


Figure S10. ^{31}P NMR of **[4][B(C_6F_5)$_4$]**

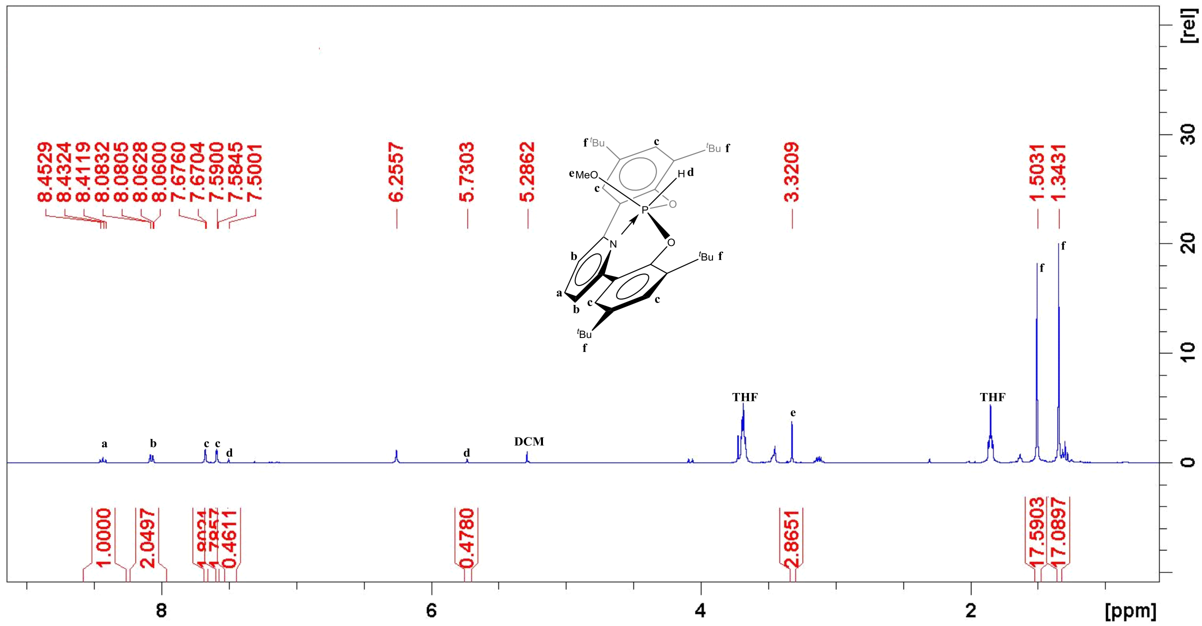


Figure S11. ^{1}H NMR of **[5][B(C$_6$F$_5$)$_4$]**

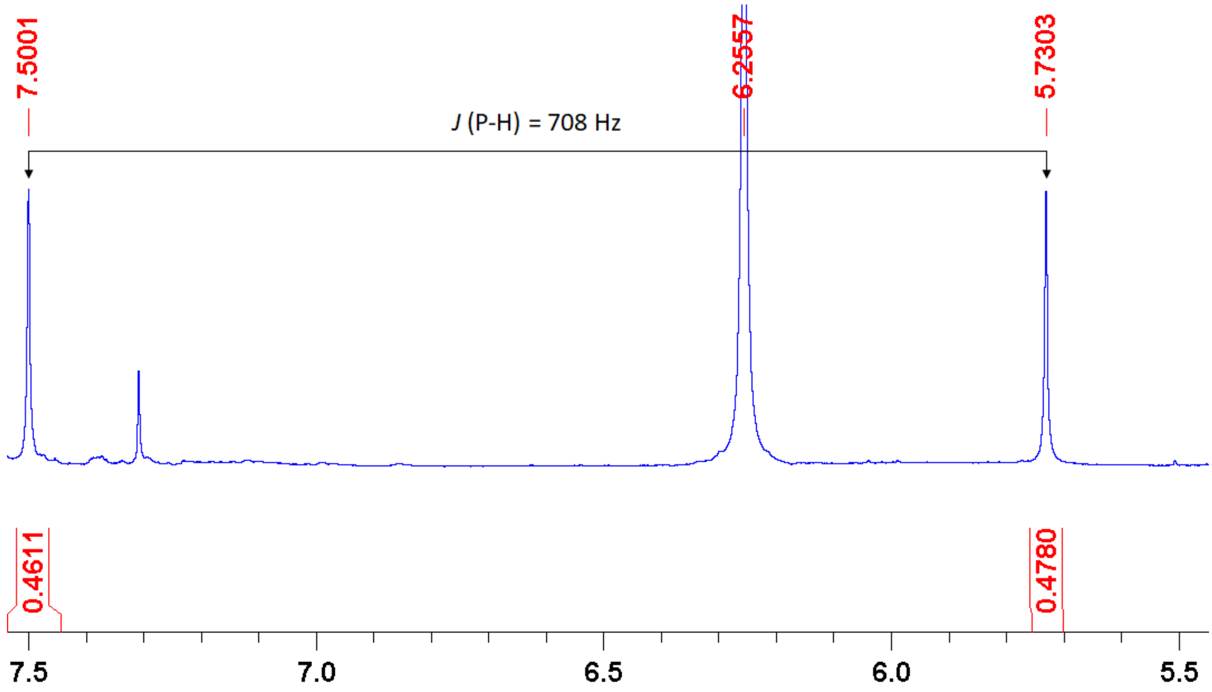


Figure S12. ^{1}H NMR of **[5][B(C$_6$F$_5$)$_4$]**, P-H coupling emphasized

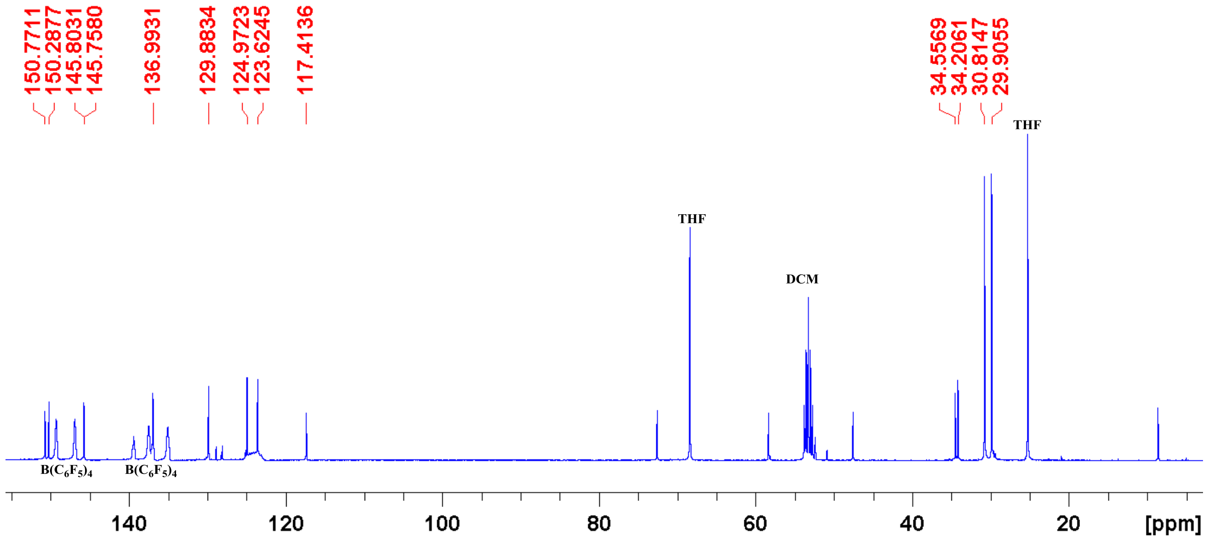


Figure S13. ^{13}C NMR of **[5][B(C$_6$F$_5$)$_4$]**

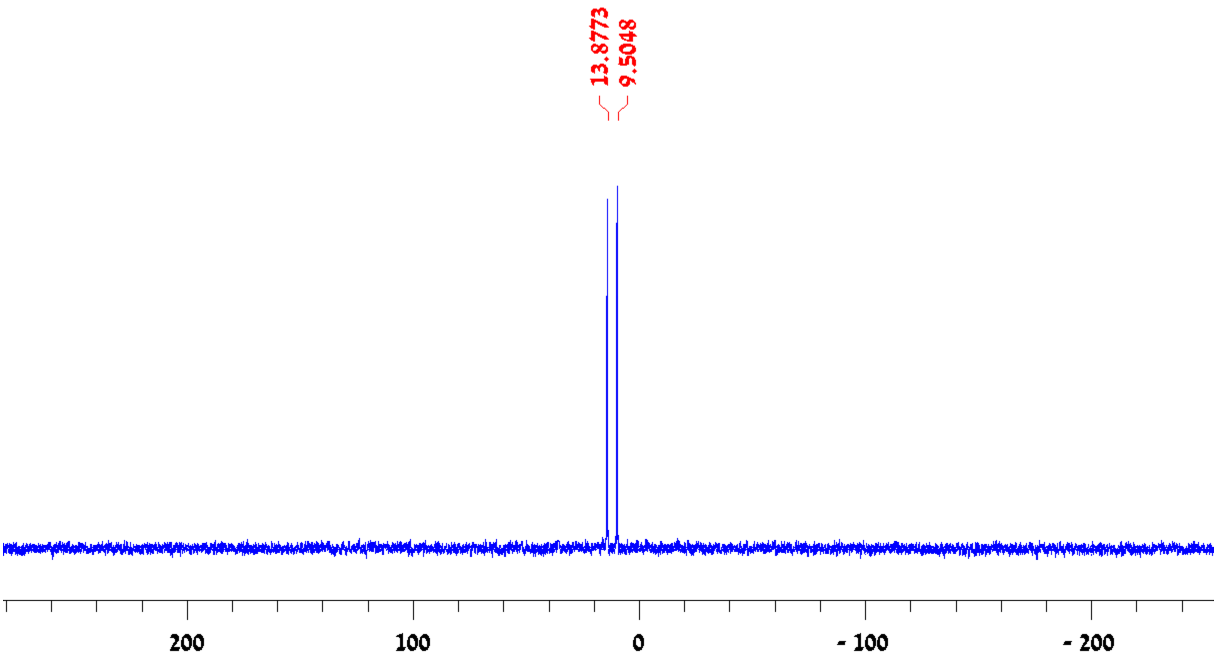


Figure S14. ^{31}P NMR of **[5][B(C$_6$F$_5$)$_4$]**

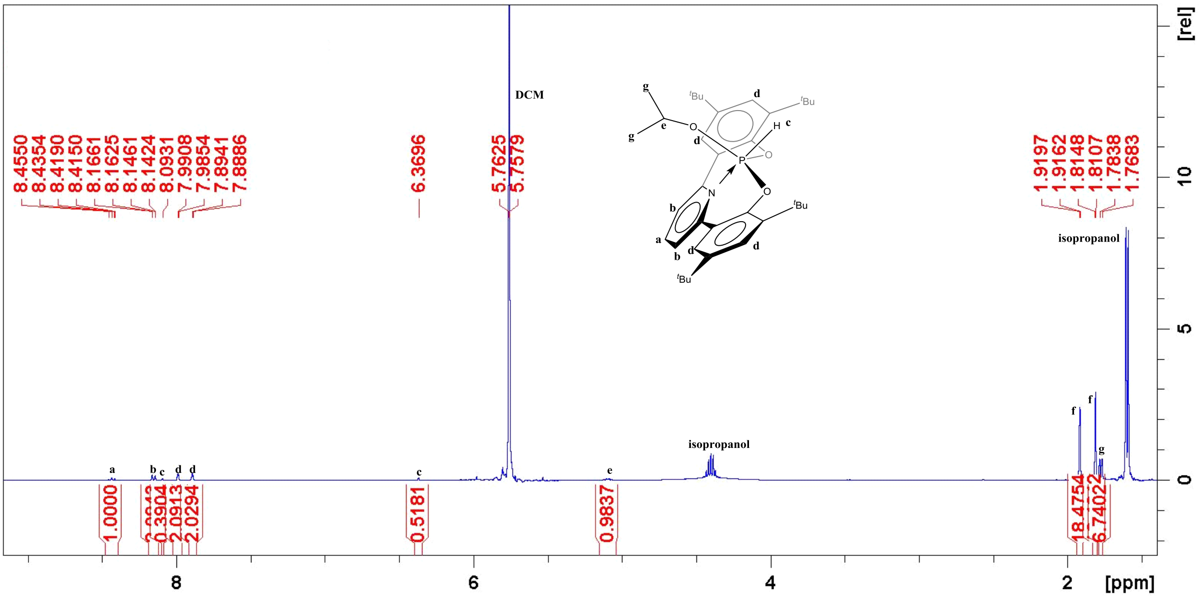


Figure S15. ^{1}H NMR of **[6][B(C$_6$F$_5$)$_4$]**

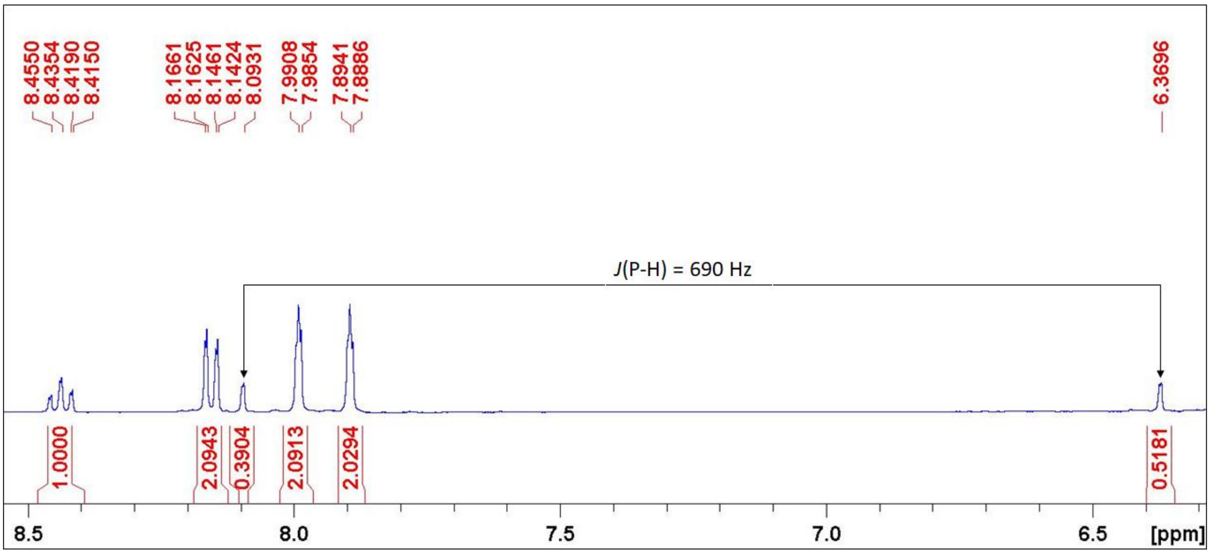


Figure S16. ^{1}H NMR of **[6][B(C$_6$F$_5$)$_4$]**, P-H coupling emphasized

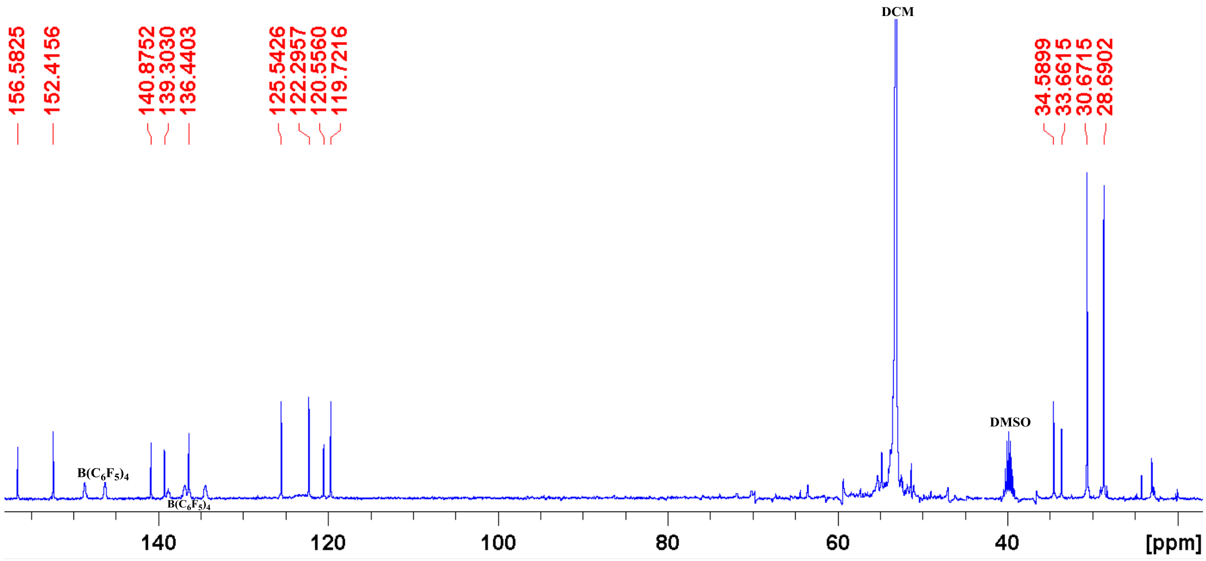


Figure S17. ^{13}C NMR of **[6][B(C_6F_5)$_4$]**

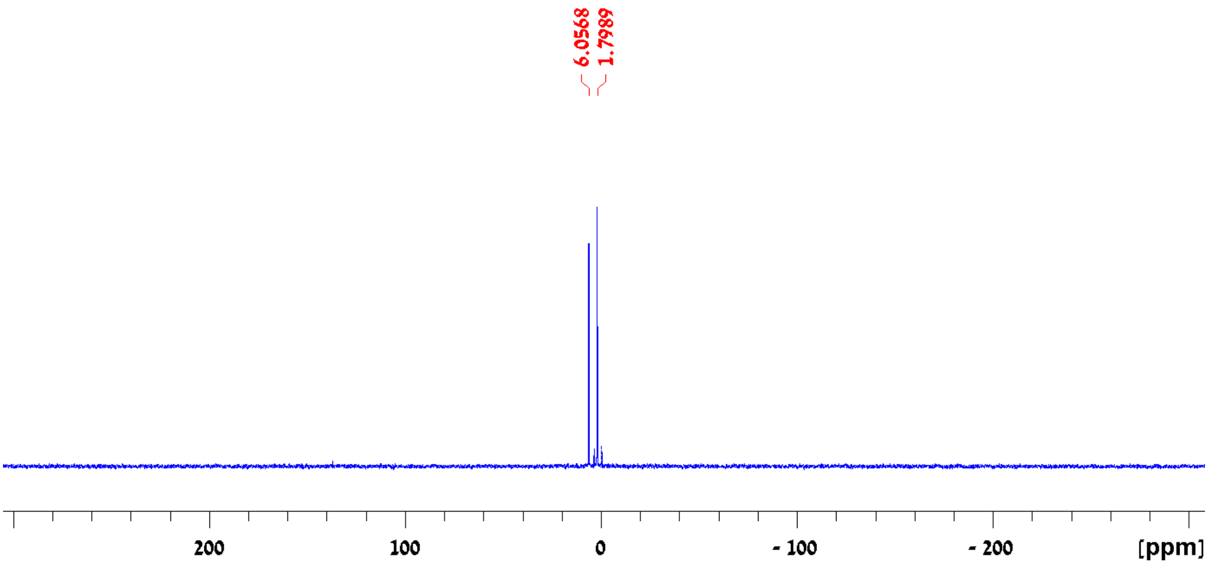


Figure S18. ^{31}P NMR of **[6][B(C_6F_5)$_4$]**

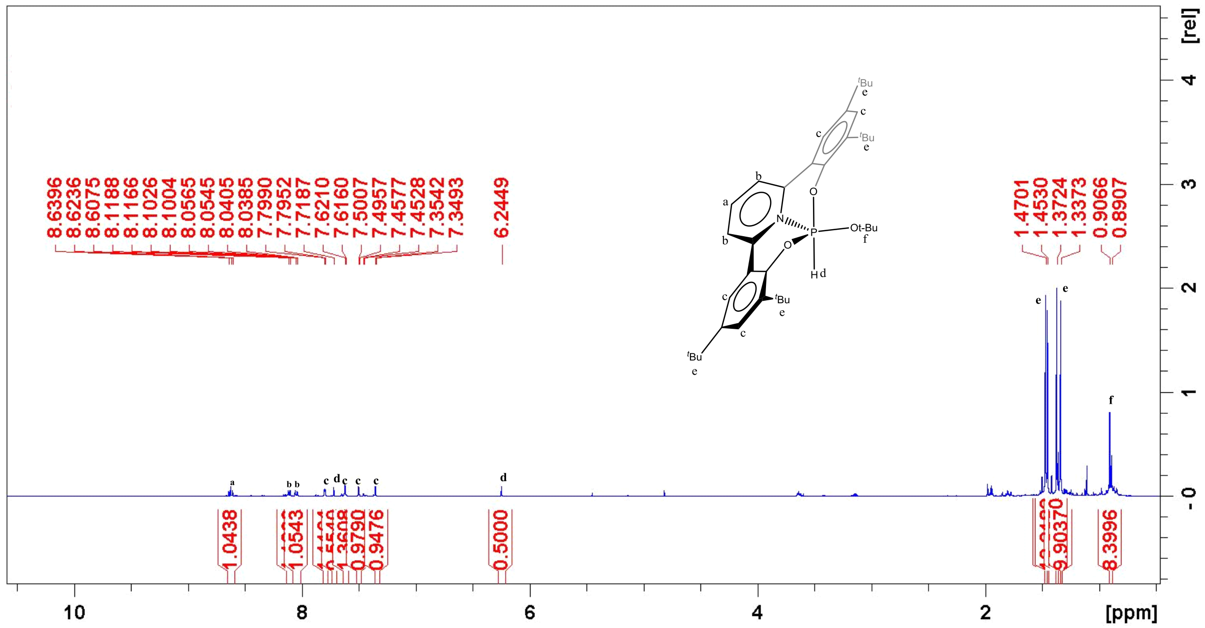


Figure S19. ^{1}H NMR of **[7][B(C$_6$F$_5$)$_4$]**

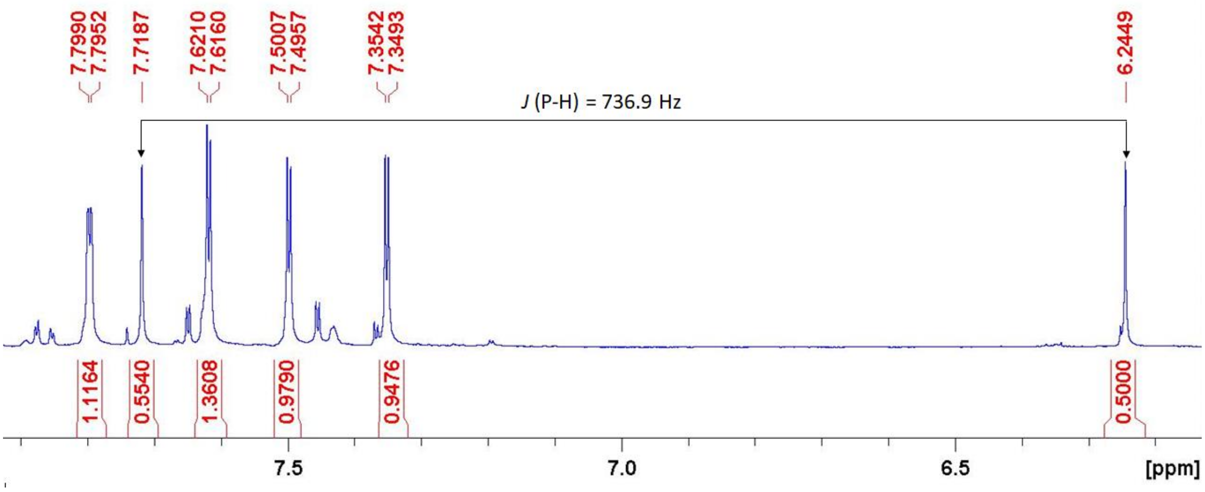


Figure S20. ^{1}H NMR of **[7][B(C$_6$F$_5$)$_4$]**, P-H coupling emphasized

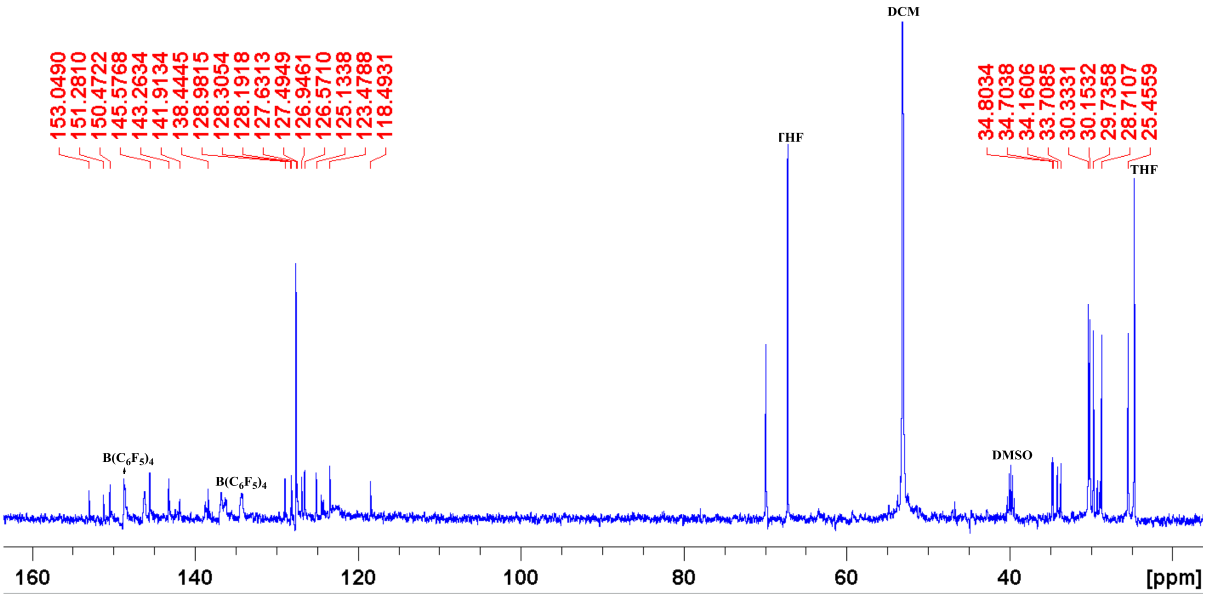


Figure S21. ^{13}C NMR of **[7][B(C$_6$F$_5$)$_4$]**

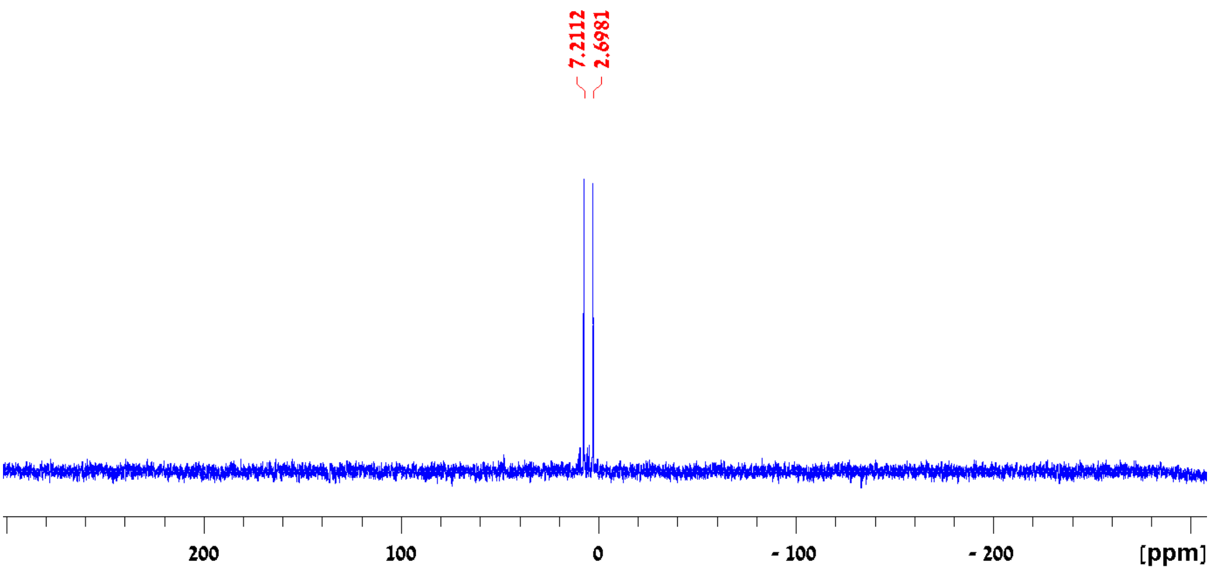
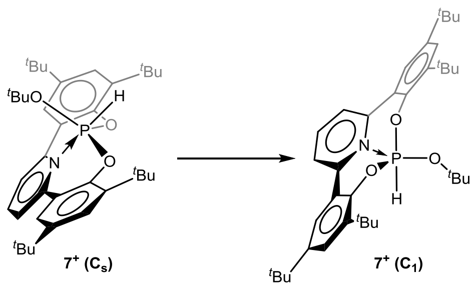


Figure S22. ^{31}P NMR of **[7][B(C$_6$F$_5$)$_4$]**

Noteworthy, the symmetry of **7** is not of a C$_s$ type, likely due to formation of a geometrical isomer in which the C$_s$ symmetry is lost.



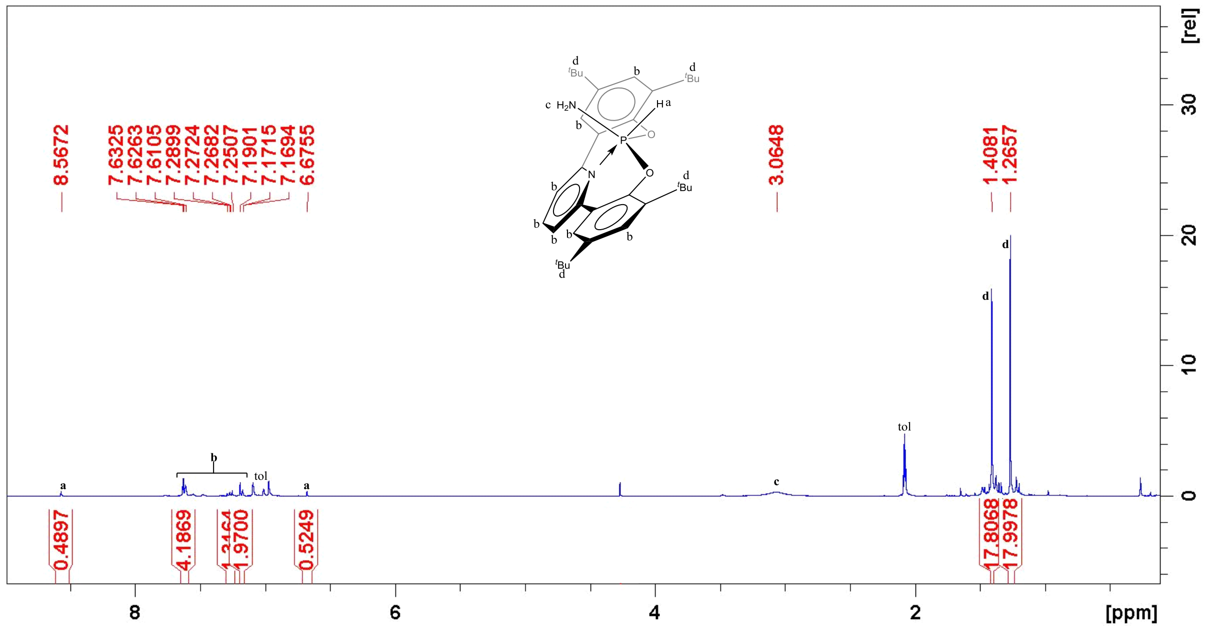


Figure S23. ^{1}H NMR of **[8][B(C$_6$F$_5$)$_4$]**

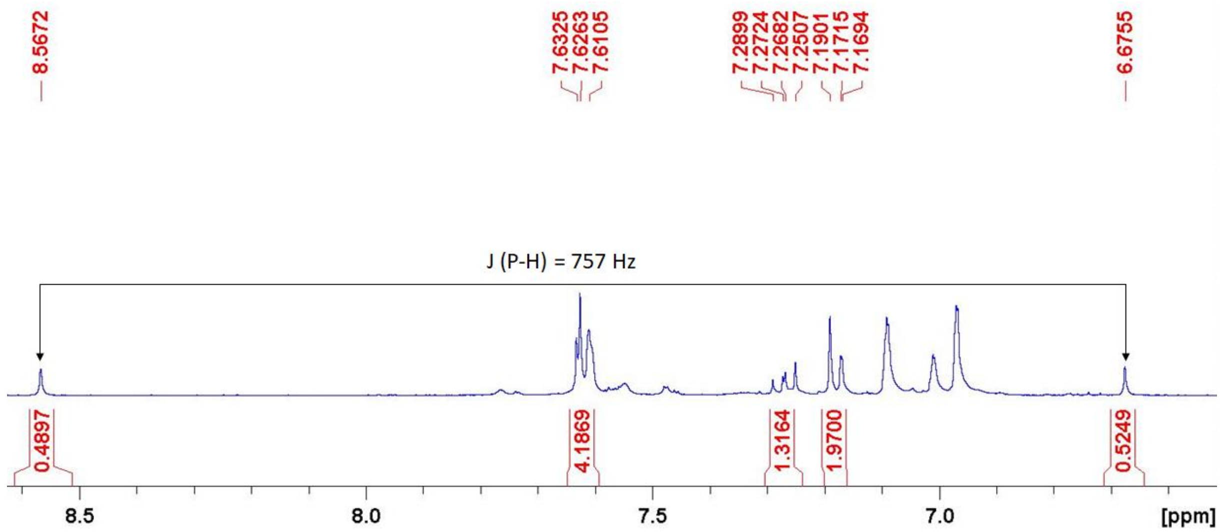


Figure S24. ^{1}H NMR of **[8][B(C$_6$F$_5$)$_4$]**, P-H coupling emphasized

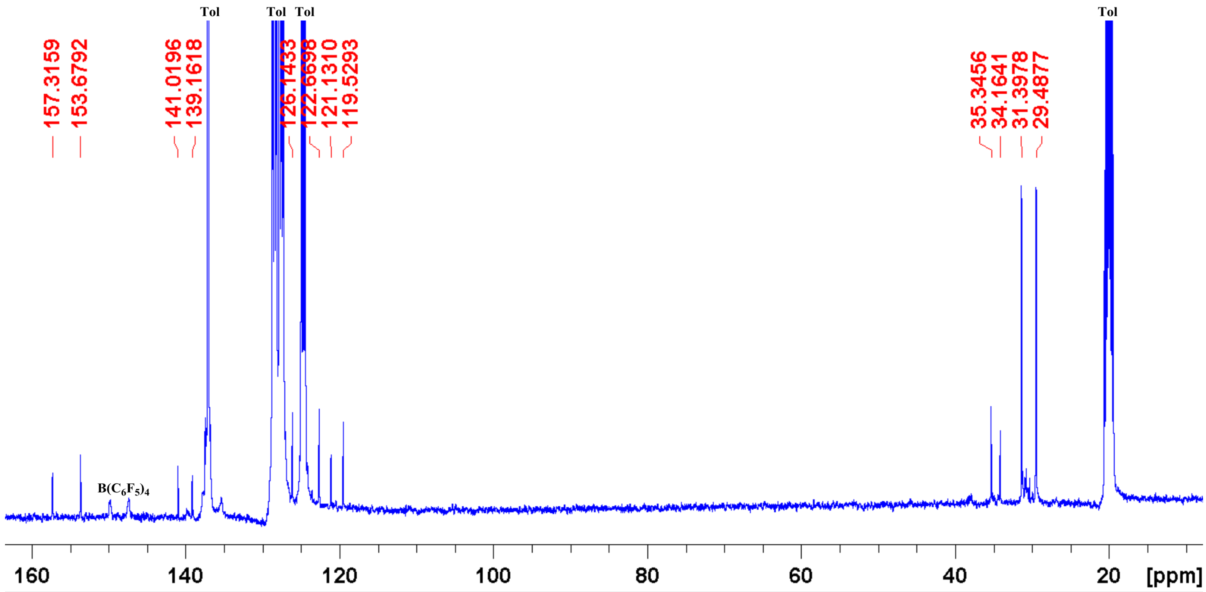


Figure S25. ^{13}C NMR of **[8][B(C_6F_5)$_4$]**

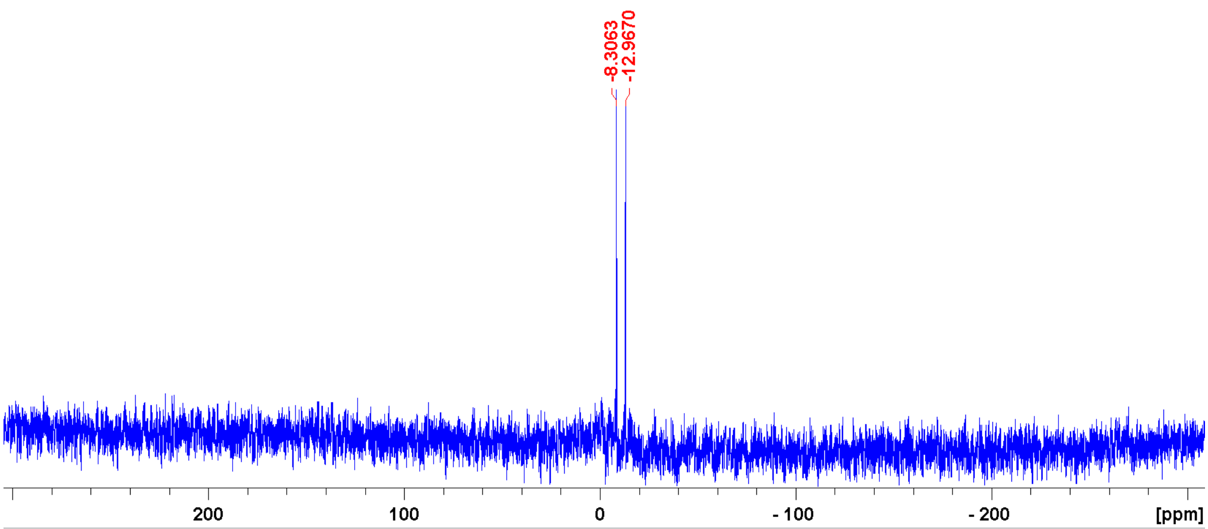
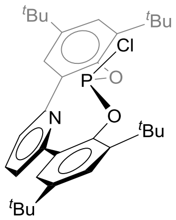


Figure S26. ^{31}P NMR of **[8][B(C_6F_5)$_4$]**

DFT calculations

DFT calculations were performed using Gaussian 09.2 Geometry optimization of all the molecules, intermediates, and the transition state were carried out using the BP86(D3)/def2-SVP basis sets implemented in the Gaussian 09 software. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all the molecules and intermediates contained no imaginary frequency showing that these are energy minima. By taking the wave functions obtained from the Gaussian output files, electron densities were computed and subjected to topological analysis using the AIMALL package,[2] which gave ρ and the Laplacian $\nabla^2\rho$, total energy density H_c, the corresponding local kinetic energy density G_c and the local potential energy density V_c.



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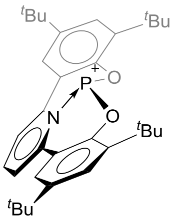

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[1] R. Fu, J. E. Bercaw, J. A. Labinger, *Organometallics*, 2011, **24**, 6751-6765.
[2] AIMPAC Program Package, R. F.W. Bader research group, McMaster University, Hamilton, Canada.