Supporting Information for

Phosphorus mediated imidazolinium to oxazolium ring rearrangement

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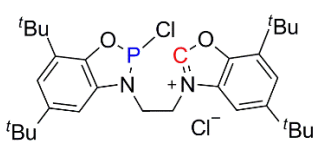
1. General experimental considerations: All preparations were carried out under an anhydrous N_2 atmosphere using standard Schlenk and glove box techniques. All glassware was oven dried and cooled under vacuum before use. Commercial reagents were purchased from Sigma Aldrich, Strem or Apollo Scientific and used without further purification unless indicated otherwise. **1** and **1-Ph** were prepared following the reported procedures.[1-2] NMR spectra were recorded at room temperature using a Bruker AvanceIII-400 MHz spectrometer. Data for ^{1}H 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.

2. X-ray Crystallography:

Single crystal X-ray diffraction data were collected on a Bruker KAPPA APEX II diffractometer equipped with an APEX II CCD detector using a TRIUMPH monochromator with a MoKα X-ray source (α = 0.710 73 Å). The crystals were mounted on a cryoloop with Paratone oil, and all data were collected at 100(2) K. Unit cell determination and refinement and data collection were done using the Bruker APPEX-II suite,[3] data reduction and integration were performed using SAINT v8.34A (Bruker, 2013)[4] and absorption corrections and scaling were done using SADABS-2014/5 (Bruker,2014/5)[5]. All the crystal structures were solved through OLEX2[6] package using SHELXT[7] and the structures were refined using SHELXL[7]. All non-hydrogen atoms were refined anisotropically. All the figures were generated using Mercury 3.10.2. CCDC no (2097388-2097398) for the X-ray structures.

3. Experimental Procedures

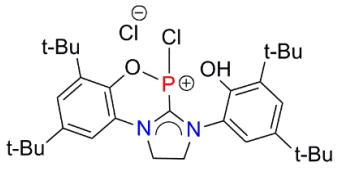
Synthesis of 3:



PCl_3 (0.46 mL, 5.3 mmol) was added to a THF (90 mL) solution of compound **1** (2 g, 3.88 mmol) at -80 °C, after 5 min followed by the addition of Et_3N (1.1 mL, 7.76 mmol) at -80 °C (the color turned from transparent to light orange at this point). This mixture was stirred at -80 °C for 15 minutes and then allowed to warm to RT. The reaction was stirred overnight (15h). The solution was filtered by cannula and thereafter all the volatiles were evaporated in vacuum. The light orange solid was washed with hexane (80 mL) that afforded white solid. This solid was crytsallized by slow evaporation of hexane-DCM mixture (10:1) at room temperature.

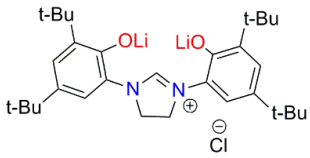
Yield: 1.41 g (62.6 %). **^{1}H NMR (400 MHz, $CDCl_3$); δ** = 12.80 (s, 1H, O-C*H*-N), 7.52 (s, 1H, Ar-*H*), 7.33 (s, 1H, Ar-*H*), 6.98 (s, 1H, Ar-*H*), 6.96 (s, 1H, Ar-*H*), 5.58 (m, 2H, -CH_2), 4.73 (m, 2H, -CH_2), 1.46 (s, 9H, -C(CH_3)$_3$), 1.35 (s, 9H, -C(CH_3)$_3$), 1.23 (s, 9H, -C(CH_3)$_3$), 1.14 (s, 9H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, $CDCl_3$); δ** = 158.82 (O-*C*H-N), 153.39, 147.86, 145.55, 137.75, 136.68, 132.45, 129.14, 124.58, 116.91, 108.35, 106.19, 45.93 (-*C*H_2), 42.65 (d, *J* = 64 Hz, -*C*H_2), 35.81 (-*C*(CH$_3$)$_3$), 35.21 (-*C*(CH$_3$)$_3$), 34.94 (-*C*(CH$_3$)$_3$), 34.59 (-*C*(CH$_3$)$_3$), 31.90 (-C(*C*H$_3$)$_3$), 31.42 (-C(*C*H$_3$)$_3$), 29.97 (-C(*C*H$_3$)$_3$), 29.80 (-C(*C*H$_3$)$_3$). **^{31}P NMR (162 MHz, $CDCl_3$); δ** = 162.25 ppm. **HRMS**: The MS for **3** and **5** is the same, see below MS of **3**/**5**.

Synthesis of 5: **5** was obtained as the minor compound in the synthesis of **3**.



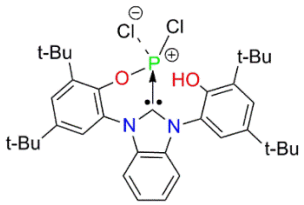
Yield: 112 mg (5%). **^{1}H NMR (400 MHz, $CDCl_3$): δ** = 9.18 (s, 1H, -O*H*), 7.38 (s, 2H, Ar-*H*), 7.08 (br, 2H, Ar-*H*), 4.68 (br, 4H, -CH_2), 1.41 (s, 18H, -C(CH_3)$_3$), 1.31 (s, 18H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, $CDCl_3$):δ** = 166.28 (d, $J_{C\text{-}P}$ = 70 Hz, N-*C*-N), 159.64, 154.33, 153.33, 149.02, 144.50, 139.94,126.48, 123.93, 122.28, 115.83, 110.83, 49.29 (-*C*H_2) 35.53 (-*C*(CH$_3$)$_3$), 34.75 (-*C*(CH$_3$)$_3$), 31.36 (-C(*C*H$_3$)$_3$), 29.91 (-C(*C*H$_3$)$_3$). **^{31}P NMR (162 MHz, $CDCl_3$): δ** = 60.07 ppm. **HRMS** (APPI$^+$): The MS for **3** and **5** is the same, furthermore **5** can rearrange to **3** during MS measurments. Calculated for $C_{31}H_{45}ClN_2O_2P$: 543.2907 [M-Cl]$^+$; Obs: 543.2916.

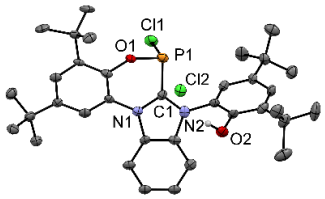
Synthesis of 1-Li$_2$:



2.1 eq. of *n*BuLi (0.28 mL, 2.5 M in hexane, 0.688 mmol) was added to a 4 mL THF solution of **1** (164 mg, 0.318 mmol) at -80 ^{o}C. The solution was allowed to warm to room temperature and stirred for 2h. The solution was concentrated up to 0.5 mL. The NMR of this solution showed exclusive formation of compound ***1-Li$_2$***. **^{1}H NMR (400 MHz, in THF); δ** = 9.78 (s, 1H, N-C*H*-N), 6.61 (s, 2H, Ar-*H*), 6.40 (s, 2H, Ar-*H*), 3.78 (s, 4H, -CH_2), 1.07 (s, 18H, -C(CH_3)$_3$), 0.87 (s, 18H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, in THF); δ** = 158.79 (N-*C*H-N), 137.17,128.26, 125.51, 120.63, 114.08, 49.08 (-*C*H_2), 34.92 (-*C*(CH$_3$)$_3$), 33.06 (-*C*(CH$_3$)$_3$), 31.13 (-C(*C*H$_3$)$_3$), 28.72 (-C(*C*H$_3$)$_3$).

Synthesis of 5-Ph:



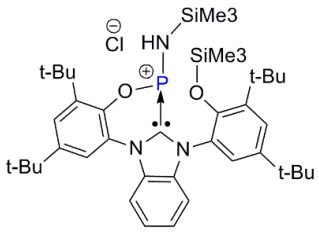


Molecular structure of ***5-Ph***

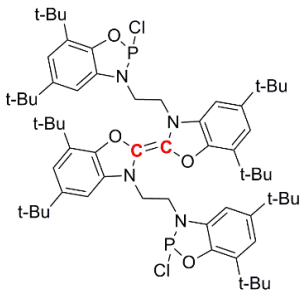
PCl_3 (0.31 mL, 3.55 mmol) was added to a THF (90 mL) solution of compound **1-Ph** (2 g, 3.55 mmol) at -80 °C, after 5 min followed by the addition of Et_3N (1.1 mL, 7.82 mmol) at -80 °C. This mixture was stirred at -80 °C for 15 minutes and then allowed to warm to RT. The reaction was stirred overnight (15h). The solution was filtered by cannula and thereafter all the volatiles were evaporated in vacuum. The off white solid was washed with hexane (80 mL) that afforded white solid which was crystallized from DCM-hexane mixture. Yield: 1.7 g (76.2 %). **^{1}H NMR (400 MHz, $CDCl_3$); *δ*** = 9.05 (s, 1H, -O*H*), 8.16 (s, 1H, Ar-*H*), 7.96 (s, 1H, Ar-*H*), 7.74 (m, 1H, Ar-*H*), 7.61 (s, 4H, Ar-*H*), 7.26 (s, 1H, Ar-*H*), 1.49 (s, 9H, -C(CH_3)$_3$), 1.47 (s, 9H, -C(CH_3)$_3$), 1.43 (s, 9H, -C(CH_3)$_3$), 1.31 (s, 9H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, $CDCl_3$); *δ*** = 151.95 (d, $J_{C\text{-}P}$ = 78 Hz, N-*C*-N), 148.78, 148.04, 144.20, 143.53, 143.04, 138.55 (d, *J* = 11 Hz), 132.61, 129.75, 128.17, 127.68, 124.96, 123.23, 122.98, 115.78, 114.97, 114.48, 35.81 (-*C*(CH_3)$_3$), 35.24 (-*C*(CH_3)$_3$), 34.66 (-*C*(CH_3)$_3$), 31.47 (-C(*C*H_3)$_3$), 30.19 (-C(*C*H_3)$_3$), 29.84 (-C(*C*H_3)$_3$). **^{31}P NMR (162 MHz, $CDCl_3$); *δ*** = 63.73 ppm. **HRMS** (APPI$^+$): Calculated for $C_{35}H_{45}ClN_2O_2P$: 591.2907 $[M\text{-}Cl]^+$; Obs: 591.2901.

Alternative synthesis route for 5-Ph*:* 2.1 equivalent of *n*BuLi (2.98 mL, 2.5 M in hexane, 7.45 mmol) was added to a THF (80 mL) solution of compound **1-Ph** (2 g, 3.55 mmol) at -80 °C. The solution was allowed to warm to room temperature and stirred for 2h. PCl_3 (0.31 mL, 3.55 mmol) was added at -80 °C. This mixture was stirred at -80 °C for 10 min and then allowed to warm to room temperature and further stirred for overnight. All the volatiles were evaporated in the vacuum and the solid obtained was extractred with DCM. All the volatiles were evaporaeted under vaccum and the obtained solid was washed with 80 mL hexane that afforded **5-Ph** as a white solid. Yield: 1.3 g (58%).

Synthesis of 5a-Ph:



KHMDS (160 mg, 0.8 mmol) was added to a 8 mL benzene solution of **5-Ph** (502 mg, 0.8 mmol) at -30 °C. The reaction was allowed to warm to room temperature very slowly and stirred overnight. On concentrating the solution to 2 mL and storing at room temperature produced crystals after 3 days. Yield: 260 mg (43.2 %). **^{1}H NMR (400 MHz, C_6D_6); δ** = 9.63 (s, 1H, -N*H*), 8.95 (s, 1H, Ar-*H*), 8.27 (s, 1H, Ar-*H*), 8.04 (s, 1H, Ar-*H*), 7.75 (s, 1H, Ar-*H*), 7.64 (s, 1H, Ar-*H*), 7.29 (s, 1H, Ar-*H*), 7.12 (s, 2H, Ar-*H*), 1.61 (s, 9H, -C(CH_3)$_3$), 1.49 (s, 9H, -C(CH_3)$_3$), 1.42 (s, 9H, -C(CH_3)$_3$), 1.22 (s, 9H, -C(CH_3)$_3$), 0.08 (s, 9H, -Si(CH_3)$_3$), -0.29 (s, 9H, -Si(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, C_6D_6); δ** = 156.3 (d, $J_{C\text{-}P}$ = 52 Hz, N-*C*-N), 146.65, 146.29, 141.81 (d, $J_{C\text{-}P}$ = 8 Hz), 140.61 (d, $J_{C\text{-}P}$ = 9 Hz), 135.42, 131.81, 128.58, 127.49, 127.21. 126.97, 125.22, 124.21, 123.98, 117.54, 114.69, 114.05, 35.70 (-*C*(CH$_3$)$_3$), 35.61 (-*C*(CH$_3$)$_3$), 35.25 (-*C*(CH$_3$)$_3$), 35.04 (-*C*(CH$_3$)$_3$), 31.76 (-C(*C*H$_3$)$_3$), 31.43 (-C(*C*H$_3$)$_3$), 30.54 (-C(*C*H$_3$)$_3$), 30.39 (-C(*C*H$_3$)$_3$), 1.32 (d, *J* = 6 Hz, -Si(*C*H$_3$)$_3$), 0.70 (-Si(*C*H$_3$)$_3$). **^{31}P NMR (162 MHz, C_6D_6); δ** = 64.36 ppm. **^{29}Si NMR (79.5 MHz, C_6D_6); δ** = 18.59, 10.30 (d, *J* = 34 Hz) ppm. **HRMS** (APCI$^+$): Calculated for $C_{38}H_{53}ClN_3O_2PSi$: 642.3639 [M - H - Me_3SiCl]$^+$; Obs: 642.3633. Elem. Anal. Calc'd(found) for $C_{41}H_{63}ClN_3O_2PSi_2$·O·$H_2O$: C 62.61(62.19), H 8.33(7.94), N 5.34(5.07) (Probably due to oxidation and hydrolysis).



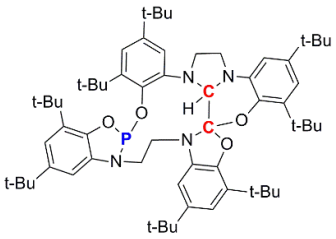
Synthesis of 7:

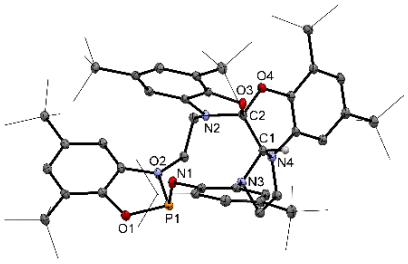
Et_3N (0.14 mL, 1 mmol) was added to a 5 mL THF solution of **3** (580 mg, 1 mmol) at -80 °C. The solution was allowed to warm to room temperature and stirred overnight. The mixture was filtered and all the volatiles were evaporated that afforded red solid. Dissolving this solid in hexane after few days afforded precpitate as **7**. Yield: (310 mg, 57 %).

Alternative route*:* PCl_3 (0.46 mL, 5.3 mmol) was added to a THF (90 mL) solution of compound **1** (2 g, 3.88 mmol) at -80 °C, after 5 min followed by the addition of Et_3N (1.9 mL, 13.58 mmol) at -80 °C (the color turned from transparent to dark red at this point). This mixture was stirred at -80 °C for 15 minutes and then allowed to warm to RT. The reaction was stirred overnight (15h). The solution was filtered by cannula and all the volatiles were evaporated in vacuum. The red solid was extracted with hexane (80 mL). This heaxne solution was concentrated up to 5 mL and the slow evapoartion after few days afforded

transparent crystals as minor compound (**7-minor**, see below). The decant hexane solution was evaporated that afforded **7** as red solid. Yield: 845 mg (40.1 %). **^{1}H NMR (400 MHz, $CDCl_3$); δ** = 7.63 (s, 1H, Ar-*H*), 7.32 (s, 1H, Ar-*H*), 7.19 (s, 1H, Ar-*H*), 6.95 (s, 1H, Ar-*H*), 5.54 (br, 3H, -CH_2), 4.64 (br, 1H, -CH_2), 1.65 (s, 9H, -C(CH_3)$_3$), 1.41 (s, 9H, -C(CH_3)$_3$), 1.11 (s, 9H, -C(CH_3)$_3$), 1.03 (s, 9H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, $CDCl_3$); δ** = 154.38, 147.65 (d, *J* = 7 Hz), 144.90, 143.94 (O-*C*-N), 137.16, 136.30, 132.58, 130.34, 126.53, 116.55, 109.97, 107.59, 48.56 (-*C*H_2), 39.47 (d, *J* = 14 Hz, -*C*H_2), 35.84 (-*C*(CH$_3$)$_3$), 35.16 (-*C*(CH$_3$)$_3$), 34.68 (-*C*(CH$_3$)$_3$), 34.52 (-*C*(CH$_3$)$_3$), 31.71 (-C(*C*H$_3$)$_3$), 31.08 (-C(*C*H$_3$)$_3$), 30.36 (-C(*C*H$_3$)$_3$), 29.74 (-C(*C*H$_3$)$_3$).**^{31}P NMR (162 MHz, $CDCl_3$); δ** = 162.54 ppm. **HRMS** (APCI$^+$): Calculated for $C_{62}H_{89}Cl_2N_4O_4P_2$: 1085.5731 $[M+H]^+$; Obs:1085.5733.

*Minor compound (**7-minor**):*



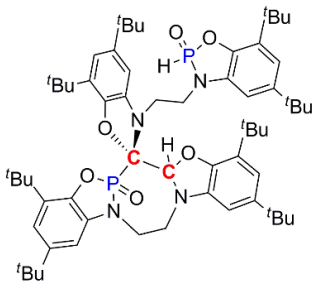


*Single crystal structure of **7-minor***

Yield: 130 mg (6.1 %). **^{1}H NMR (400 MHz, $CDCl_3$); δ** = 7.23 (s, 1H, Ar-*H*), 7.06 (s, 1H, Ar-*H*), 6.94 (m, 2H, Ar-*H*), 6.89 (s, 1H, Ar-*H*), 6.70 (s, 1H, Ar-*H*), 6.23 (s, 1H, Ar-*H*), 5.96 (s, 2H, Ar-*H*), 4.51 (s, 1H, N-C*H*-N), 4.42 (m, 1H, -CH_2), 4.16 (m, 1H, -CH_2), 3.87 (m, 2H, -CH_2), 3.63 (m, 4H, -CH_2), 1.42 (s, 9H, -C(CH_3)$_3$), 1.41 (s, 9H, -C(CH_3)$_3$), 1.37 (s, 9H, -C(CH_3)$_3$), 1.30 (s, 9H, -C(CH_3)$_3$), 1.25 (s, 9H, -C(CH_3)$_3$), 0.96 (s, 9H, -C(CH_3)$_3$), 0.85 (s, 9H, -C(CH_3)$_3$), 0.83 (s, 9H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, $CDCl_3$); δ** = 148.23, 145.24, 144.35, 143.84, 143.27, 141.56, 140.99, 139.81, 138.13, 137.09, 137.05, 135.84, 135.48, 133.77, 128.73, 122.91, 121.11, 118.12 (O-*C*-N), 115.51, 113.99, 111.28, 107.79, 102.56, 101.83, 82.46 (N-*C*H-N), 57.00 (d, *J* = 15 Hz, -*C*H_2), 45.96 (-*C*H_2), 45.15 (d, *J* = 16 Hz, -*C*H_2), 41.09 (-*C*H_2), 35.18 (-*C*(CH$_3$)$_3$), 35.01 (-*C*(CH$_3$)$_3$), 34.80 (-*C*(CH$_3$)$_3$), 34.68 (-*C*(CH$_3$)$_3$), 34.59 (-*C*(CH$_3$)$_3$), 34.46 (-*C*(CH$_3$)$_3$), 34.35 (-*C*(CH$_3$)$_3$), 33.34 (-*C*(CH$_3$)$_3$), 32.07 (-C(*C*H$_3$)$_3$), 31.73 (-C(*C*H$_3$)$_3$), 31.54 (-C(*C*H$_3$)$_3$), 30.31 (-C(*C*H$_3$)$_3$), 30.24 (-C(*C*H$_3$)$_3$), 29.87 (-C(*C*H$_3$)$_3$), 29.61 (-C(*C*H$_3$)$_3$). **^{31}P NMR (162 MHz, $CDCl_3$); δ** = 140.66

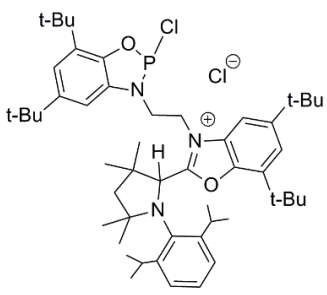
(d, *J* =13 Hz) ppm. **HRMS** (APPI$^+$): Calculated for $C_{62}H_{89}N_4O_4P$: 984.6621 $[M]^+$; Obs: 984.6638. Elem. Anal. Calc'd(found) for $C_{62}H_{89}N_4O_4P$·0.3hexane: C 75.78(75.78), H 9.29(9.00), N 5.54(5.68).

Synthesis of 9:



H_2O (7.2 µL, 0.4 mmol) was added to a 5 mL THF solution of **7** (217 mg, 0.2 mmol) followed by the addition of Et_3N (56 µL, 0.4 mmol) at -80 °C. The reaction was allowed to warm to room temperature. The mixture was stirred overnight and filtered. All the volatiles were evaporated that gave off white solid. This solid was further dissolved in hexane-DCM mixture that afforded colorless crystals on slow evaporation at room temperature. Yield: 40 mg (23.8% %). **^{1}H NMR (400 MHz, $CDCl_3$); *δ*** = 8.53 (d, $J_{H\text{-}P}$ = 708 Hz, -P*H*), 7.15 (s, 1H, Ar-*H*), 6.89 (s, 1H, Ar-*H*), 6.69 (s, 1H, Ar-*H*), 6.58 (s, 1H, Ar-*H*), 6.43 (s, 1H, Ar-*H*), 6.36 (s, 1H, Ar-*H*), 6.35 (s, 1H, O-C*H*-N), 6.30 (s, 1H, Ar-*H*), 6.27 (s, 1H, Ar-*H*), 4.35 (m, 1H, -CH_2), 4.08 (m, 5H, -CH_2), 3.64 (m, 2H, -CH_2), 1.41 (s, 9H, -C(CH_3)$_3$), 1.38 (s, 9H, -C(CH_3)$_3$), 1.26 (s, 9H, -C(CH_3)$_3$), 1.25 (s, 9H, -C(CH_3)$_3$), 1.12 (s, 9H, -C(CH_3)$_3$), 0.99 (s, 9H, -C(CH_3)$_3$), 0.95 (s, 9H, -C(CH_3)$_3$), 0.36 (s, 9H, -C(CH_3)$_3$) ppm. **^{13}C NMR (100 MHz, $CDCl_3$); *δ*** = 146.96, 146.32, 145.61, 144.99, 144.18, 143.32, 141.87, 140.99, 137.99, 136.53, 136.42, 134.34, 134.28, 134.05, 133.90, 133.59, 133.53, 130.03, 129.54, 115.07, 114.82, 113.50, 112.46, 105.34, 105.25, 103.99, 103.91, 100.97, 98.54, 92.81 (d, $J_{C\text{-}P}$ = 44 Hz, O-*C*H-N), 44.13 (-*C*H$_2$), 42.61 (d, *J* = 8 Hz, -*C*H$_2$), 40.77 (-*C*H$_2$), 40.02 (-*C*H$_2$), 35.18 (-*C*(CH$_3$)$_3$), 34.93 (-*C*(CH$_3$)$_3$), 34.66 (-*C*(CH$_3$)$_3$), 34.52 (-*C*(CH$_3$)$_3$), 34.43 (-*C*(CH$_3$)$_3$), 33.99 (-*C*(CH$_3$)$_3$), 33.58 (-*C*(CH$_3$)$_3$), 33.16 (-*C*(CH$_3$)$_3$), 31.79 (-C(*C*H$_3$)$_3$), 31.70 (-C(*C*H$_3$)$_3$), 31.62 (-C(*C*H$_3$)$_3$), 29.66 (-C(*C*H$_3$)$_3$), 29.06 (-C(*C*H$_3$)$_3$), 28.86 (-C(*C*H$_3$)$_3$). **^{31}P NMR (162 MHz, $CDCl_3$); *δ*** = 32.11 (s), 19.34 (d, $J_{P\text{-}H}$ = 708 Hz) ppm. **HRMS** (APPI$^+$): Calculated for $C_{62}H_{91}N_4O_6P_2$: 1049.6414 $[M+H]^+$; Obs: 1049.6416. Elem. Anal. Calc'd(found) for $C_{62}H_{90}N_4O_6P_2$: C 70.96(70.13), H 8.65(8.19), N 5.34(5.08).

Synthesis of 10:



A cold (-30 °C) toluene (4mL) solution of cAAC carbene (86 mg, 0.3 mmol) was added to a toluene solution (12 mL) of compound **3** (174 mg, 0.3 mmol) at -30 °C. This mixture was slowly allowed to warm to RT and heated at 100 °C for 6h that afford a red color solution. Evaporation of all the volatiles afforded a white solid, that on dissolving in minimum amount of benzene and

on storing afforded colorless crystals. Washing of these crystals with pentane afforded pure compound. Yield: 200 mg (80 %). **^{1}H NMR (400 MHz, $CDCl_3$); δ** = 8.43 (s, 1H, Ar-*H*), 7.63 (s, 1H, Ar-*H*), 7.28 (m, 1H, Dipp-Ar-*H*), 7.23 (m, 1H, Dipp-Ar-*H*, 7.01 (d, $J_{H\text{-}H}$ = 8 Hz, 1H, Ar-*H*), 6.91 (s, 1H, Ar-*H*), 5.72 (d, $J_{H\text{-}H}$ = 8 Hz, 1H, -CH_2), 4.89 (s, 1H, C-C*H*-N), 4.59 (m, 1H, -CH_2), 4.18 (m, 1H, -CH_2), 3.76 (m, 1H, -CH_2), 3.20 (sep, 1H, -C*H*$(CH_3)_2$), 2.99 (sep, 1H, -C*H*$(CH_3)_2$), 2.28 (two merge doublets, 2H, -CH_2), 1.57 (s, 3H, -CH_3), 1.56 (s, 9H, -C(CH_3)$_3$), 1.44 (s, 3H, -CH_3), 1.43 (d, 3H, -CH(CH_3)$_2$), 1.34 (s, 9H, -C(CH_3)$_3$), 1.31 (d, 3H, -CH(CH_3)$_2$), 1.29 (s, 9H, -C(CH_3)$_3$), 1.06 (s, 9H, -C(CH_3)$_3$), 0.99 (d, 3H, -CH(CH_3)$_2$), 0.95 (s, 3H, -CH_3), 0.05 (d, 3H, -CH(CH_3)$_2$), ppm. **^{13}C NMR (100 MHz, $CDCl_3$); δ** = 169.19 (N-*C*-O), 154.51, 150.46, 148.65, 147.87, 144.45, 136.77, 135.77, 132.72, 131.66, 130.09, 129.18, 125.99, 125.33, 125.22, 125.09, 116.86, 111.27, 105.44, 72.22 (C-*C*H-N), 66.87 (N*C*$(CH_3)_2$), 57.22 (-CH_2, pyrrolidine), 48.87 (d, -*C*H_2, oxazolidin), 45.02 (NC*C*$(CH_3)_2$), 41.40 (d, -*C*H_2, oxazolidin), 36.16 (-*C*$(CH_3)_3$), 34.88 (-*C*$(CH_3)_3$), 34.65 (-*C*$(CH_3)_3$), 34.40 (-*C*$(CH_3)_3$), 32.40, 31.90, 31.59 (-C(*C*H_3)$_3$), 31.51 (-C(*C*H_3)$_3$), 30.16 (-C(*C*H_3)$_3$), 29.63 (-C(*C*H_3)$_3$), 28.43, 28.04, 27.72, 27.59, 27.45, 26.89, 26.77, 26.35, 25.20, 24.85, 24.69. **^{31}P NMR (162 MHz, $CDCl_3$); δ** = 161.31 ppm. **HRMS** (APPI, APCI, ASAP, ES): repeated attempts to observe molecular peak for the desired compound were not successful, products of hydrolysis and fragmentation were obsereved using a variety of MS methods.

4. Selected spectra:

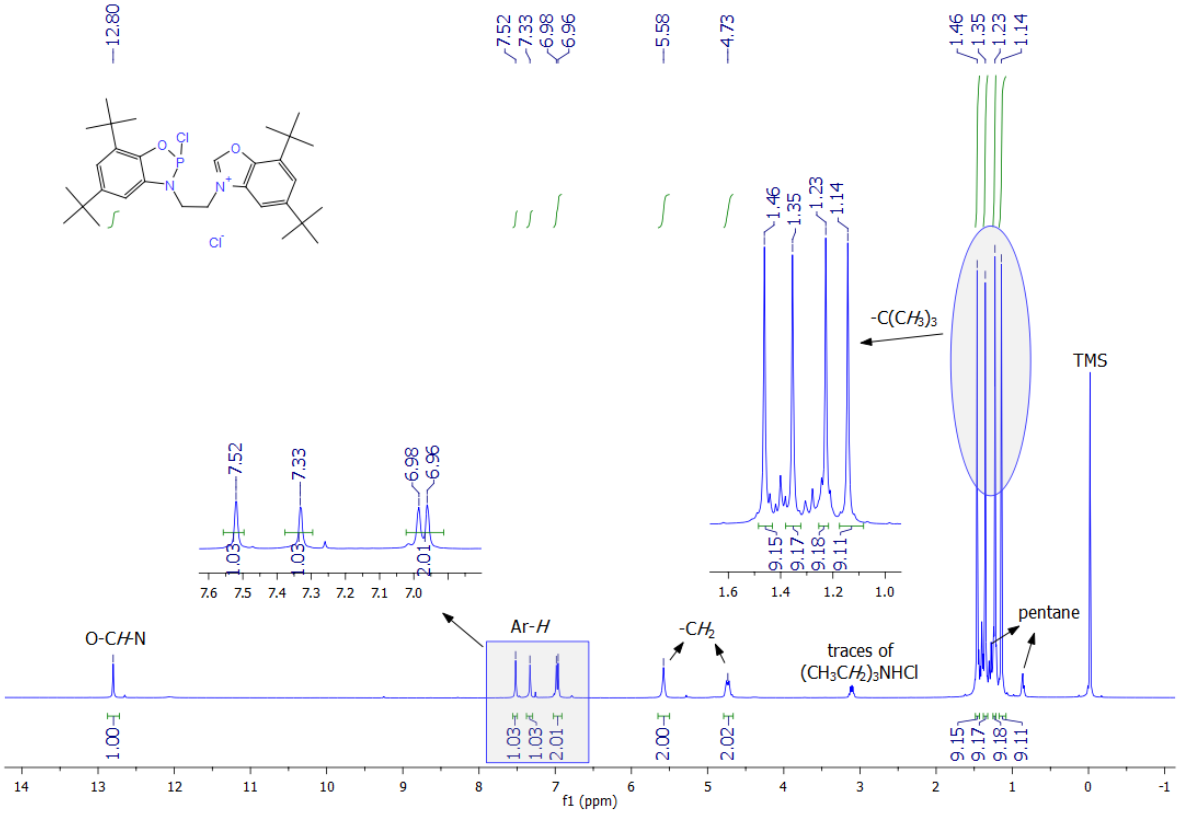


Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3**.

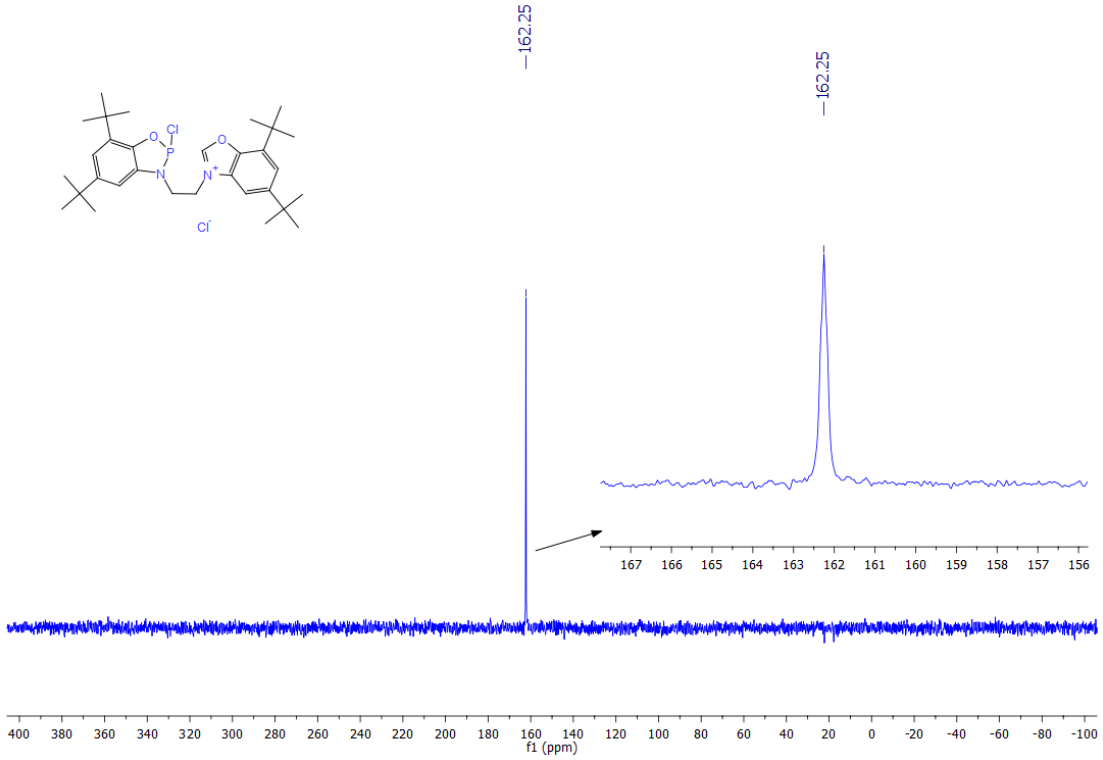


Figure S2. ^{31}P NMR spectrum (162 MHz, $CDCl_3$) of **3**.

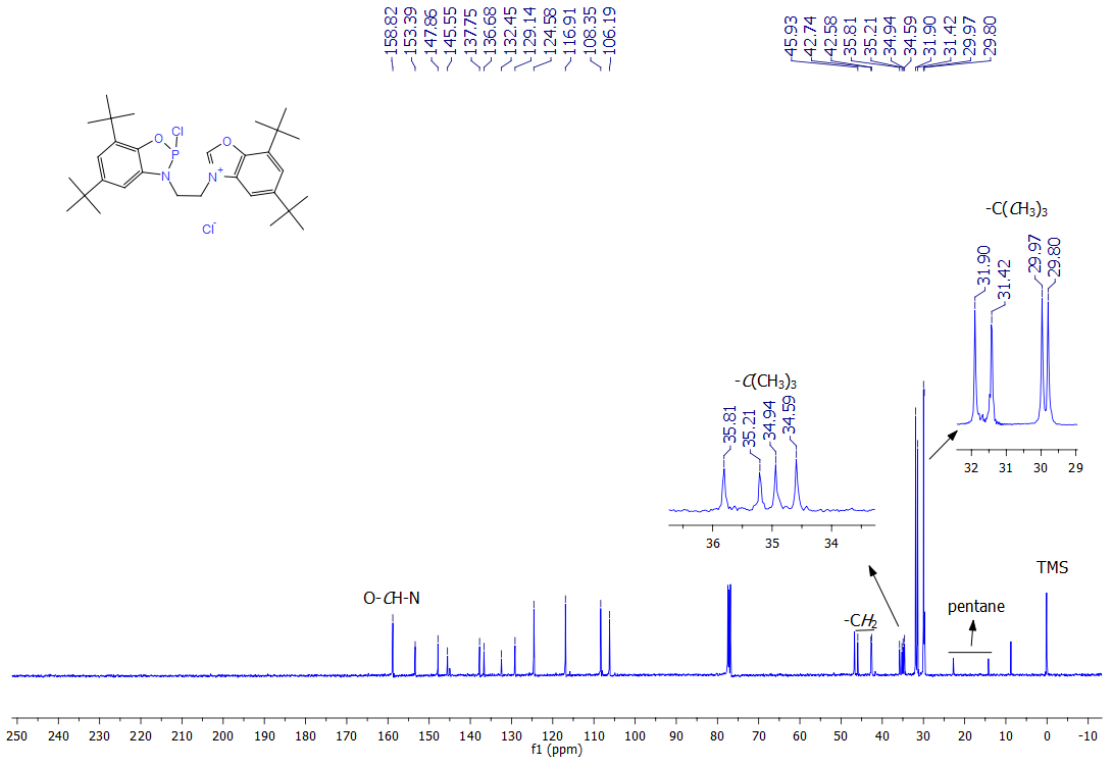


Figure S3. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **3**.

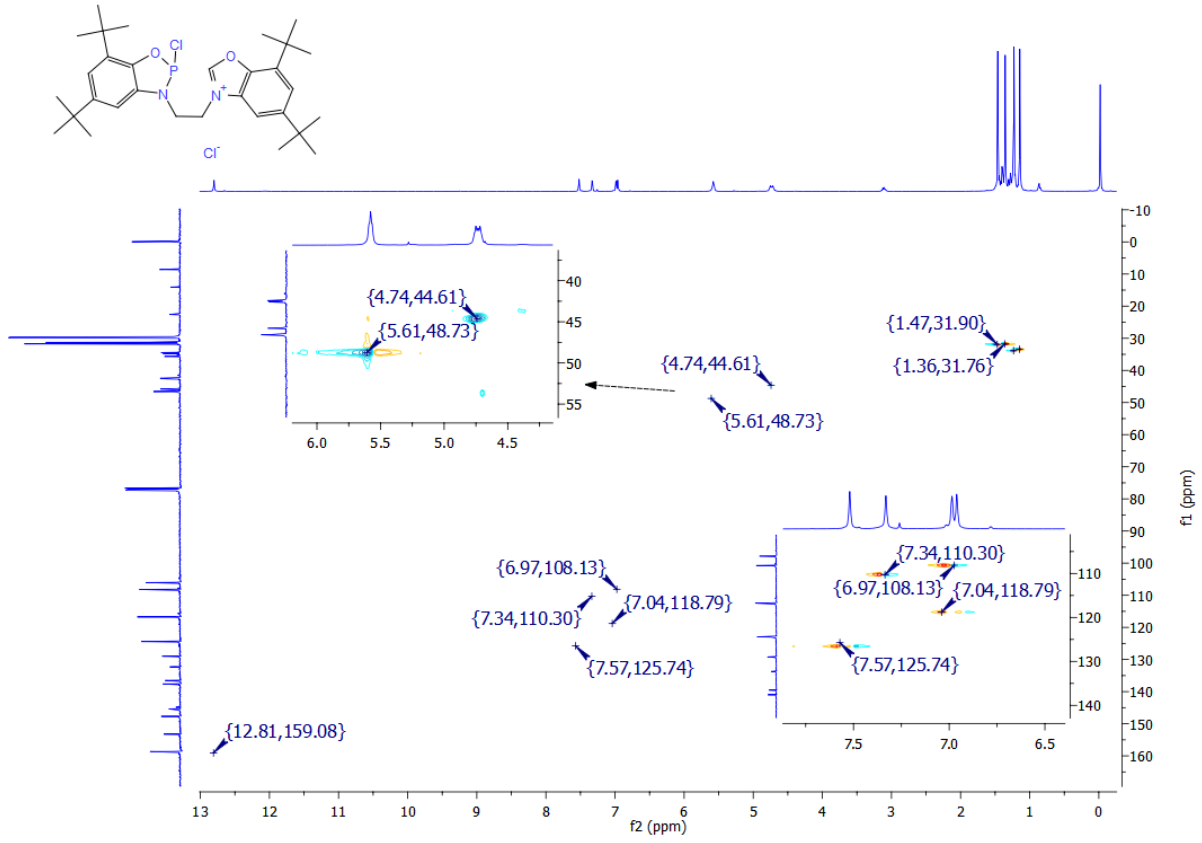


Figure S4. ^{1}H-^{13}C HSQC NMR spectrum ($CDCl_3$) of **3**.

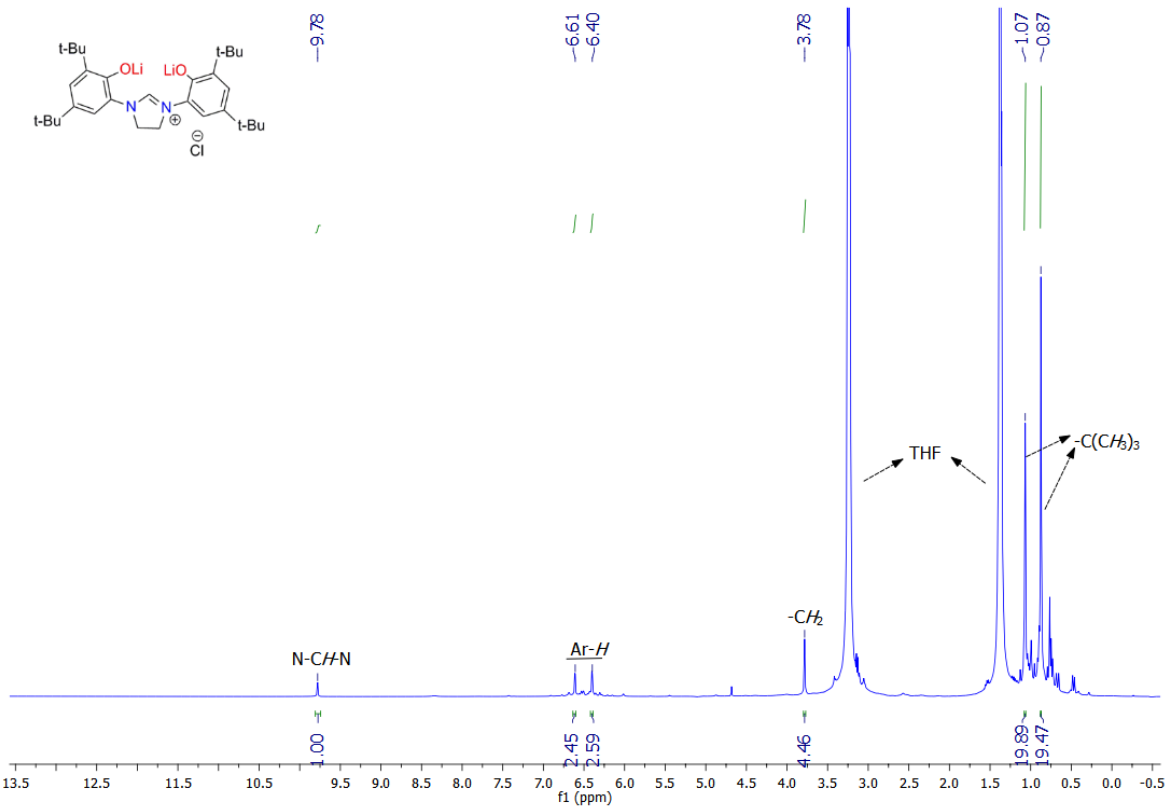


Figure S5. ^{1}H NMR spectrum (400 MHz, in THF reaction mixture) of **1-Li$_2$**.

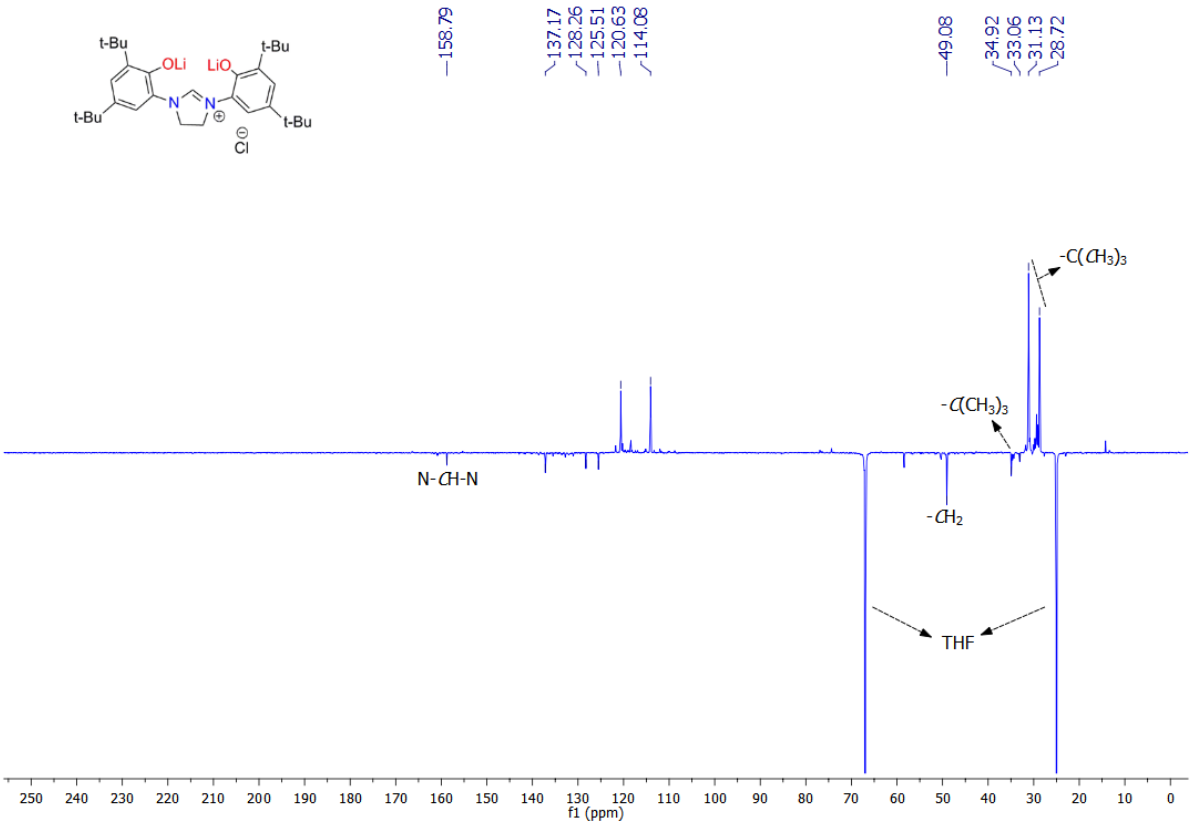


Figure S6. ^{13}C-JMOD NMR spectrum (100 MHz, in THF reaction mixture) of **1-Li$_2$**.

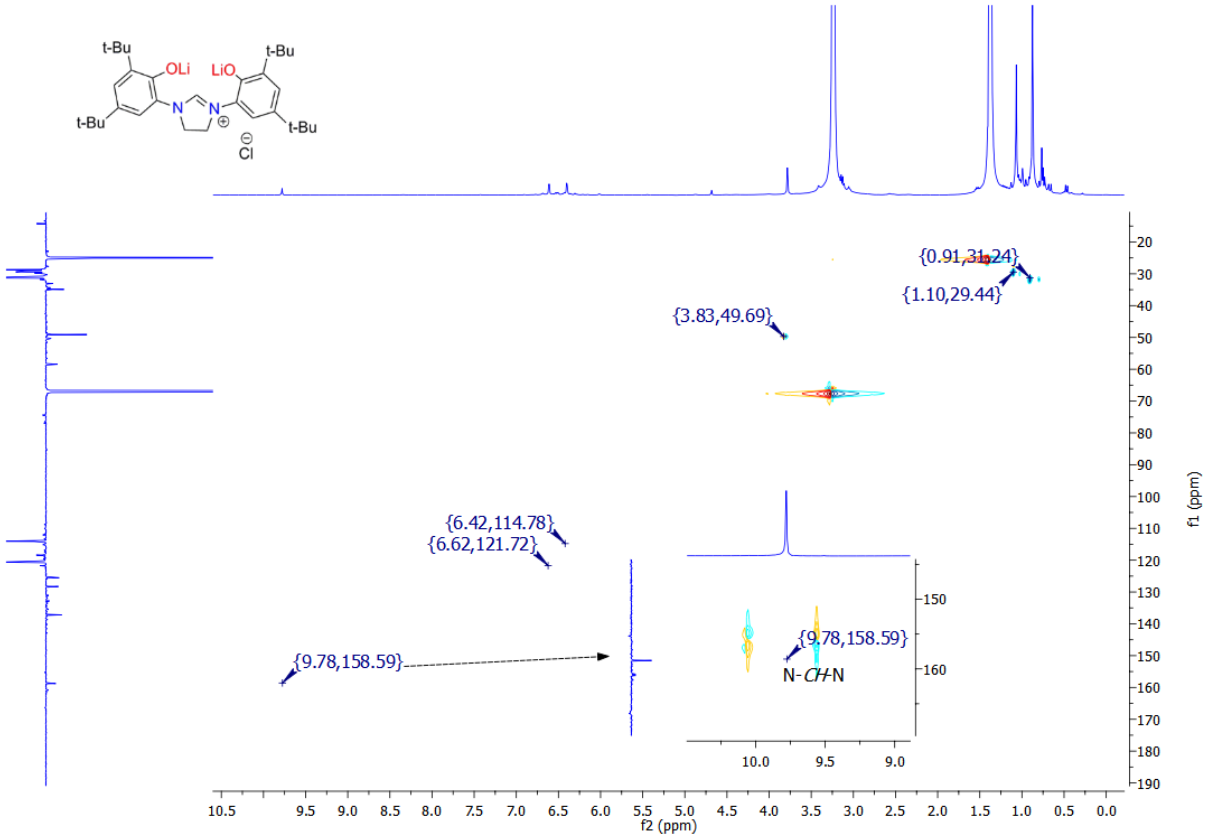


Figure S7. ^{1}H-^{13}C HSQC NMR spectrum (in THF reaction mixture) of **1-Li$_2$**.

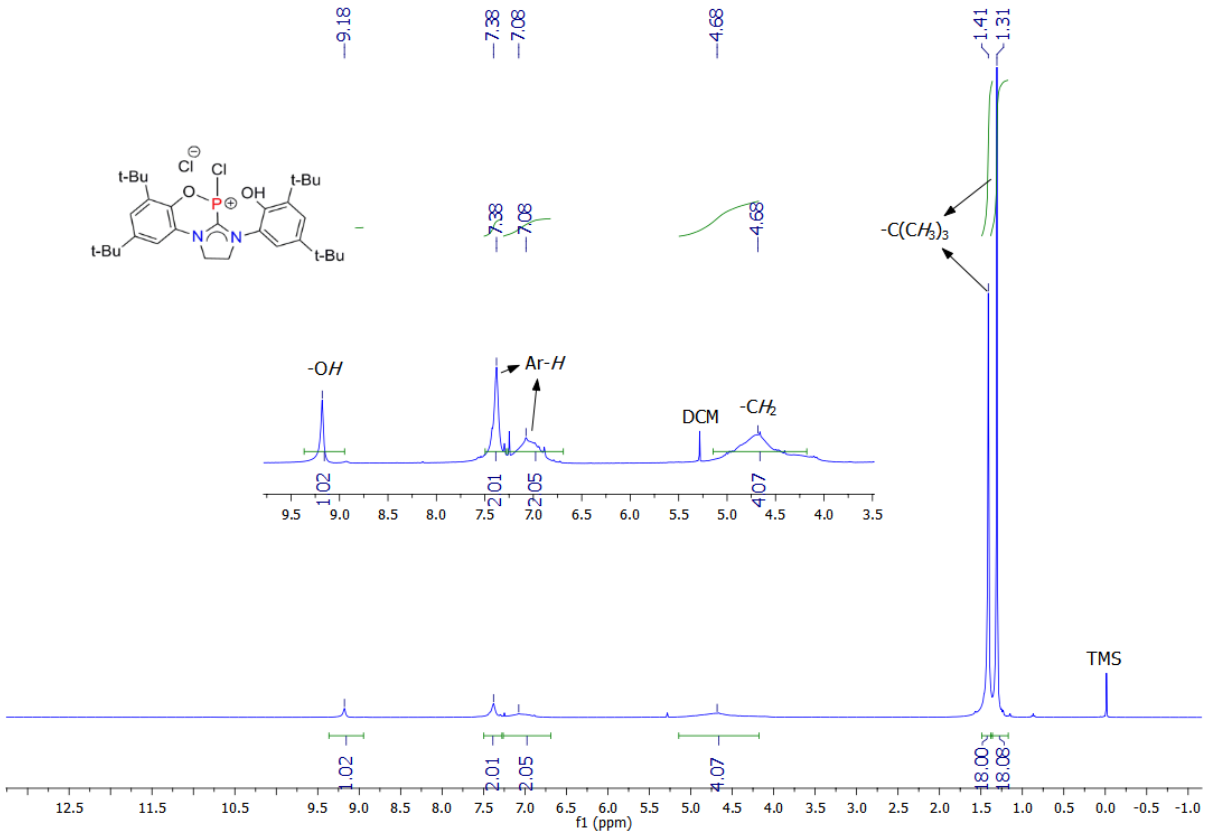


Figure S8. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **5**.

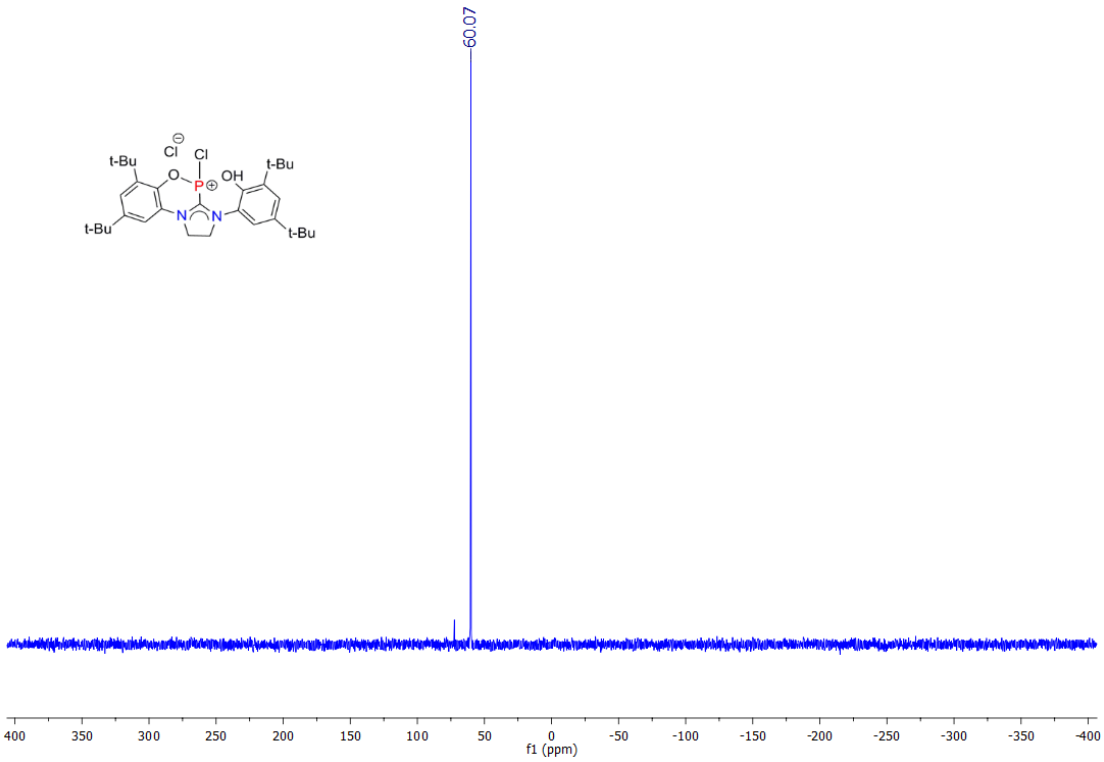


Figure S9. ^{31}P NMR spectrum (162 MHz, $CDCl_3$) of **5**.

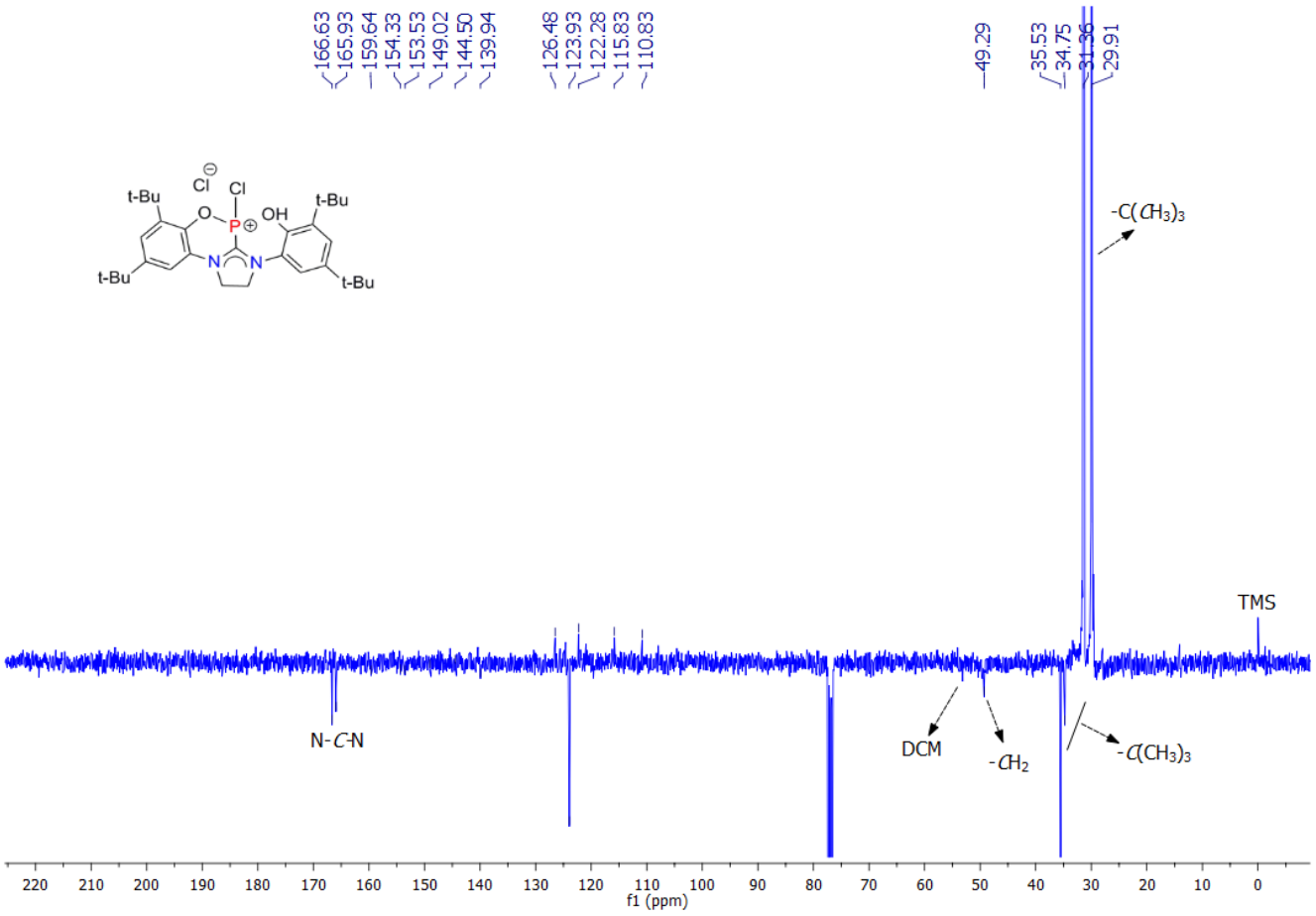


Figure S10. ^{13}C-JMOD NMR spectrum (100 MHz, $CDCl_3$) of **5**.

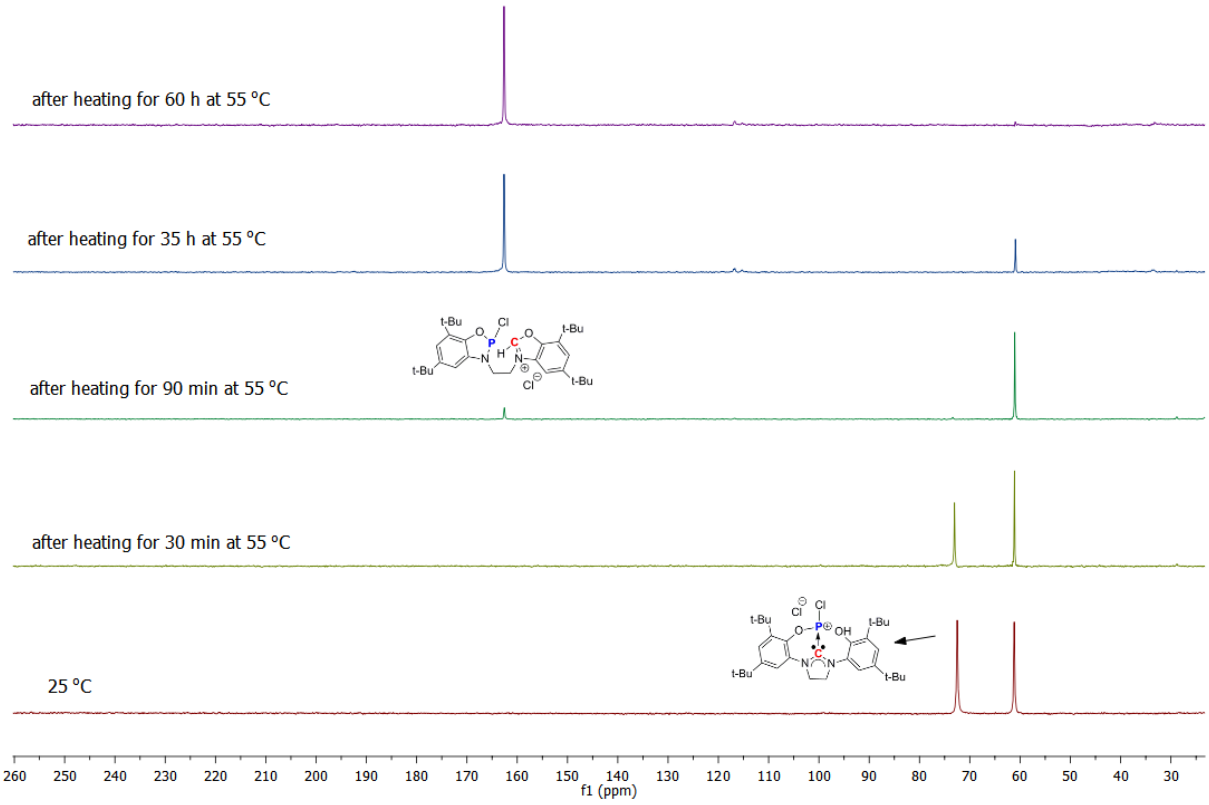


Figure S11. Stacked ^{31}P NMR spectra (162 MHz, $CDCl_3$) to show the conversion of **5** to **3**.

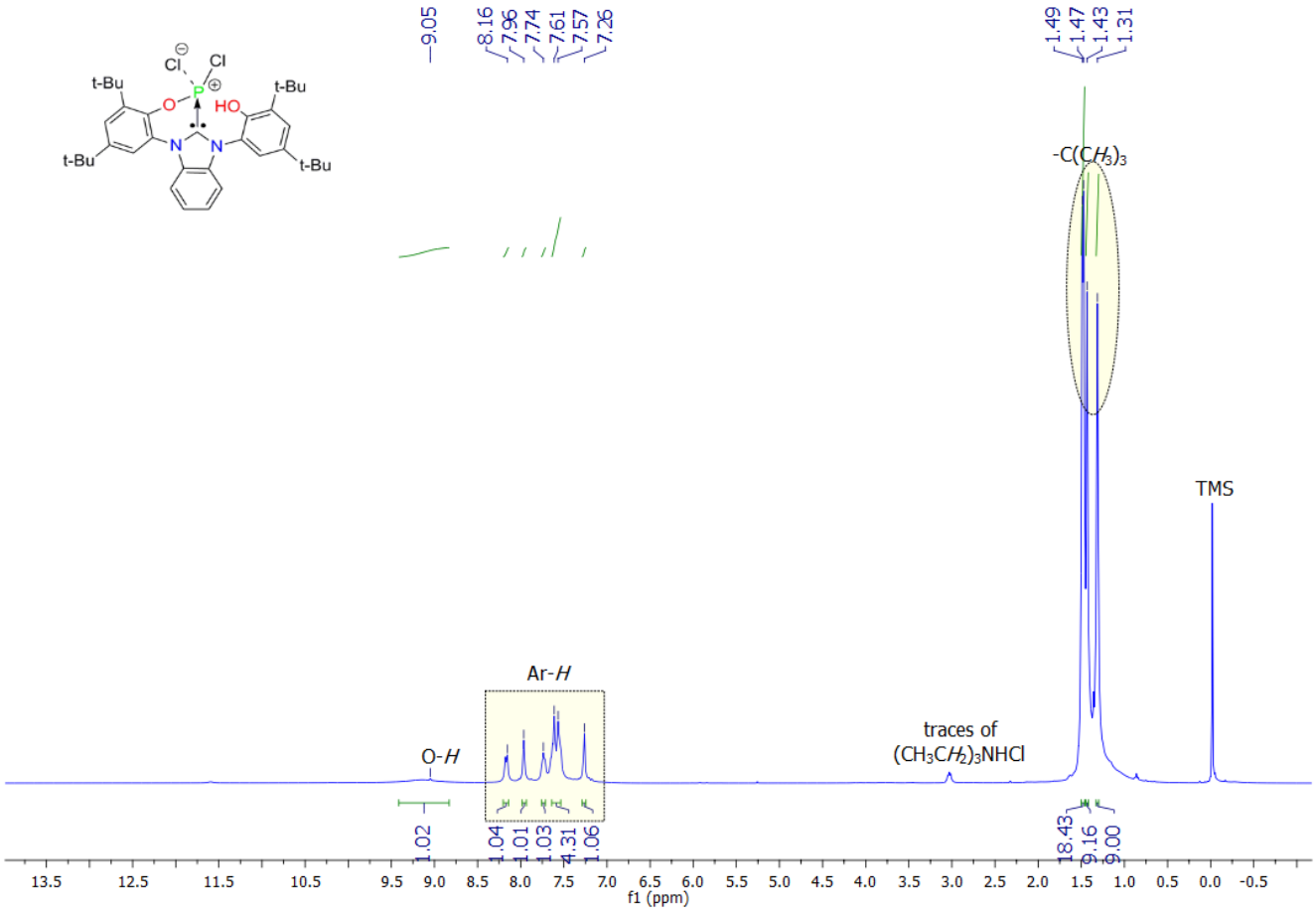


Figure S12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **5-Ph**.

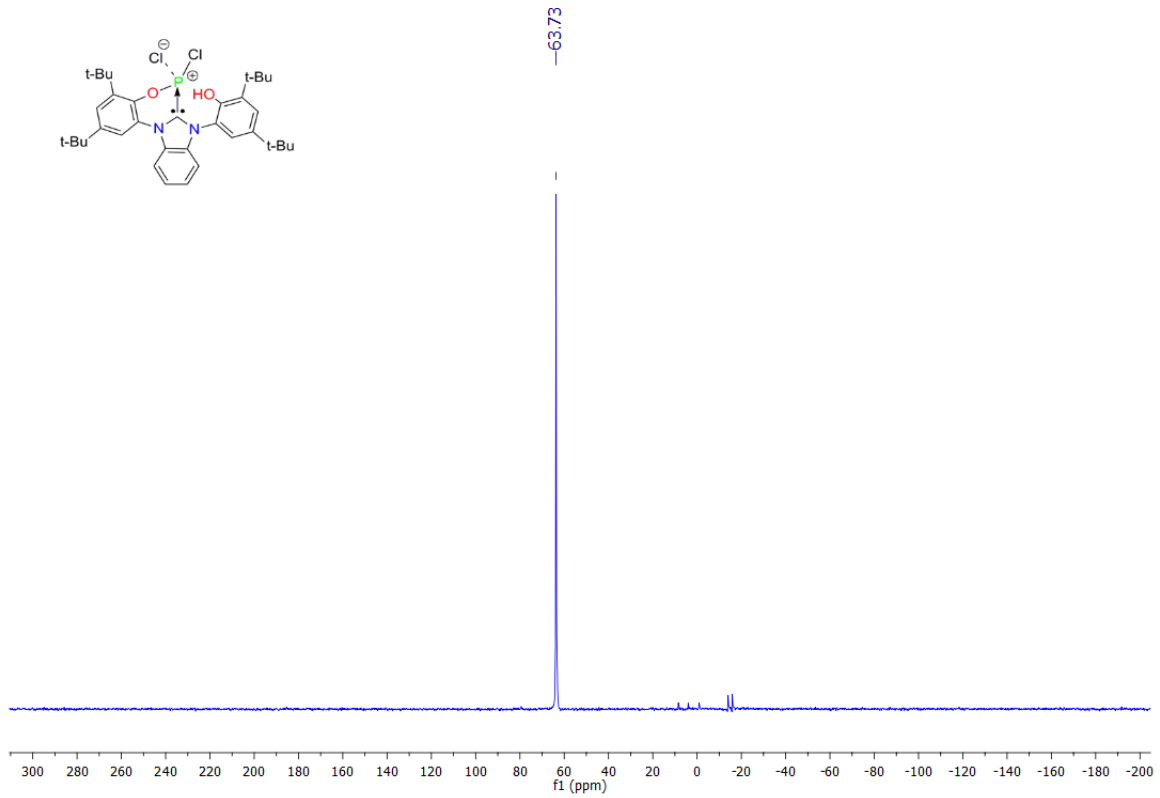


Figure S13. ^{31}P NMR spectrum (162 MHz, $CDCl_3$) of **5-Ph**.

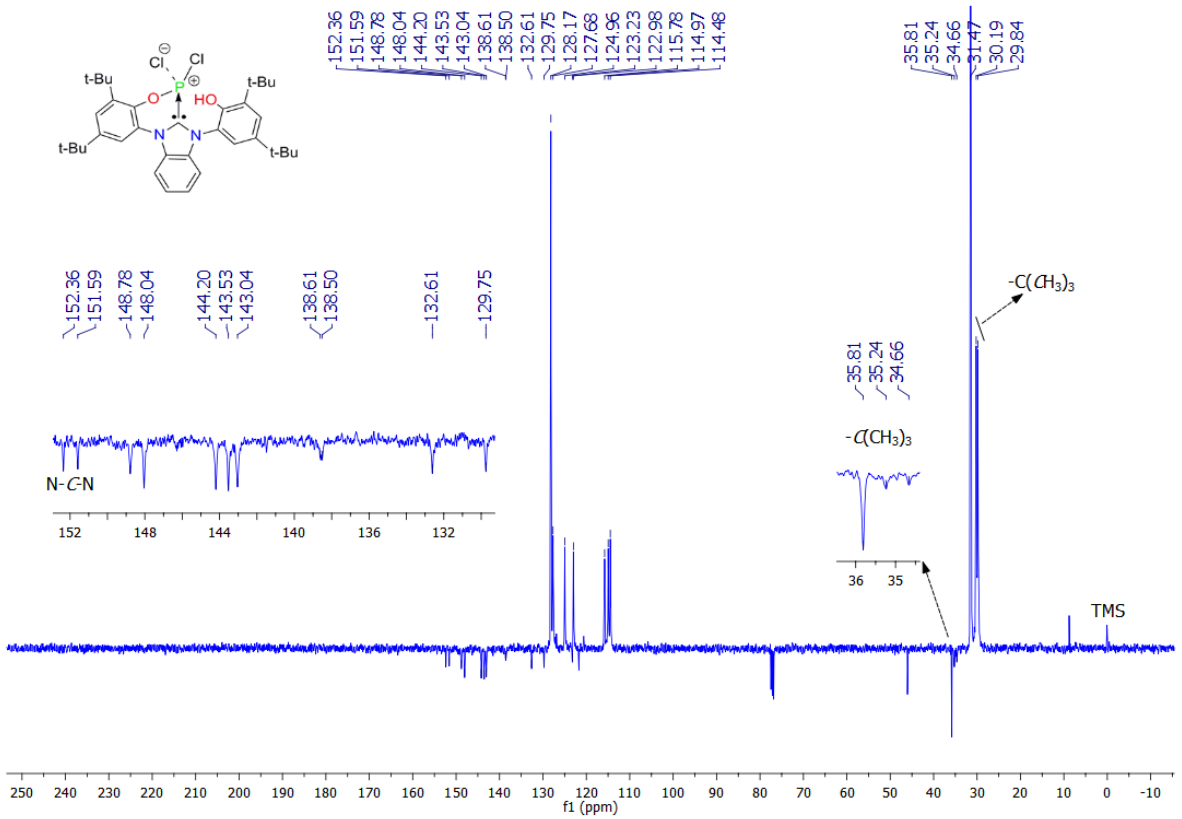


Figure S14. ^{13}C-JMOD NMR spectrum (100 MHz, $CDCl_3$) of **5-Ph**.

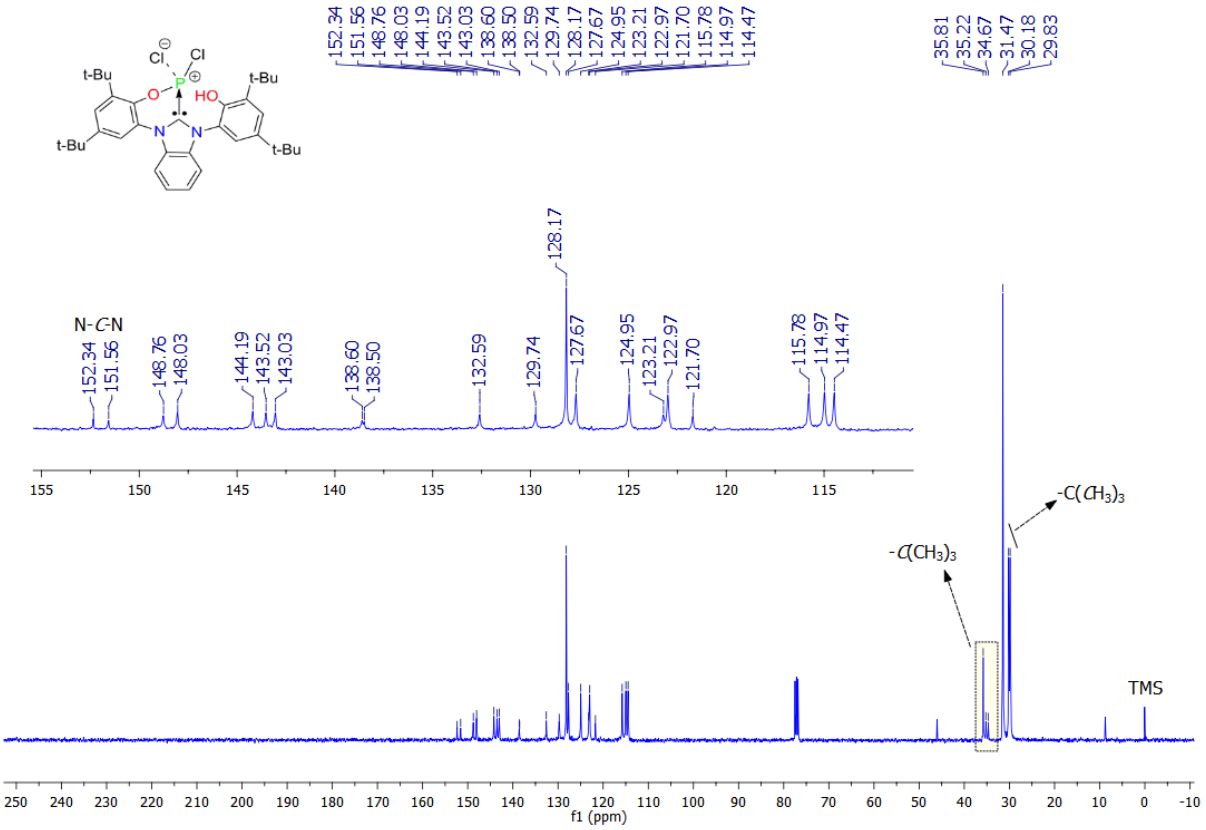


Figure S15. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **5-Ph**.

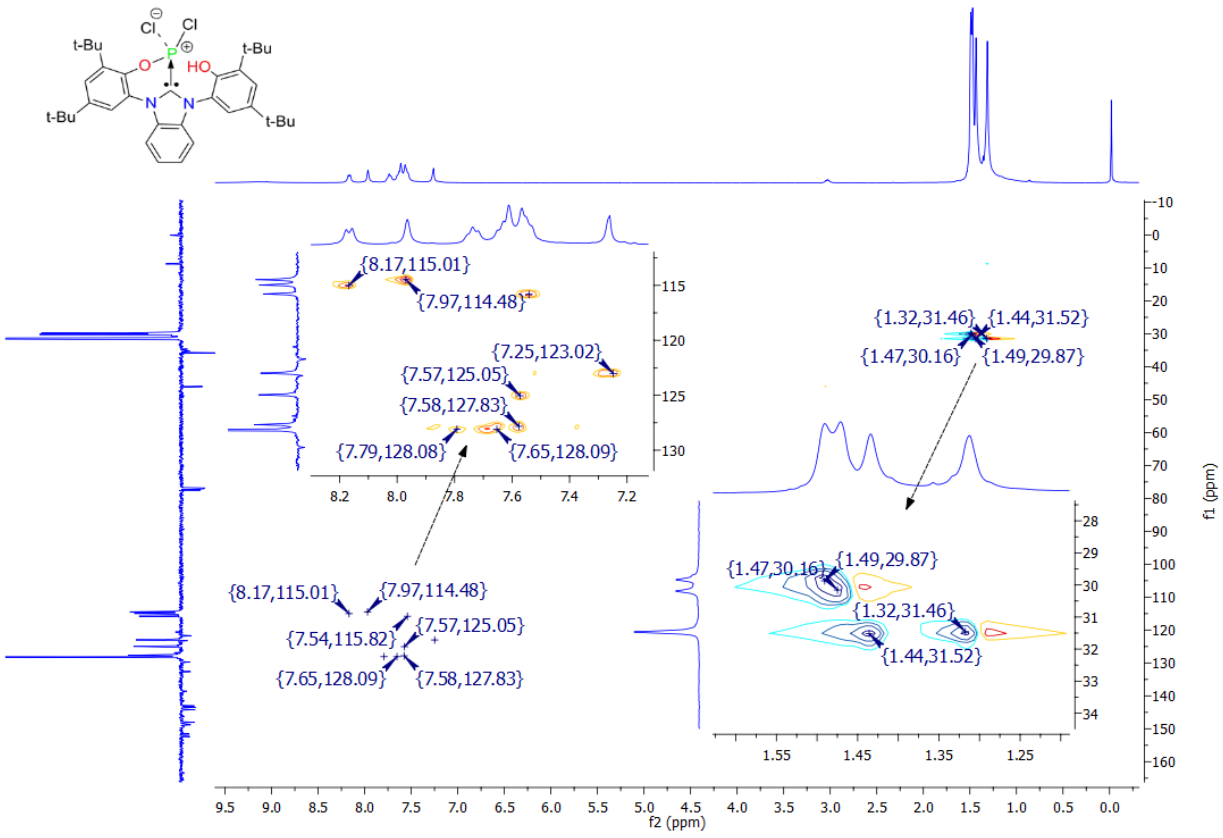


Figure S16. ^{1}H-^{13}C-HSQC NMR spectrum ($CDCl_3$) of **5-Ph**.

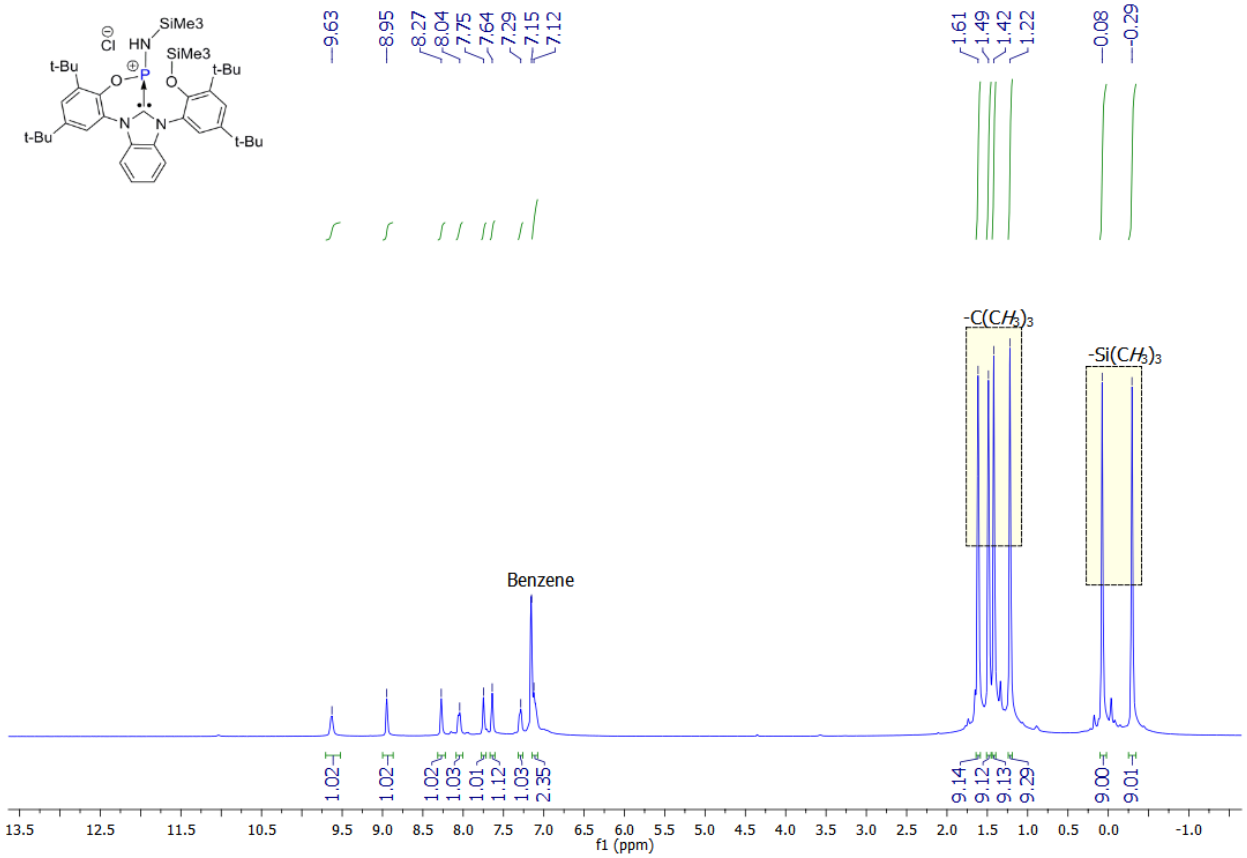


Figure S17. ^{1}H NMR spectrum (400 MHz, C_6D_6) of **5a-Ph**.

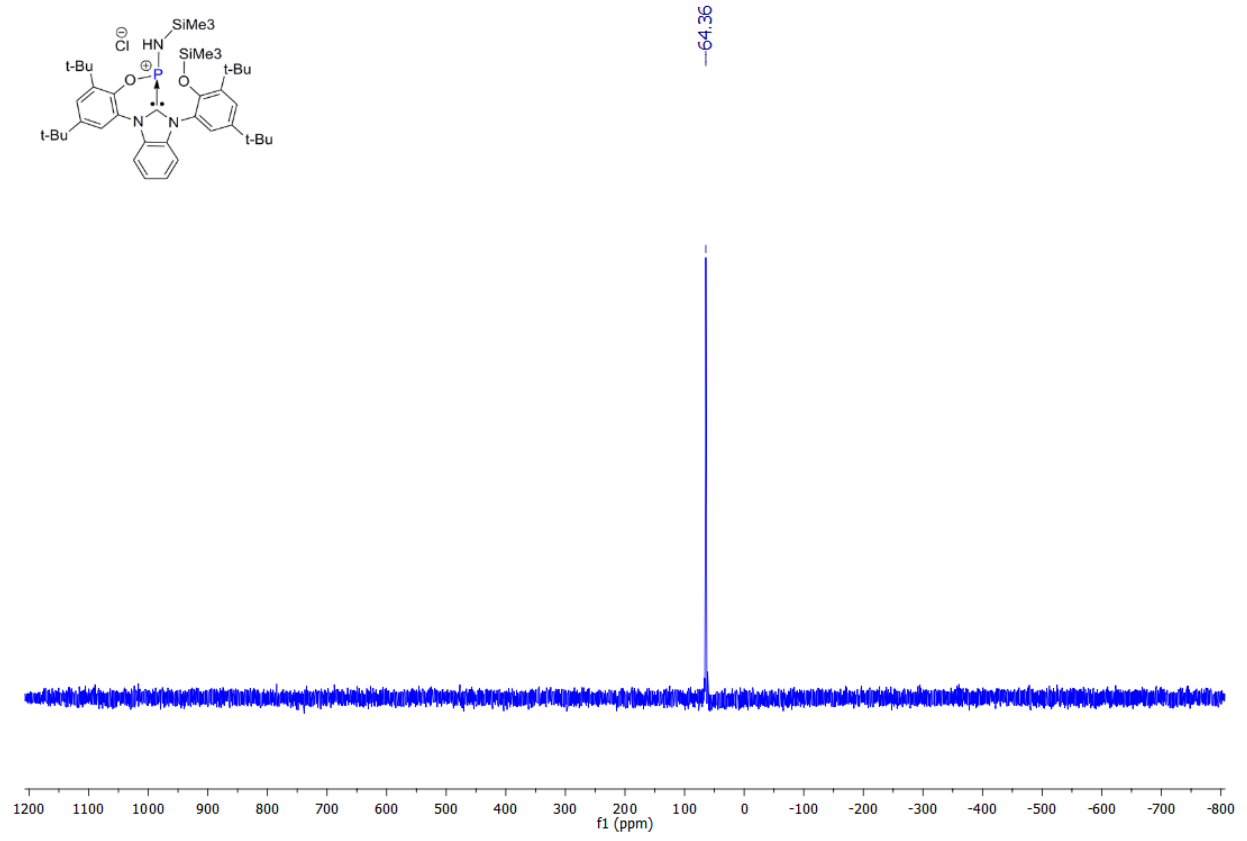


Figure S18. ^{31}P NMR spectrum (162 MHz, C_6D_6) of **5a-Ph**.

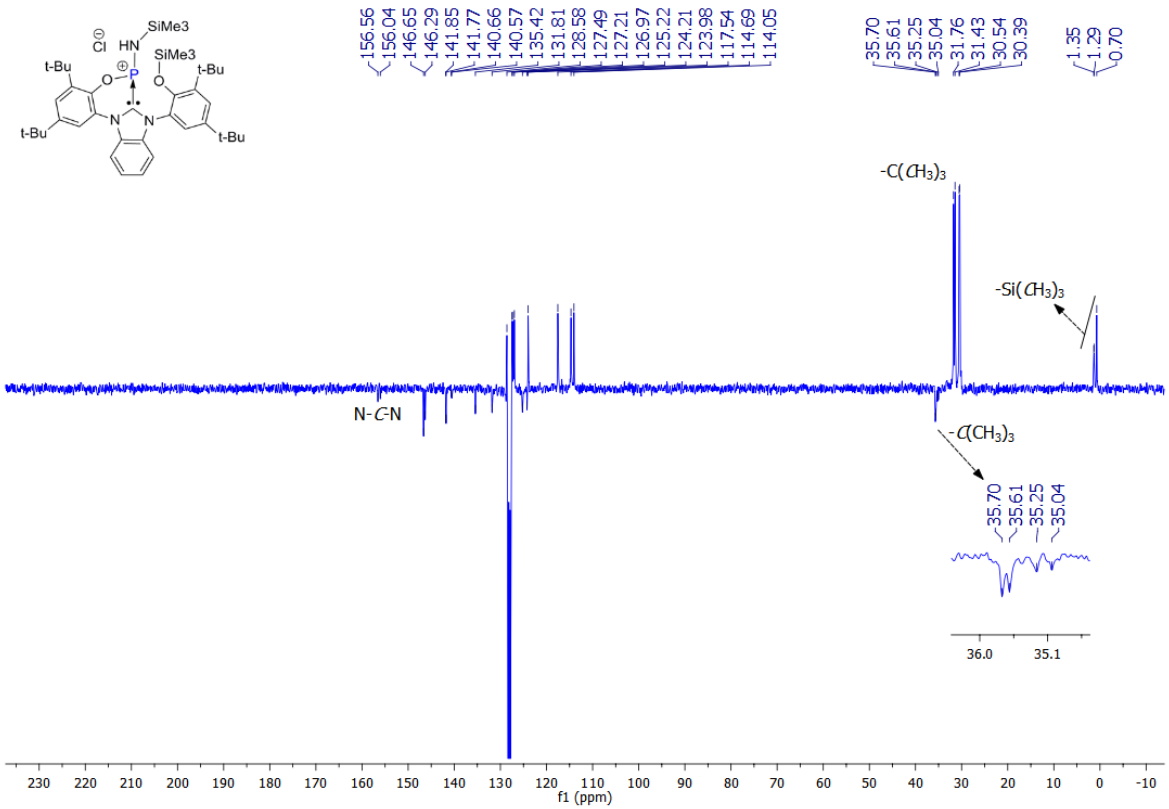


Figure S19. ^{13}C-JMOD NMR spectrum (100 MHz, C_6D_6) of **5a-Ph**.

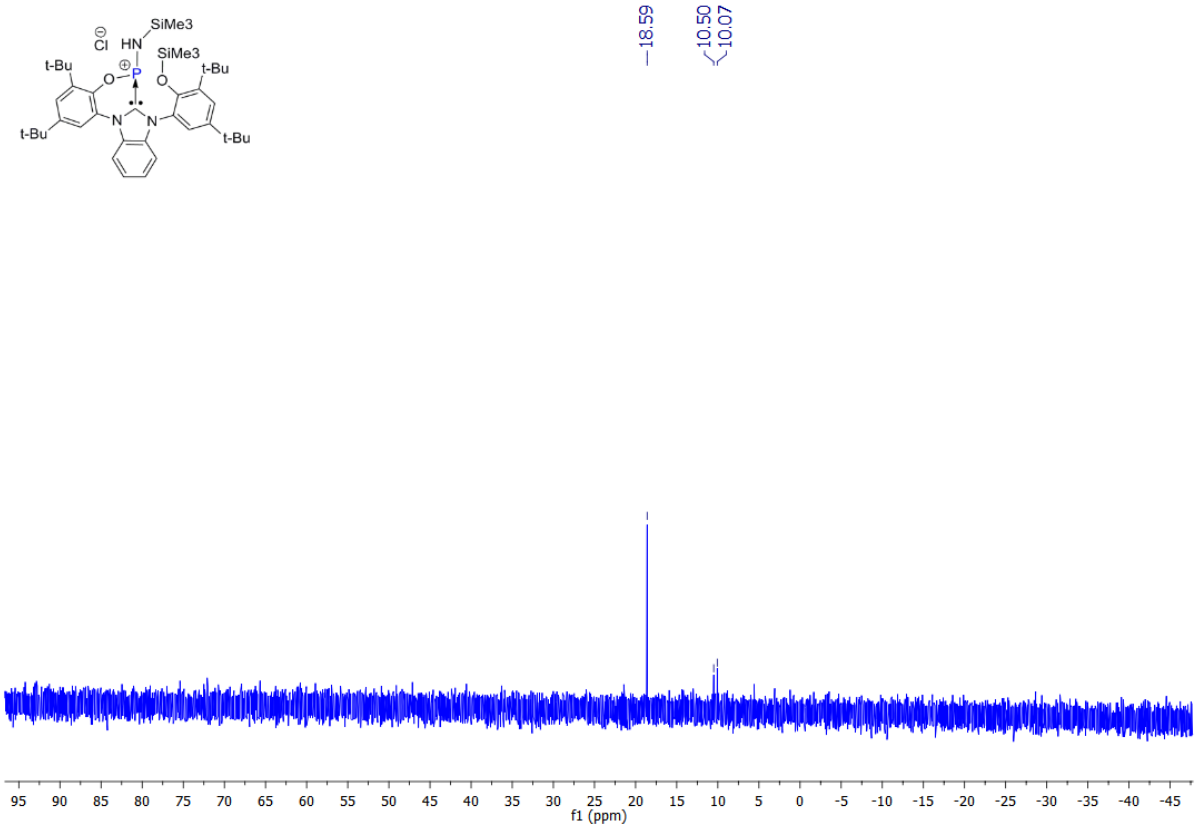


Figure S20. ^{29}Si NMR spectrum (79.5 MHz, C_6D_6) of **5a-Ph**.

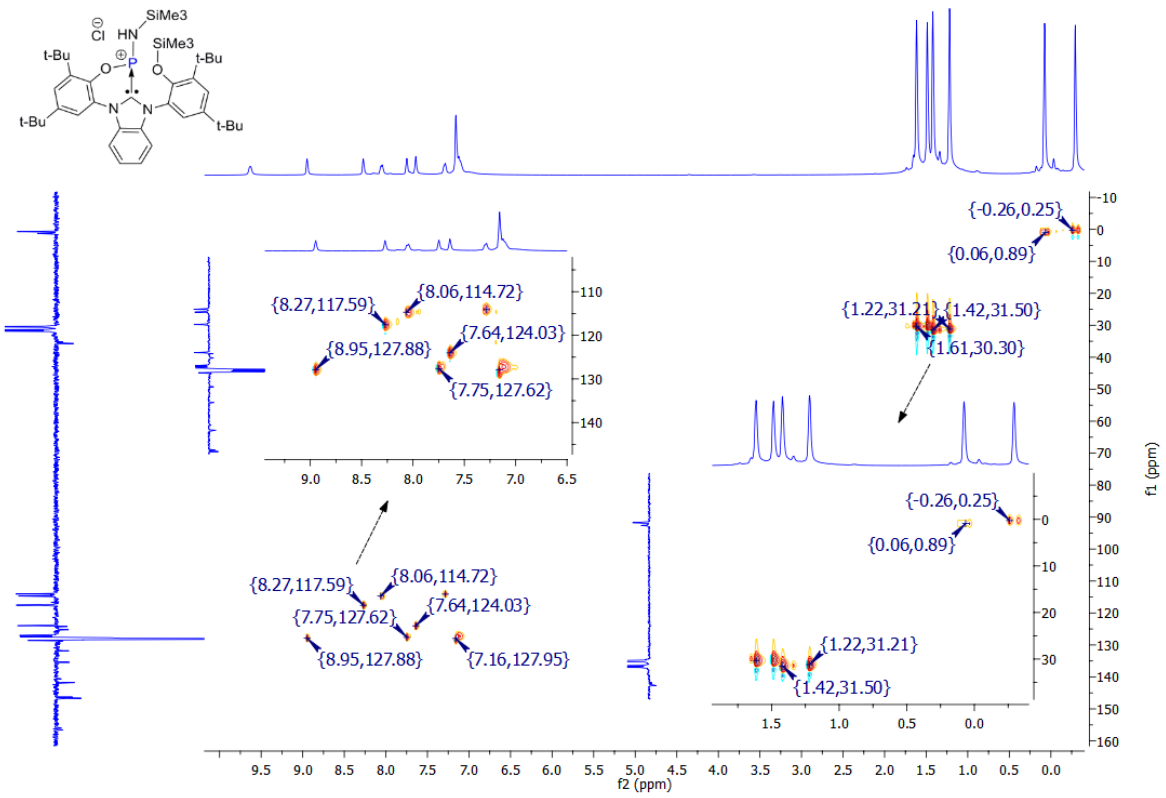


Figure S21. ^{1}H-^{13}C-HSQC NMR spectrum (C_6D_6) of **5a-Ph**.

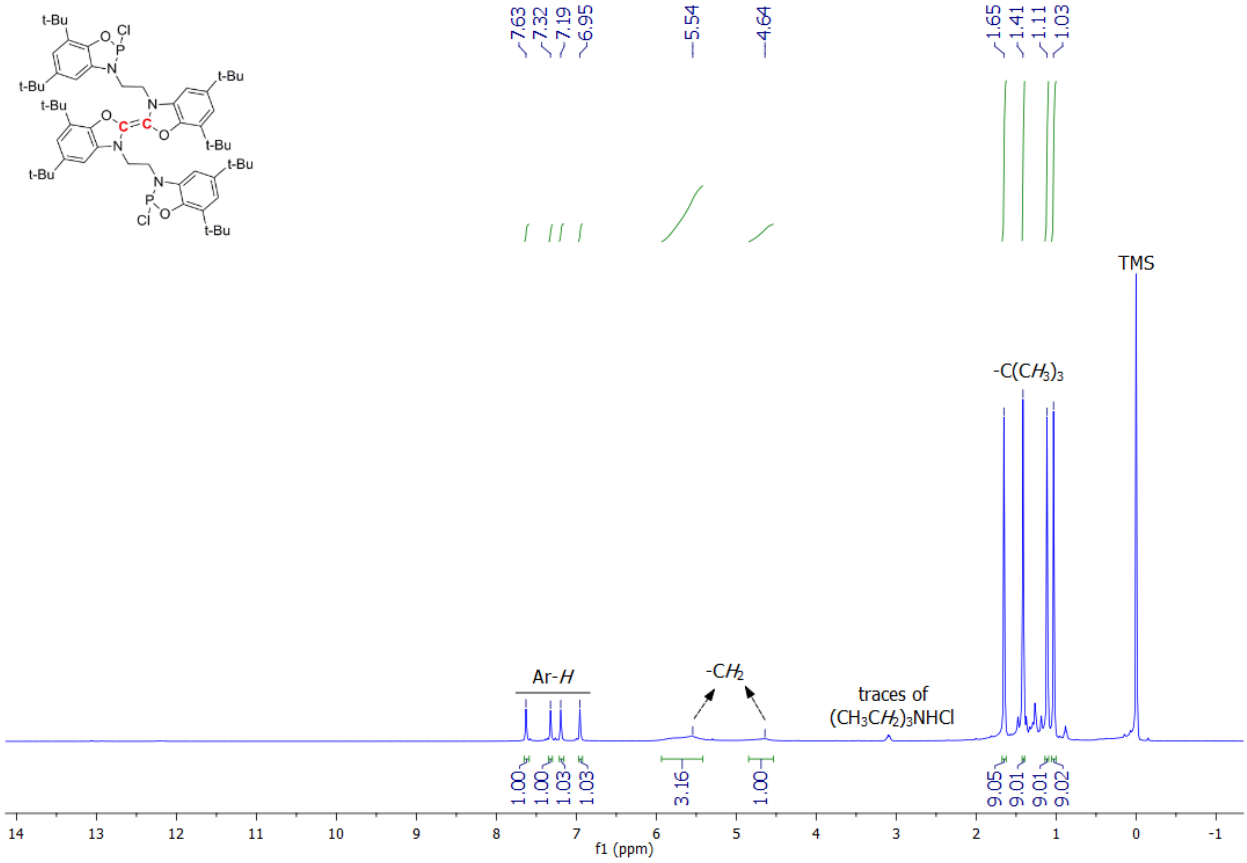


Figure S22. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **7**.

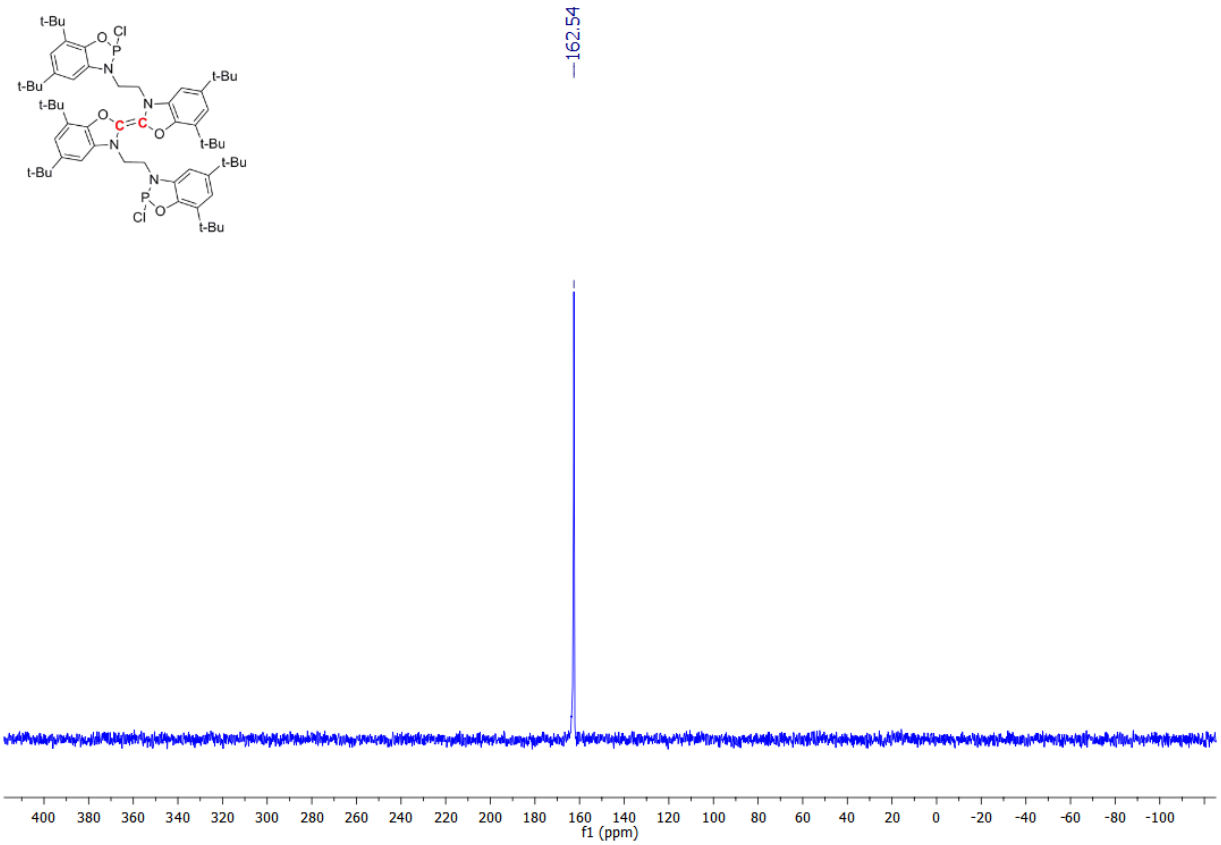


Figure S23. ^{31}P NMR spectrum (162 MHz, $CDCl_3$) of **7**.

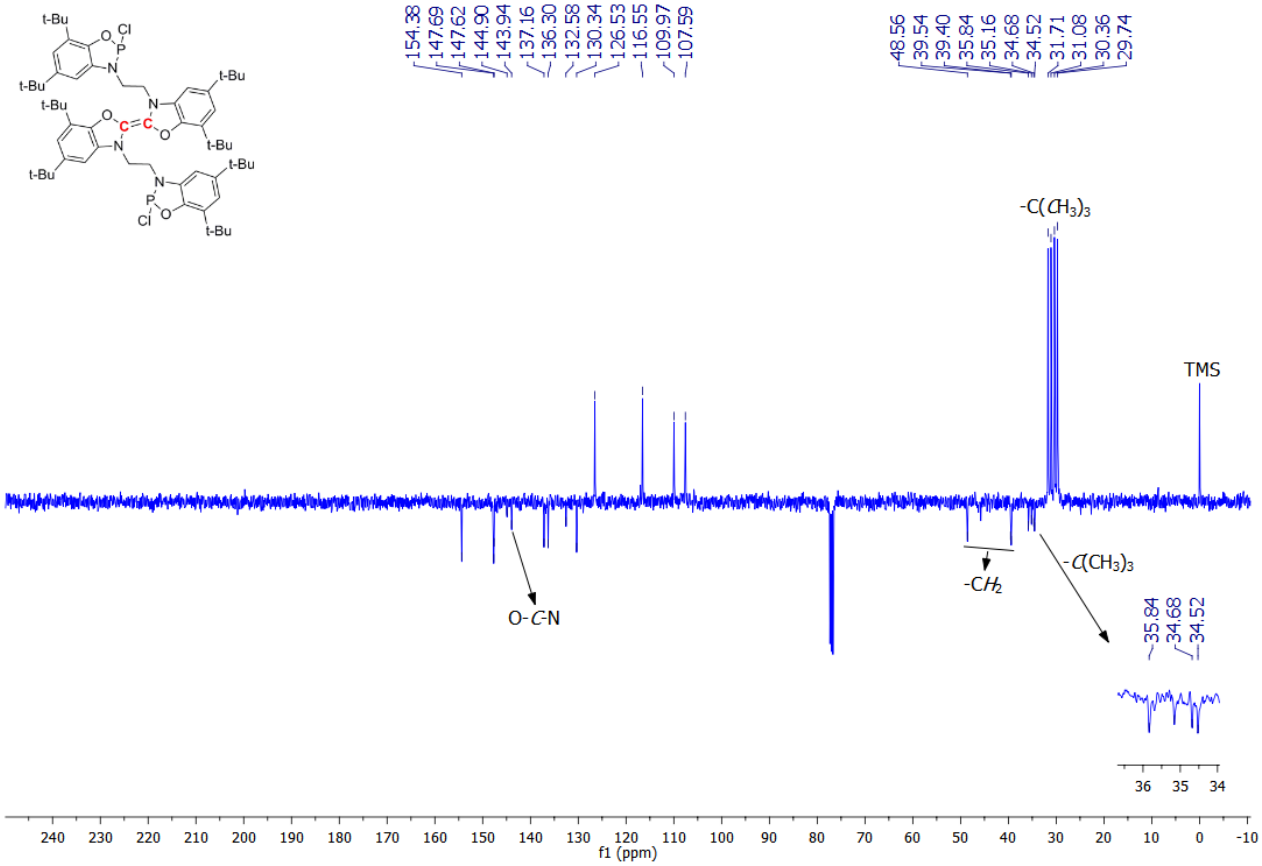


Figure S24. ^{13}C-JMOD NMR spectrum (100 MHz, $CDCl_3$) of **7**.

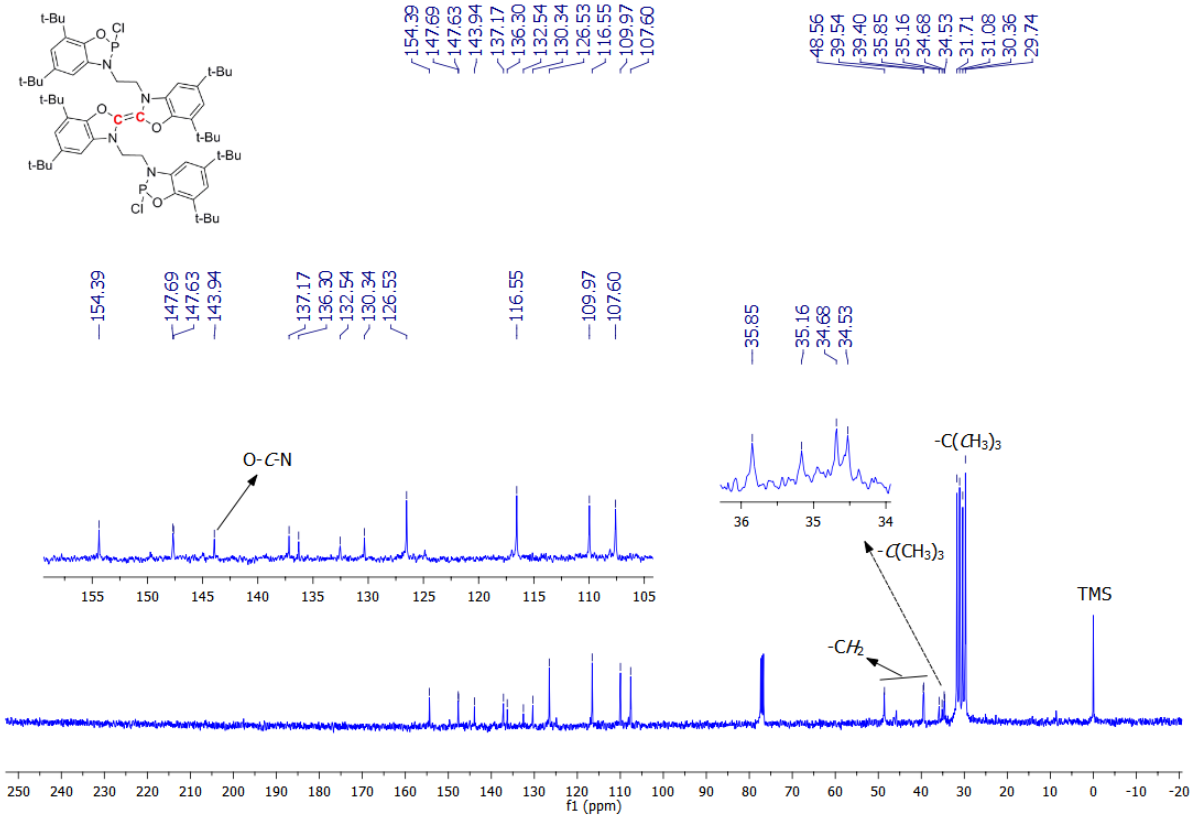


Figure S25. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **7**.

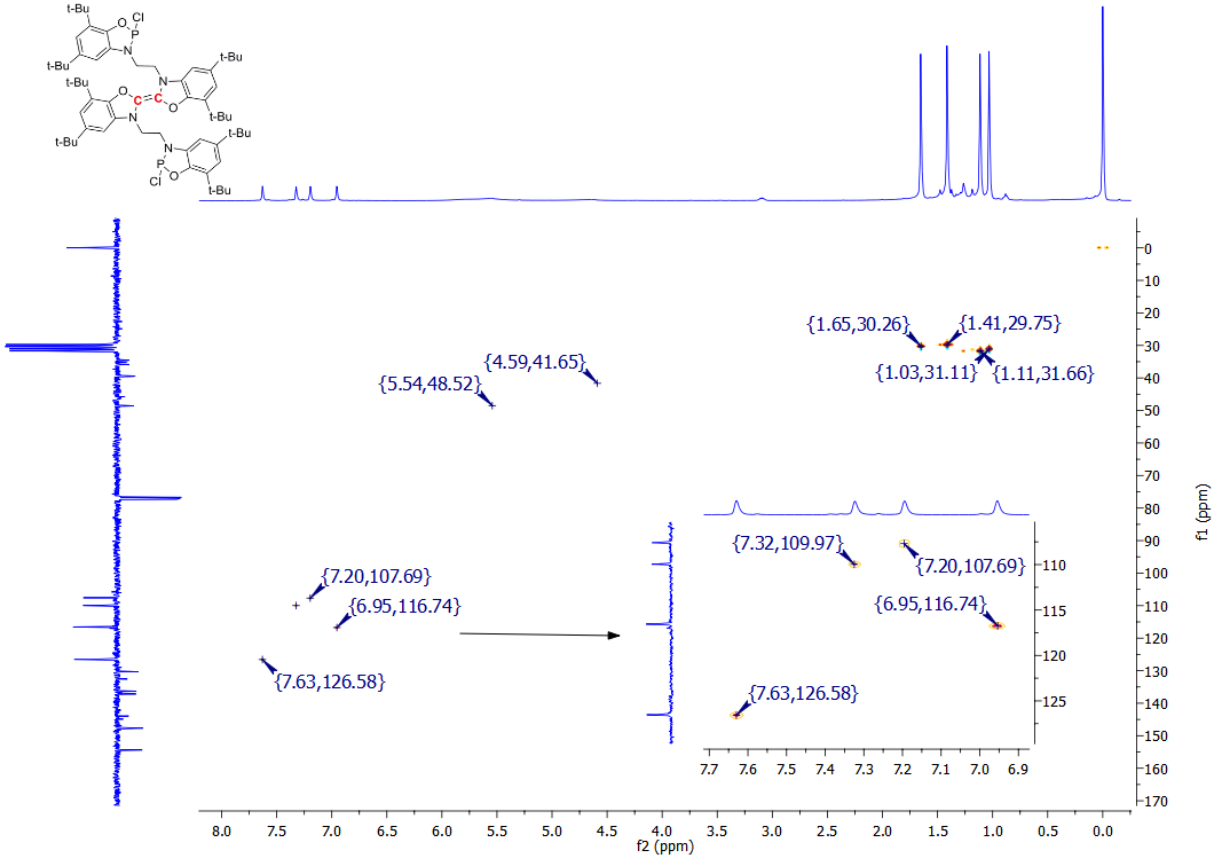


Figure S26. ^{1}H-^{13}C-HSQC NMR spectrum ($CDCl_3$) of **7**.

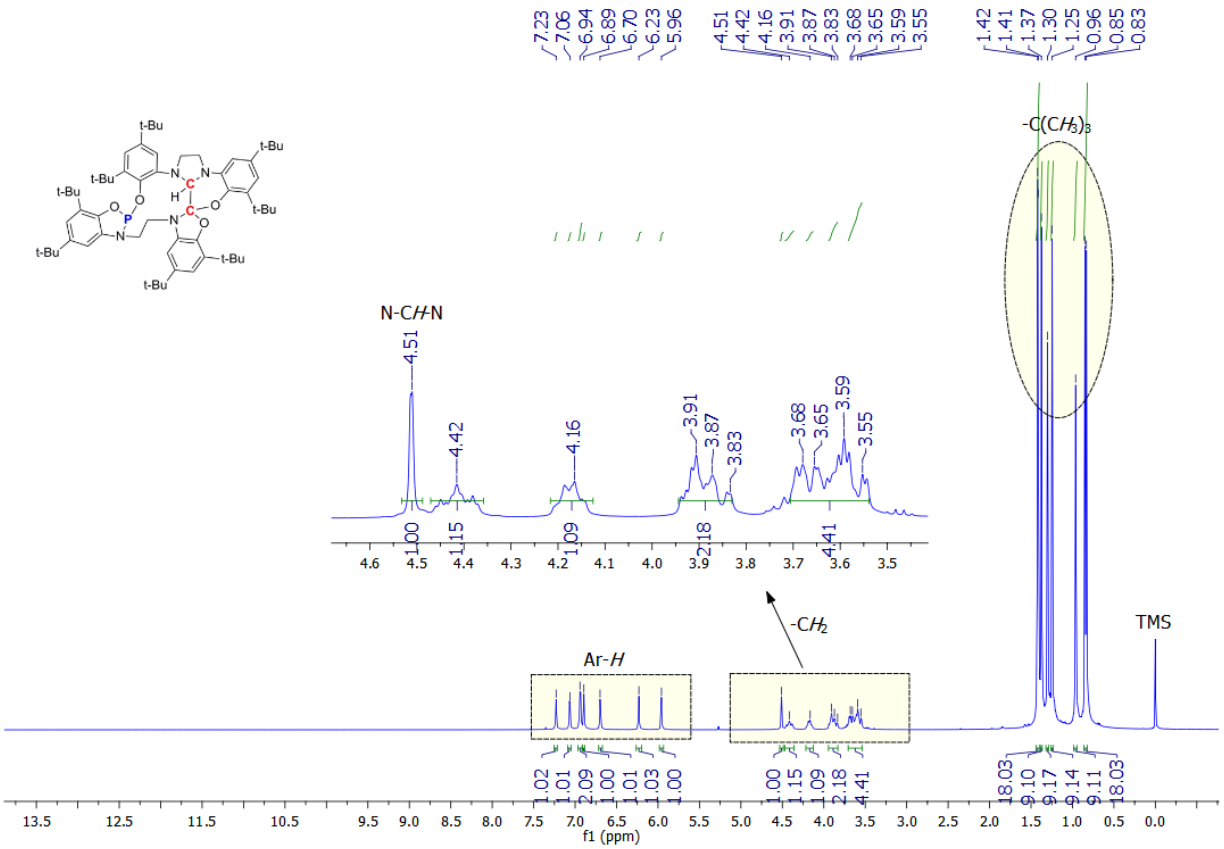


Figure S27. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **7-minor**.

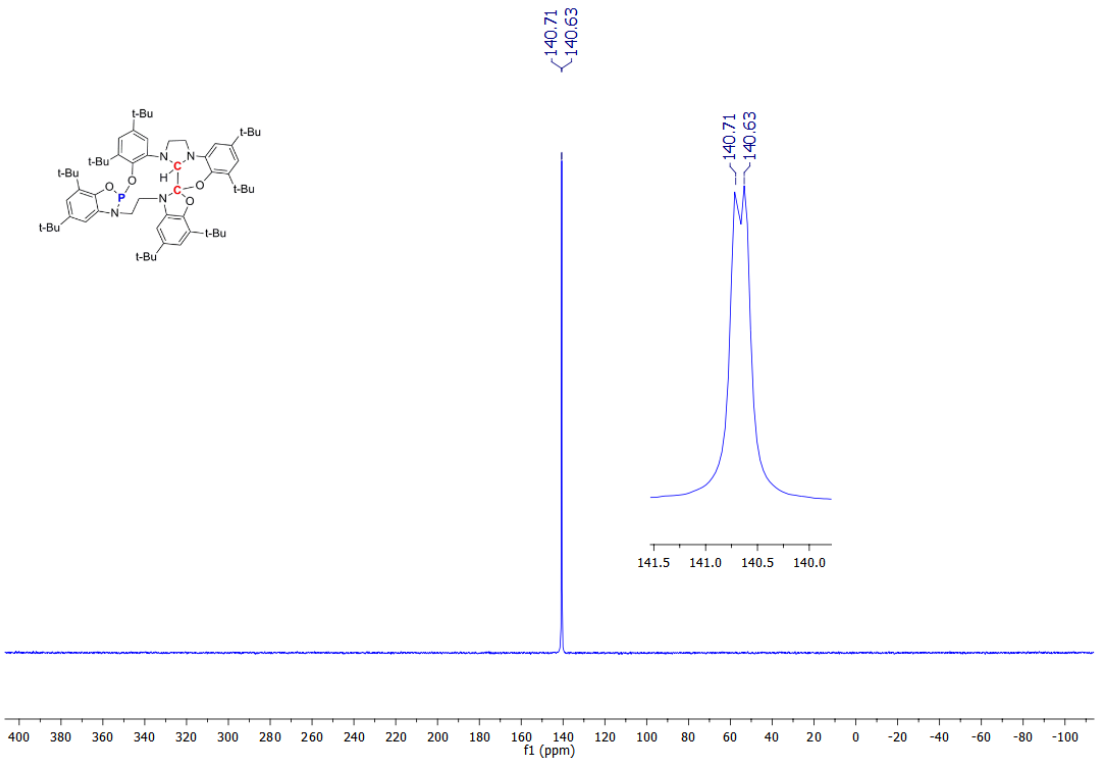


Figure S28. ^{31}P NMR spectrum (162 MHz, $CDCl_3$) of **7-minor**.

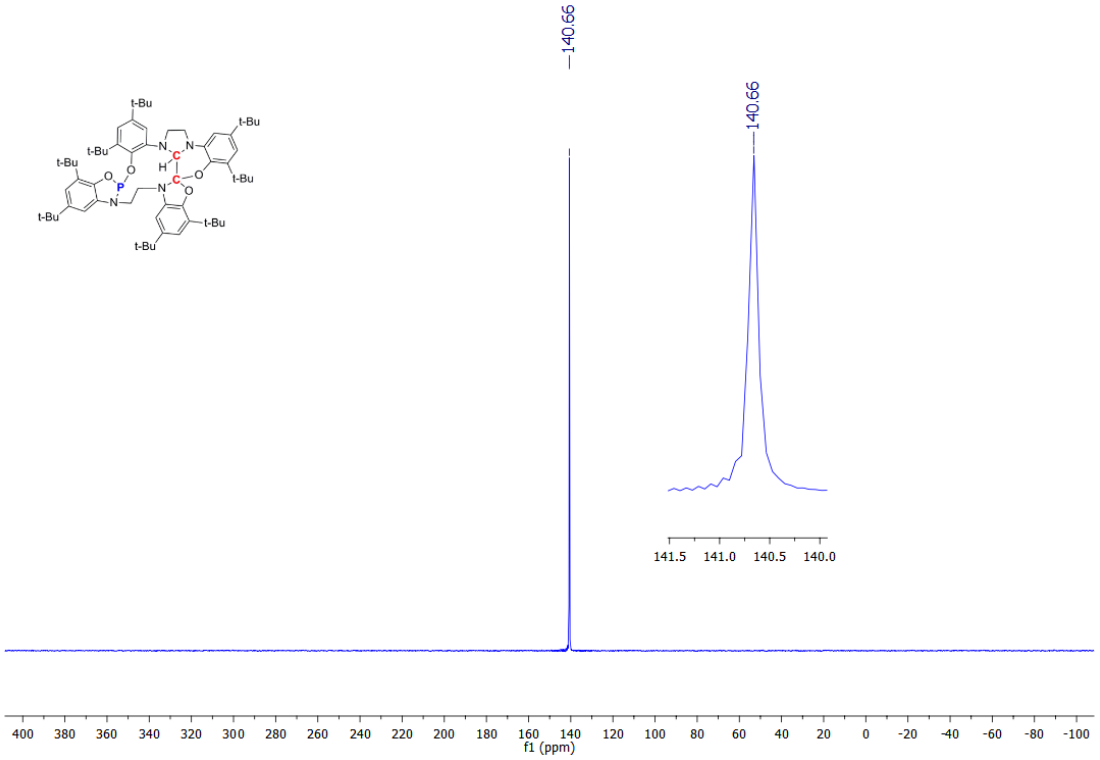


Figure S29. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, $CDCl_3$) of **7-minor**.

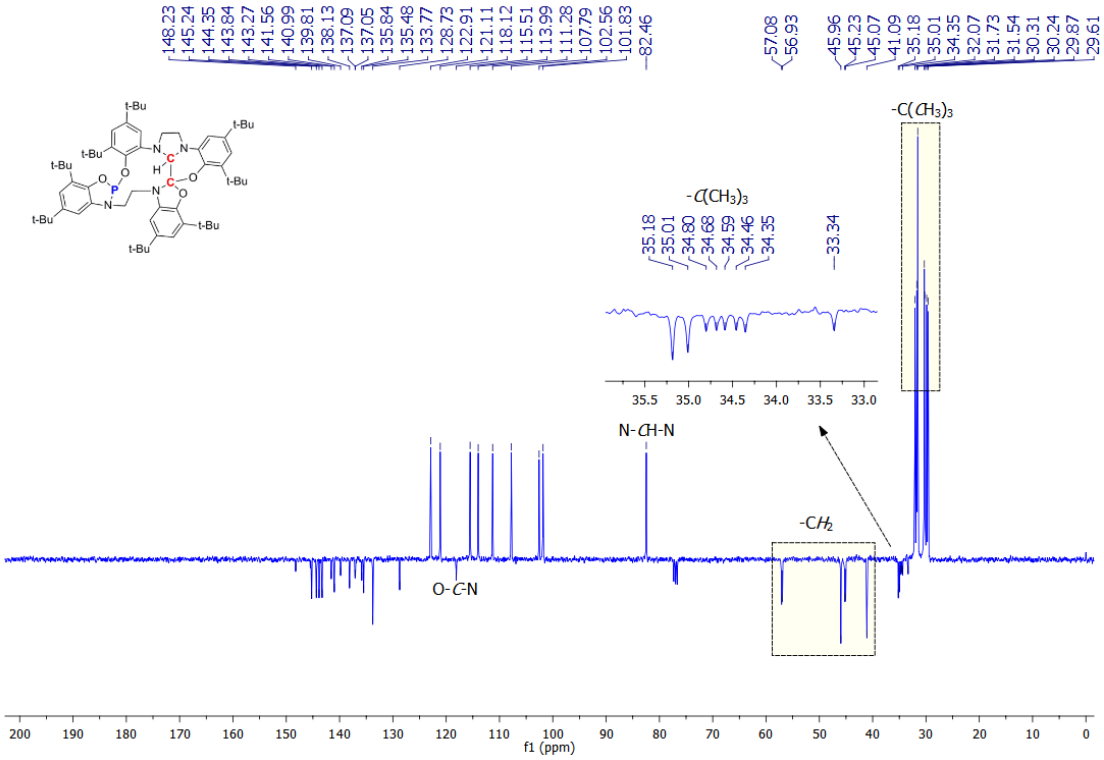


Figure S30. ^{13}C-JMOD NMR spectrum (100 MHz, $CDCl_3$) of **7-minor**.

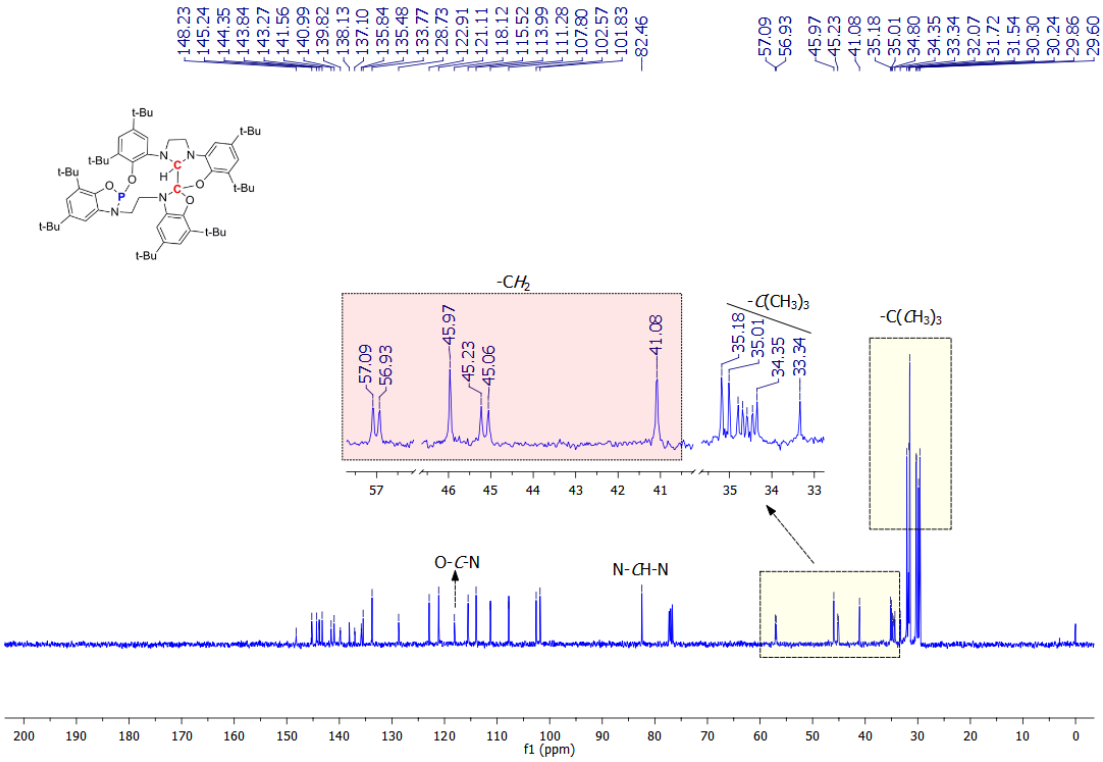


Figure S31. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **7-minor**.

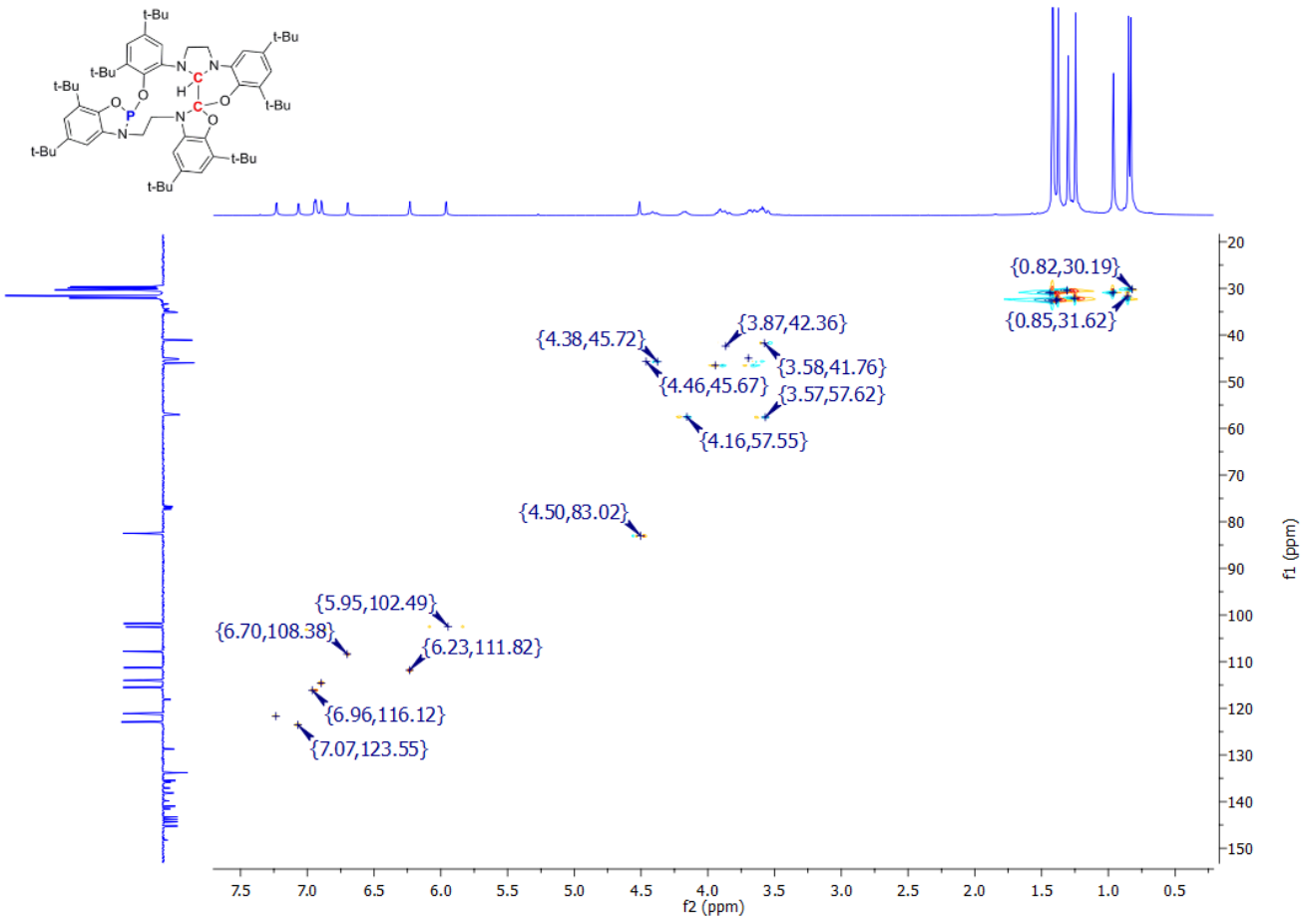


Figure S32. ^{1}H-^{13}C HSQC NMR spectrum ($CDCl_3$) of **7-minor**.

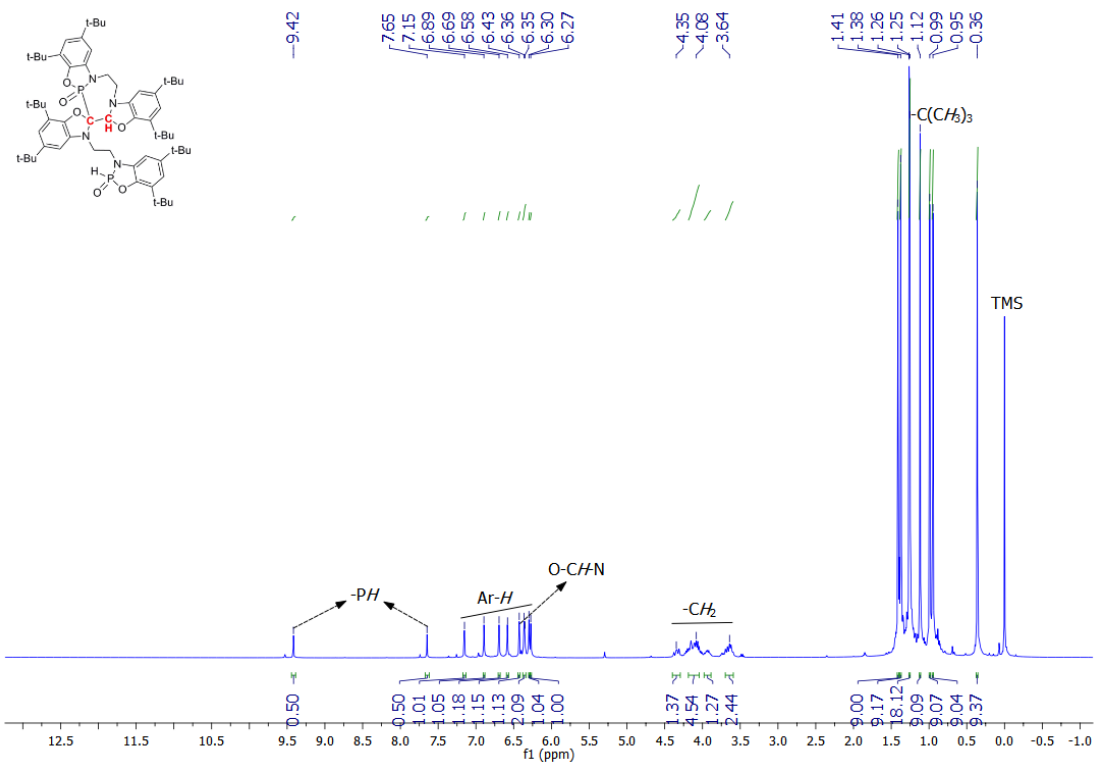


Figure S33. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9**.

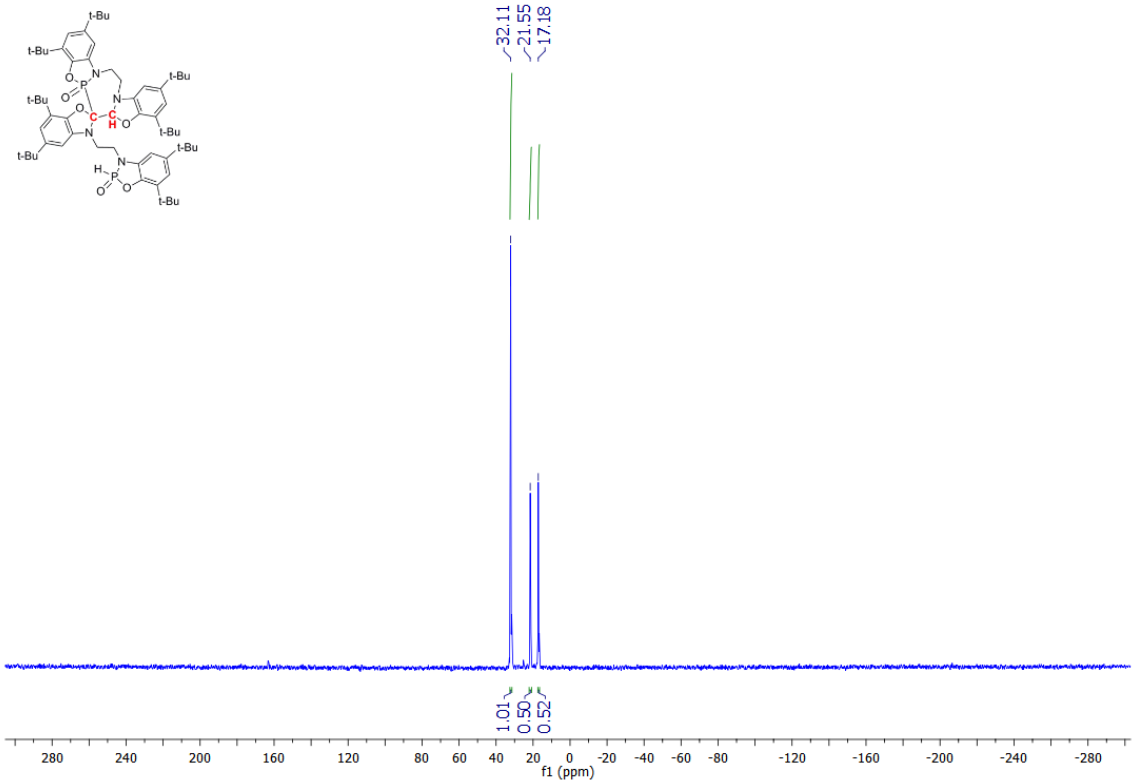


Figure S34. ^{31}P NMR spectrum (162 MHz, $CDCl_3$) of **9**.

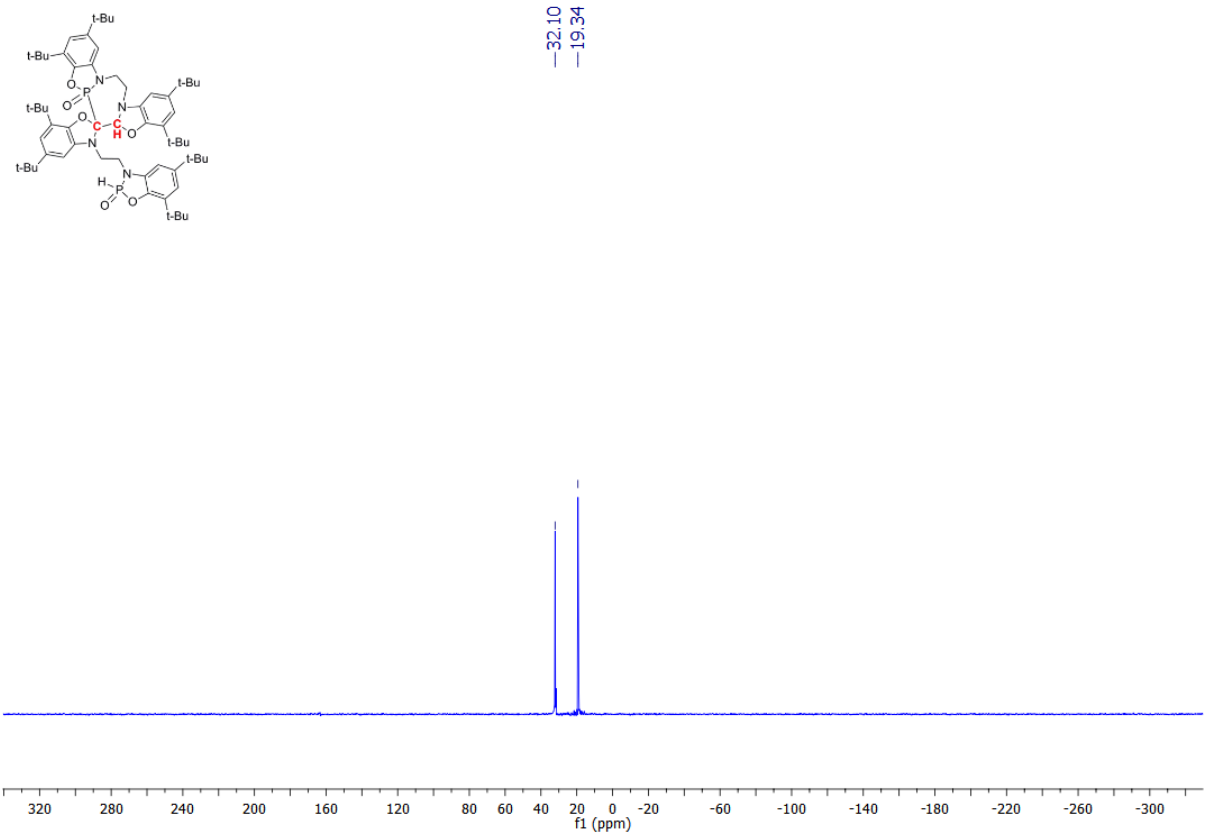


Figure S35. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, $CDCl_3$) of **9**.

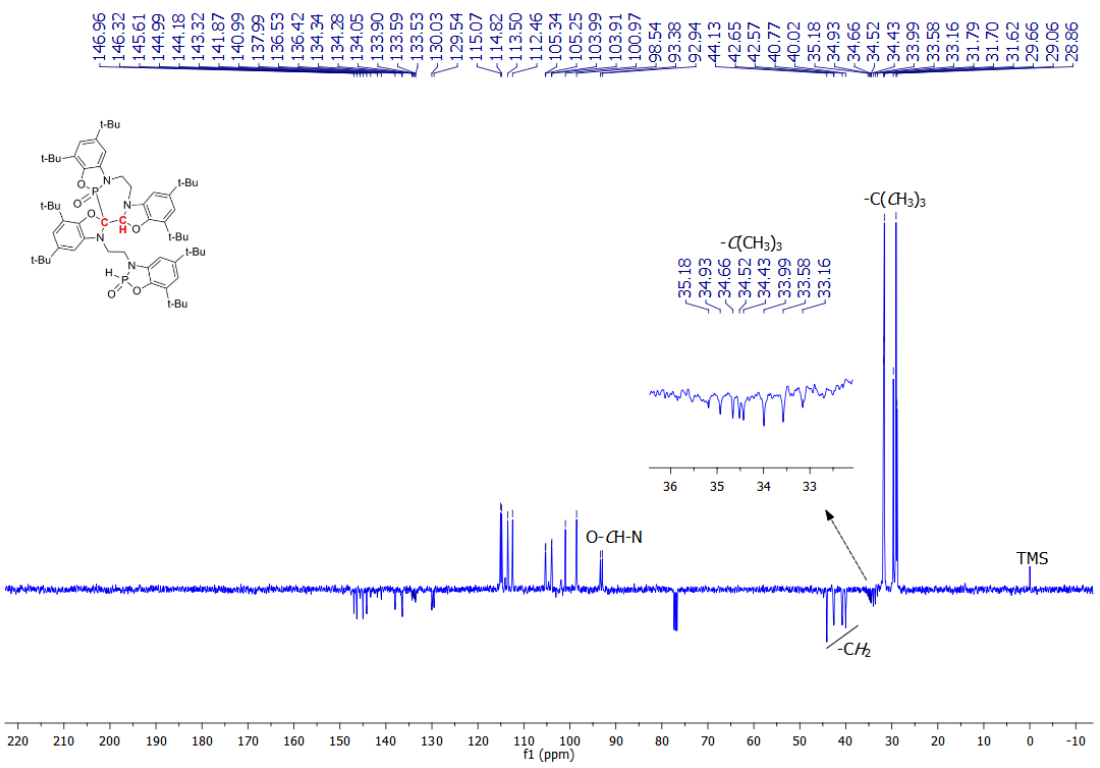


Figure S36. ^{13}C-JMOD NMR spectrum (100 MHz, $CDCl_3$) of **9**.

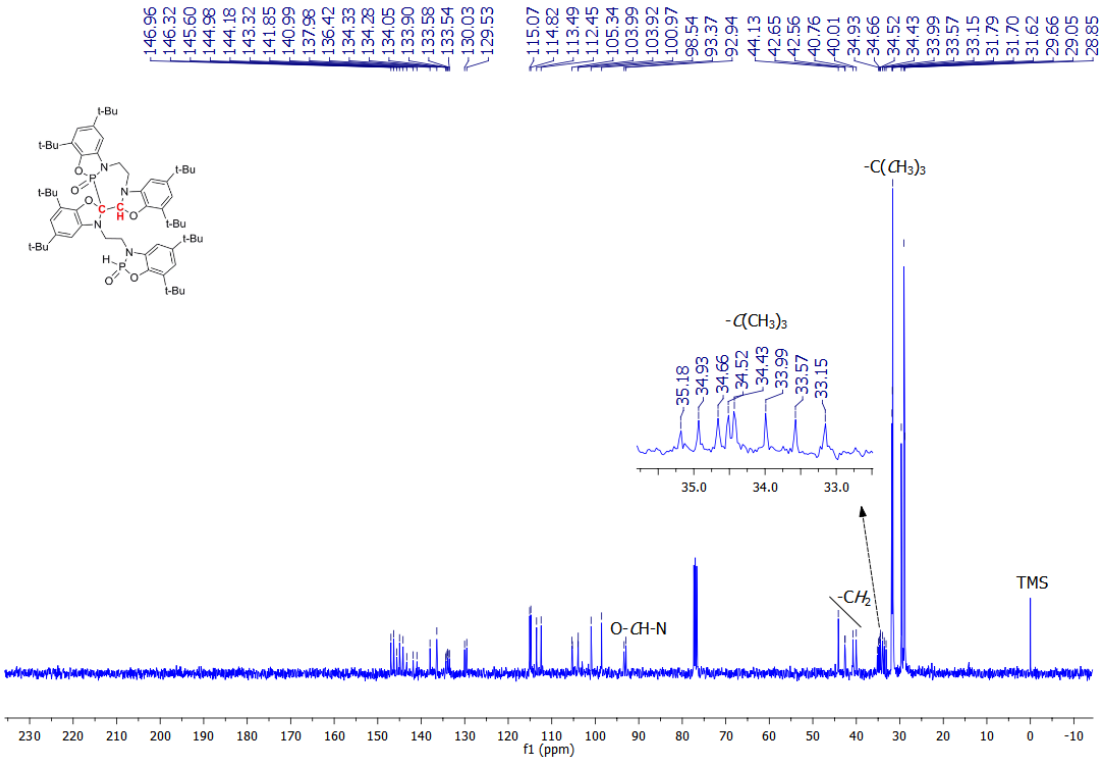


Figure S37. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **9**.

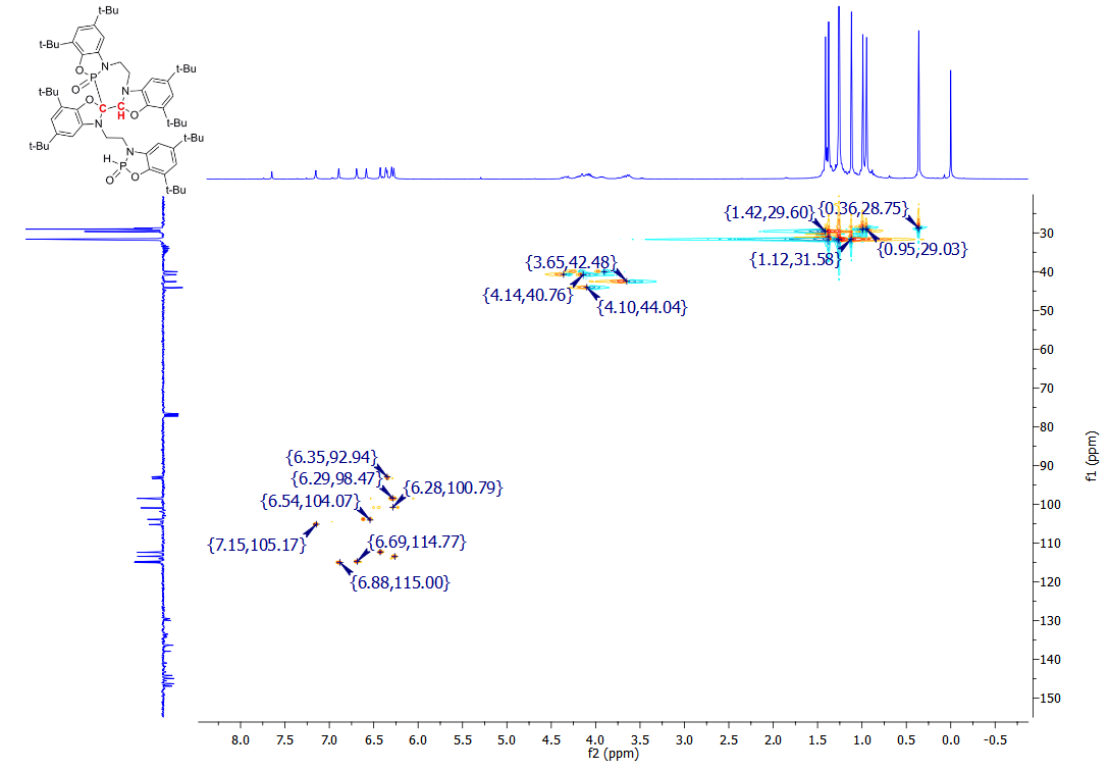


Figure S38. ^{1}H-^{13}C HSQC NMR spectrum ($CDCl_3$) of **9**.

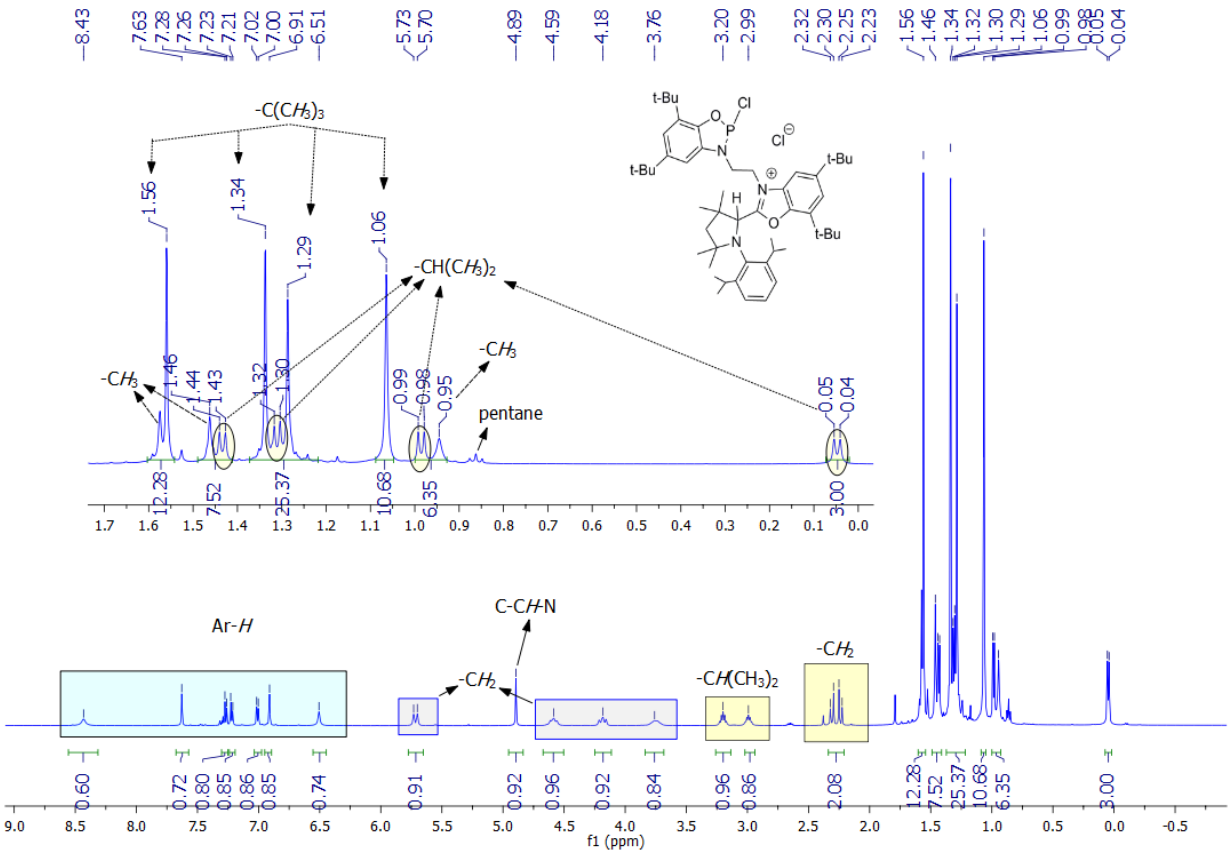


Figure S39. ^{1}H NMR spectrum (400 MHz, in $CDCl_3$) of **10**.

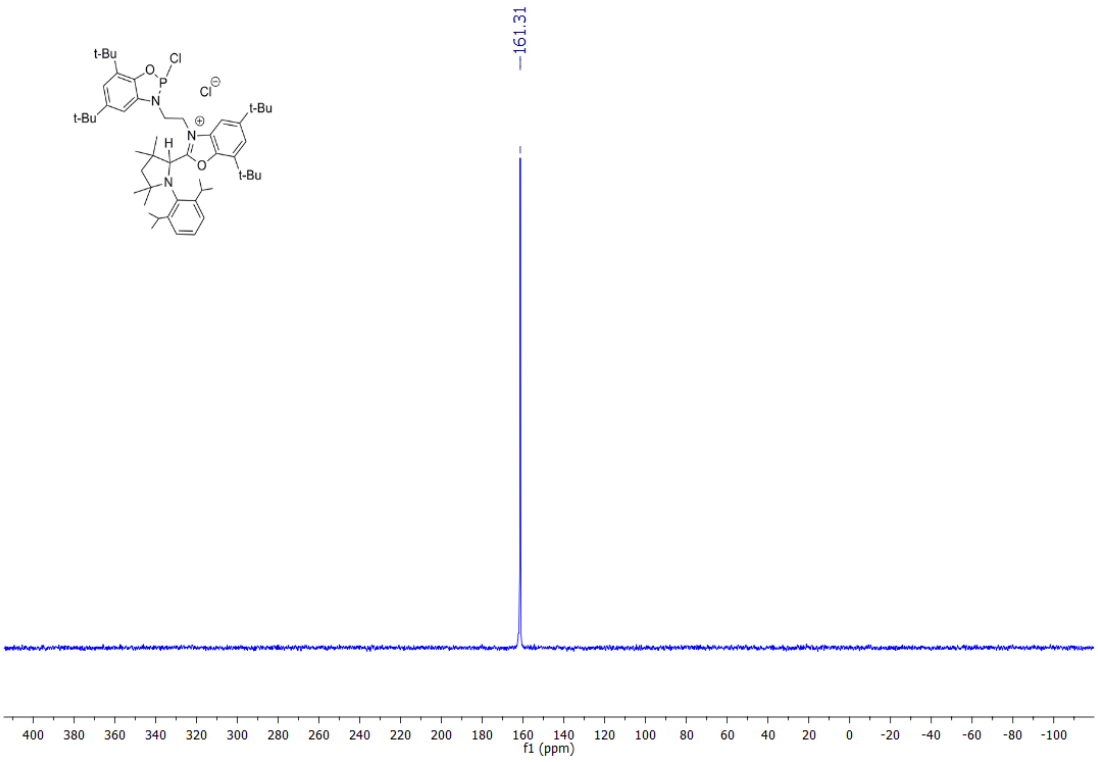


Figure S40. ^{31}P NMR spectrum (162 MHz, in $CDCl_3$) of **10**.

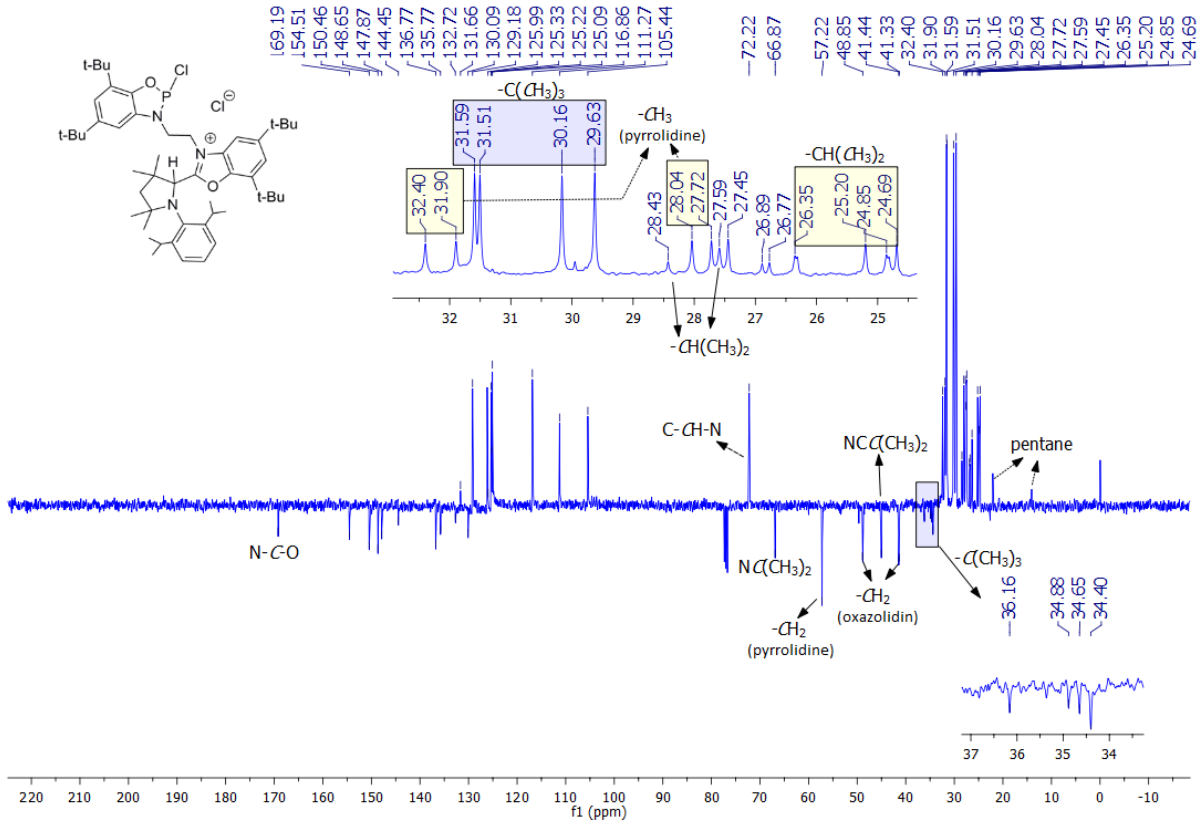


Figure S41. ^{13}C-JMOD NMR spectrum (100 MHz, in $CDCl_3$) of **10**.

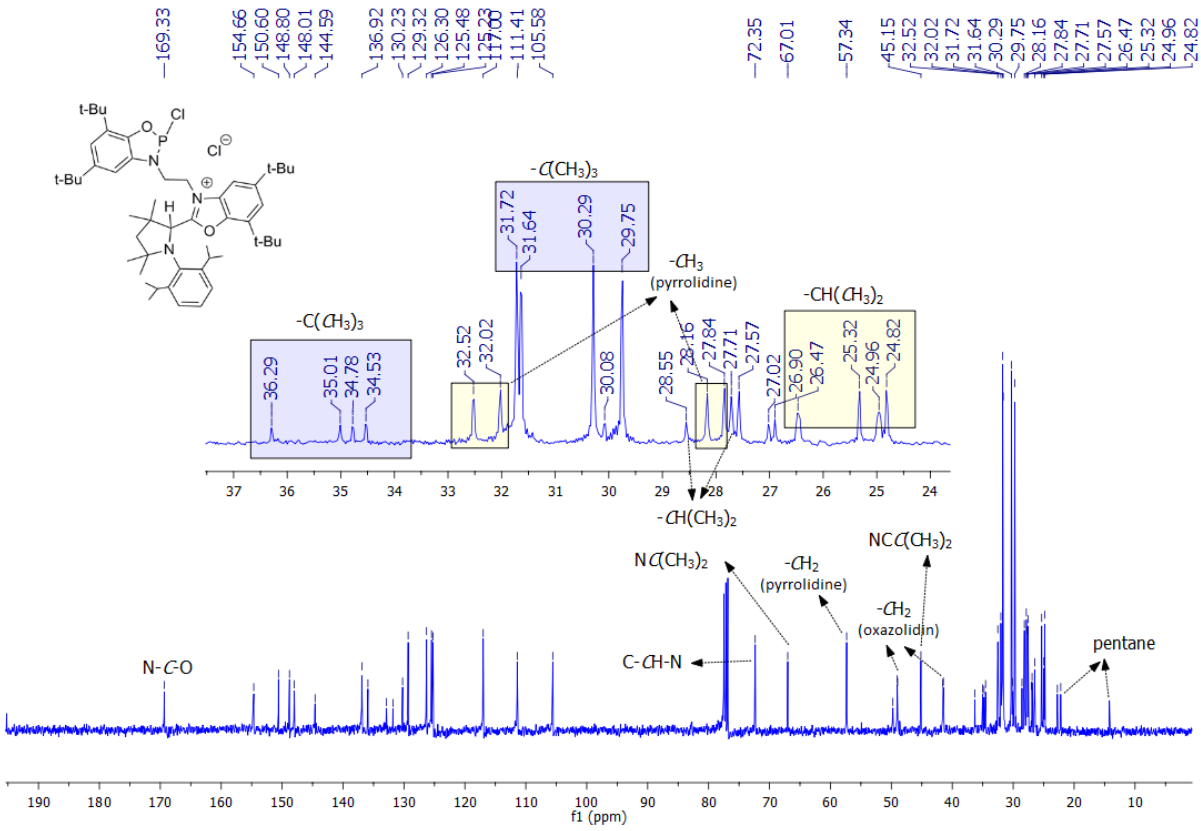


Figure S42. ^{13}C NMR spectrum (100 MHz, in $CDCl_3$) of **10**.

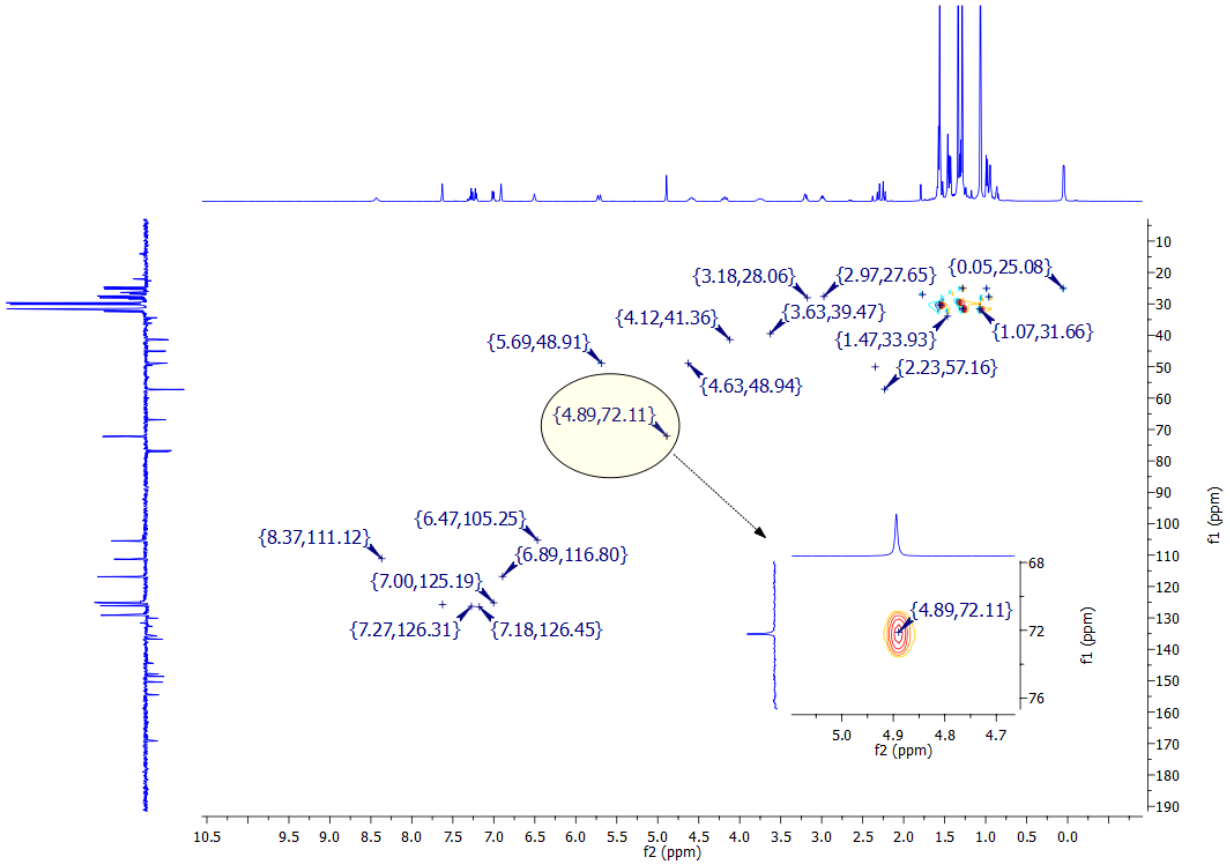
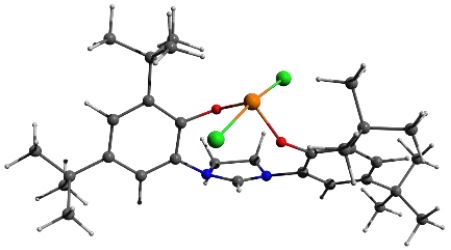


Figure S43. ^{1}H-^{13}C HSQC NMR spectrum (in $CDCl_3$) of **10**.

5. DFT Computations

DFT calculations were performed using Gaussian 09.2.[8] Geometry optimization of all the molecules were carried out using the BP86-D3 method[9] with Ahlrichs' def2-SVP basis set,[10] implemented in the Gaussian 09 software. Conductor-like polarizable continuum model (CPCM)[11] was used to account for the effect of THF. 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. The transition states geometries gave one imaginary frequency at expected reaction coordinates confirming that it is a first-order saddle point.

4:



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C	-3.54037	-1.88655	0.50367
H	-3.47997	-2.92256	0.86799
C	-2.37057	-1.27156	0.05591
C	-3.68430	2.11753	-1.34062
C	-2.99127	2.00818	-2.72652
H	-3.11412	2.96238	-3.28111
H	-3.45434	1.20038	-3.33155
H	-1.90876	1.79785	-2.64237
C	-3.04523	3.26340	-0.51911
H	-3.22004	4.23409	-1.02986
H	-1.94999	3.14243	-0.40270
H	-3.47558	3.31375	0.50117
C	-5.16127	2.50325	-1.59319
H	-5.19566	3.44462	-2.17877
H	-5.71669	2.68543	-0.65000
H	-5.70211	1.72748	-2.17416
C	-6.04301	-1.82826	1.01697
C	-5.84012	-2.15680	2.51880
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H	-5.63067	-1.23507	3.10066
H	-4.99522	-2.85803	2.67811
C	-6.32536	-3.13633	0.23395
H	-7.24981	-3.62025	0.61394
H	-5.49872	-3.86893	0.33679
H	-6.46375	-2.92772	-0.84743
C	-7.27110	-0.90389	0.88123
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H	-7.48812	-0.65492	-0.17833
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N	-1.14015	-2.00218	-0.07586
C	-0.78309	-2.63418	-1.38120
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H	-1.01404	-3.71698	-1.33706
C	0.73067	-2.34416	-1.51710
H	1.32083	-3.25105	-1.74458
H	0.96060	-1.54498	-2.25280
N	1.08400	-1.80962	-0.17220
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C	4.76699	-1.23094	-0.02041
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C	2.34163	0.18651	0.46682
C	6.11466	-1.92829	-0.29564
C	5.92577	-3.38058	-0.78096
H	6.91532	-3.84313	-0.97485

H	5.34615	-3.42857	-1.72645
H	5.40936	-4.00666	-0.02366
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H	7.85010	-1.62742	-1.61116
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H	7.16647	-0.92841	1.38152
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C	3.07605	3.28723	0.19030
H	3.18704	4.32953	0.55719
H	2.00094	3.11870	-0.01337
H	3.60970	3.19539	-0.77752
C	2.85368	2.41117	2.56791
H	2.95025	3.44105	2.97244
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C	-0.02443	-1.58555	0.52839
Cl	-1.21232	1.59554	1.93030

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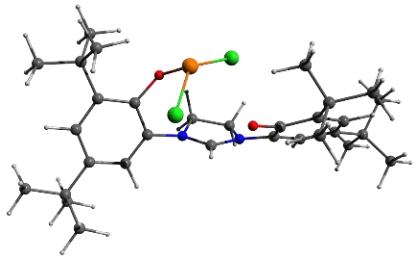

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H	3.25979	-1.94586	-2.93555
C	3.94402	-3.20127	-0.49754
H	4.42278	-4.14236	-0.84029
H	2.86627	-3.28386	-0.74522
H	4.03334	-3.14231	0.60599
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H	6.48664	-3.07711	-1.45482

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C	4.93819	2.66524	2.80684
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H	3.93937	3.14679	2.77441
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H	6.01825	3.60012	-0.39944
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H	6.90850	0.84989	2.08267
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H	-1.22712	3.20170	-1.59529
H	-1.61457	1.62534	-2.38490
N	-1.24398	1.50779	-0.29708
C	-2.52756	1.03330	0.07371
C	-3.66982	1.71802	-0.37682
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C	-4.95138	1.18000	-0.17365
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H	-5.32983	3.11709	-2.22628
H	-5.43939	3.94346	-0.63318
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H	-7.92671	1.46685	-1.99521
H	-7.26583	0.00162	-1.20299
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O	-1.51091	-0.79249	1.21585
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Cl	1.26909	-1.72346	1.44603

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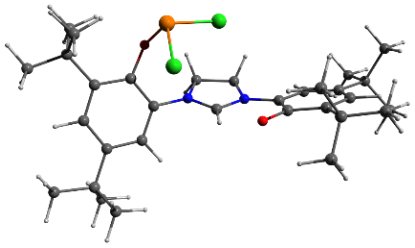

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C	5.32598	-2.91952	-0.64663
H	6.00423	-3.72972	-0.30615
H	5.68306	-2.56714	-1.63660
H	4.31567	-3.35012	-0.77677
C	4.87265	-2.26428	1.77205
H	5.60219	-2.99878	2.17251
H	3.89507	-2.78797	1.73210
H	4.78456	-1.42808	2.49495
C	6.79943	-1.27995	0.53219
H	7.43323	-2.13856	0.83391
H	6.91034	-0.49941	1.31285
H	7.20622	-0.88352	-0.42089
C	4.65521	3.24090	-0.73404
C	3.80726	4.16177	0.18113
H	4.18553	5.20462	0.13280
H	3.85749	3.82428	1.23727
H	2.73986	4.17870	-0.12036
C	4.55486	3.72987	-2.20201
H	4.94561	4.76555	-2.28948
H	3.50735	3.73604	-2.56731
H	5.14804	3.07870	-2.87735
C	6.12962	3.33189	-0.28769
H	6.47755	4.38242	-0.36312
H	6.79560	2.71505	-0.92621
H	6.26387	3.01210	0.76665
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H	-1.42276	-0.23226	-3.33787
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H	-6.21148	0.47859	0.75030
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Cl	1.36049	-0.85692	2.19970

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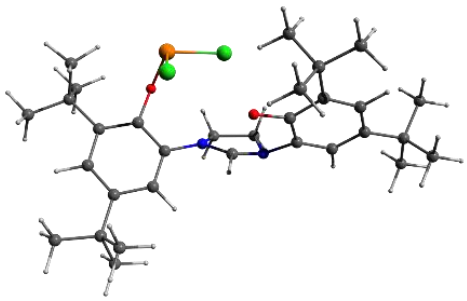

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C	5.23959	-1.49544	-0.65725
C	5.26550	-1.81995	-2.17411
H	5.96562	-2.65943	-2.36915
H	5.61429	-0.94095	-2.75511
H	4.26703	-2.11067	-2.55095
C	4.81115	-2.74742	0.15083
H	5.59214	-3.53254	0.07529
H	3.87613	-3.20341	-0.23466
H	4.65986	-2.50550	1.22225

C	6.68386	-1.14886	-0.22746
H	7.35007	-2.00166	-0.47027
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H	3.19539	4.63674	-0.01455
H	4.83851	4.31993	-0.66233
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C	-4.97051	-0.02676	0.60860
H	-5.89080	-0.43947	1.04727
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H	-3.49943	-0.17915	3.85468
H	-1.91232	-0.66164	3.15491
C	-5.02696	-2.12282	2.61644
H	-4.90266	-2.91729	3.38205
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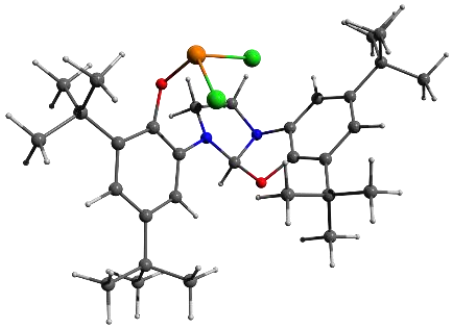

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H	-4.91717	-2.82907	1.45735
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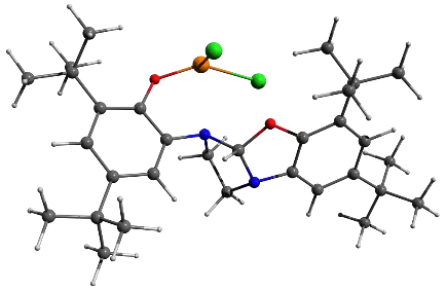
H	-6.40468	-2.71070	-1.21085
H	-5.86893	-1.10970	-1.79685
H	-6.33764	-1.32984	-0.07352
C	-3.96166	2.86663	0.25786
C	-2.92911	3.72702	-0.51679
H	-3.30034	4.76755	-0.63193
H	-2.74744	3.30940	-1.52900
H	-1.95130	3.77280	0.00504
C	-4.18031	3.46354	1.67157
H	-4.57871	4.49773	1.59761
H	-3.23694	3.50993	2.25341
H	-4.90696	2.85418	2.24867
C	-5.30359	2.91452	-0.50236
H	-5.65368	3.96464	-0.57991
H	-6.09566	2.33782	0.01909
H	-5.20811	2.51748	-1.53435
N	-0.37871	-0.26349	1.77787
C	-0.14835	-1.38786	2.69302
H	-0.21534	-2.35678	2.16720
H	-0.89945	-1.39257	3.51753
C	1.28875	-1.12422	3.23352
H	1.31527	-1.16518	4.34091
H	2.01141	-1.86633	2.84173
N	1.64899	0.21921	2.74795
C	2.52986	0.35468	1.64680
C	3.73420	-0.29656	1.36218
H	4.13010	-1.04121	2.06504
C	4.38370	-0.00048	0.13802

C	3.81403	0.96620	-0.72450
H	4.33060	1.18545	-1.66858
C	2.59850	1.64767	-0.45784
C	1.99176	1.29572	0.75314
C	5.65795	-0.75081	-0.30910
C	6.18738	-1.70243	0.78415
H	7.11022	-2.20688	0.43008
H	5.45142	-2.49478	1.03316
H	6.43994	-1.15689	1.71731
C	5.31147	-1.59618	-1.56316
H	6.19682	-2.17473	-1.90416
H	4.97727	-0.95706	-2.40610
H	4.49187	-2.31015	-1.33692
C	6.77948	0.26051	-0.65499
H	7.69664	-0.27425	-0.98206
H	7.03888	0.88087	0.22852
H	6.48371	0.94575	-1.47537
C	1.95135	2.67108	-1.40794
C	0.54641	2.16214	-1.82277
H	0.05678	2.89476	-2.49940
H	-0.11398	2.01181	-0.94590
H	0.62469	1.19413	-2.35665
C	1.81654	4.03016	-0.67314
H	1.34148	4.78176	-1.33931
H	2.81301	4.41707	-0.37288
H	1.19230	3.93655	0.23750
C	2.79238	2.88229	-2.68310
H	2.29320	3.62465	-3.33979
H	2.90322	1.94314	-3.26427
H	3.80702	3.26798	-2.45111
O	0.78334	1.77192	1.25189
H	-0.11037	1.45063	3.07231
C	0.41260	0.86557	2.27945
Cl	-0.74261	-1.24090	-2.32481

Sum of electronic and zero-point Energies= -2728.264380
Sum of electronic and thermal Energies= -2728.222860
Sum of electronic and thermal Enthalpies= -2728.221916
Sum of electronic and thermal Free Energies= -2728.337134

TS3:



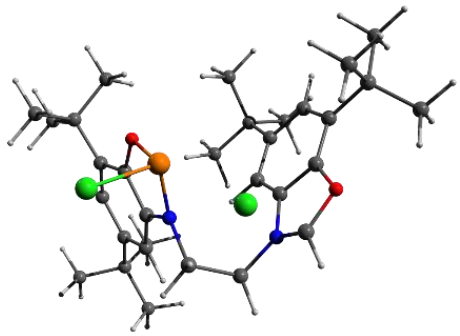
P	0.90933	-2.32446	-1.03378
Cl	-1.38172	-2.01782	-1.62329
O	2.46770	-1.67107	-1.29749
C	2.99652	-0.56616	-0.67678
C	4.37847	-0.43247	-0.41833
C	4.78403	0.78582	0.17410
H	5.85114	0.92136	0.38090
C	3.89633	1.82722	0.51321
C	2.52162	1.63098	0.25779
H	1.79949	2.42215	0.50594
C	2.07000	0.43592	-0.31974
C	5.36882	-1.57234	-0.73419
C	5.32204	-1.91015	-2.24736
H	6.04768	-2.71886	-2.47681

H	5.59521	-1.02249	-2.85551
H	4.31780	-2.25152	-2.56175
C	4.98016	-2.81758	0.10709
H	5.67137	-3.65788	-0.11507
H	3.94826	-3.15572	-0.10594
H	5.04877	-2.59248	1.19178
C	6.82021	-1.18673	-0.37674
H	7.49399	-2.03521	-0.61474
H	6.93975	-0.96219	0.70340
H	7.17246	-0.30872	-0.95714
C	4.36449	3.15313	1.14924
C	3.68544	3.31936	2.53324
H	4.01072	4.26771	3.01066
H	3.95575	2.48133	3.20897
H	2.57941	3.34767	2.45188
C	3.95734	4.33074	0.22616
H	4.28259	5.29652	0.66753
H	2.85871	4.38370	0.08053
H	4.42944	4.23110	-0.77344
C	5.89401	3.19643	1.34748
H	6.18362	4.16596	1.80234
H	6.43881	3.10436	0.38501
H	6.24713	2.39234	2.02590
N	0.68913	0.13557	-0.62198
C	0.23584	0.78282	-1.89915
H	-0.48621	0.09954	-2.38859
H	1.10655	0.95010	-2.55959
C	-0.46770	2.06804	-1.43419
H	0.25017	2.89835	-1.26960
H	-1.23673	2.41685	-2.14949
N	-1.08883	1.66486	-0.16682
C	-2.42714	1.20850	-0.11340
C	-3.59229	1.75170	-0.66415
H	-3.53616	2.66310	-1.27382
C	-4.81977	1.09650	-0.40041
C	-4.81466	-0.04763	0.43301
H	-5.77900	-0.52125	0.65957
C	-3.64813	-0.62183	0.99989
C	-2.45831	0.03595	0.65503
C	-6.16147	1.60325	-0.97620
C	-5.97750	2.84733	-1.87075
H	-6.95994	3.17175	-2.27234
H	-5.31613	2.63900	-2.73756
H	-5.55049	3.70263	-1.30667
C	-6.80584	0.48184	-1.83162
H	-7.77100	0.82606	-2.26103
H	-7.00986	-0.42889	-1.23210
H	-6.13833	0.19228	-2.67013
C	-7.11471	1.97827	0.18738
H	-8.08469	2.34823	-0.20823
H	-6.67135	2.77734	0.81774
H	-7.32864	1.10899	0.84252
C	-3.67215	-1.83343	1.95039
C	-2.88898	-3.01421	1.32765
H	-2.88758	-3.87813	2.02670
H	-1.84113	-2.73859	1.10721
H	-3.35264	-3.33648	0.37304
C	-3.00617	-1.42484	3.29127
H	-3.02632	-2.27715	4.00349
H	-3.54516	-0.57368	3.75816
H	-1.94945	-1.12837	3.14171
C	-5.11229	-2.30163	2.24608
H	-5.08542	-3.15920	2.94986
H	-5.63438	-2.64222	1.32774
H	-5.72206	-1.50146	2.71554
O	-1.16869	-0.31380	1.02816

H	0.37300	0.98506	1.30230
C	-0.27629	0.63207	0.47472
Cl	0.96320	-2.53404	1.09786

Sum of electronic and zero-point Energies= -2728.238223
Sum of electronic and thermal Energies= -2728.197296
Sum of electronic and thermal Enthalpies= -2728.196352
Sum of electronic and thermal Free Energies= -2728.309567

3:

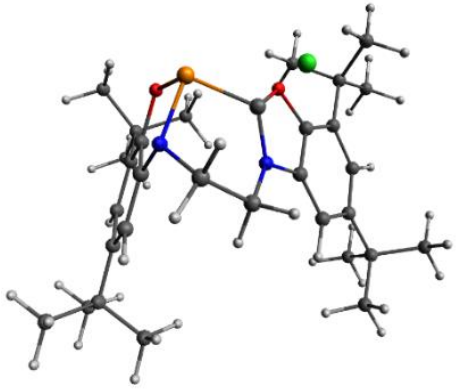


P	-0.26523	1.96505	1.28209
Cl	0.70220	3.89038	1.89351
O	0.89353	0.85632	1.86157
C	1.88387	0.55093	0.94367
C	3.05526	-0.17900	1.22136
C	3.86606	-0.45753	0.09767
H	4.77606	-1.05151	0.25305
C	3.57330	-0.02066	-1.21733
C	2.42866	0.77690	-1.42958
H	2.18295	1.16679	-2.42480
C	1.59358	1.06584	-0.33591
C	3.42347	-0.59552	2.65655
C	3.54796	0.68726	3.52176
H	3.78781	0.41824	4.57232
H	2.60933	1.27537	3.52035
H	4.36172	1.33834	3.13930
C	2.32502	-1.52109	3.23510
H	2.58259	-1.81724	4.27406
H	2.23408	-2.44452	2.62767
H	1.33858	-1.01896	3.25492
C	4.76772	-1.35065	2.71010
H	5.00166	-1.61409	3.76220
H	5.60663	-0.73393	2.32605
H	4.73652	-2.29637	2.12963
C	4.50239	-0.44240	-2.37610
C	5.94756	0.03823	-2.08858
H	6.62617	-0.25955	-2.91594
H	6.35206	-0.39710	-1.15205
H	5.98392	1.14355	-1.99315
C	4.47902	-1.98900	-2.48938
H	5.12606	-2.32860	-3.32602
H	3.44741	-2.35332	-2.67747
H	4.84300	-2.47473	-1.56097
C	4.05459	0.15083	-3.72820
H	4.74782	-0.17667	-4.53016
H	4.06128	1.26069	-3.71478
H	3.03611	-0.18735	-4.01176
N	0.40524	1.81461	-0.32639
C	0.01348	2.65138	-1.45654
H	0.91534	3.10323	-1.92285
H	-0.62262	3.47225	-1.07234
C	-0.76824	1.87681	-2.53554
H	-1.07543	2.56979	-3.34329
H	-0.14912	1.08169	-2.99586

N	-1.96257	1.23198	-1.99573
C	-1.98680	0.00120	-1.31675
C	-1.00278	-0.97026	-1.09300
H	0.02243	-0.82285	-1.45247
C	-1.38902	-2.11489	-0.36900
C	-2.72778	-2.22242	0.10521
H	-2.99381	-3.11763	0.68206
C	-3.73406	-1.25387	-0.09824
C	-3.29943	-0.15025	-0.84978
O	-4.03542	0.96237	-1.25571
C	-3.16344	1.83386	-1.79319
H	-3.55006	2.64529	-2.41915
C	-0.39019	-3.25100	-0.06508
C	1.03479	-2.90789	-0.54813
H	1.72727	-3.73764	-0.29883
H	1.43141	-1.99053	-0.06777
H	1.07583	-2.76524	-1.64785
C	-0.34727	-3.49232	1.46494
H	0.41304	-4.26262	1.71246
H	-1.32058	-3.84766	1.86036
H	-0.08043	-2.55917	1.99932
C	-0.86121	-4.54047	-0.78492
H	-0.16328	-5.37701	-0.56934
H	-0.89172	-4.39131	-1.88452
H	-1.87392	-4.85136	-0.45466
C	-5.15591	-1.33558	0.47494
C	-5.38536	-2.64810	1.25073
H	-6.41913	-2.66408	1.65260
H	-4.69198	-2.74807	2.11130
H	-5.26462	-3.53906	0.59993
C	-5.35367	-0.13967	1.44573
H	-6.38772	-0.14384	1.84997
H	-5.18029	0.83475	0.94670
H	-4.64864	-0.21207	2.29976
C	-6.18448	-1.25734	-0.68287
H	-7.21605	-1.32019	-0.27746
H	-6.04253	-2.09783	-1.39382
H	-6.09904	-0.30798	-1.24683
Cl	-2.86832	3.37365	0.03231

Sum of electronic and zero-point Energies= -2728.295683
Sum of electronic and thermal Energies= -2728.253769
Sum of electronic and thermal Enthalpies= -2728.252825
Sum of electronic and thermal Free Energies= -2728.368398

6:



6: In Gas Phase

C	-1.47451900	-1.00395900	-3.15182800
C	-0.40580000	0.05079300	-2.76344300
H	0.25221600	0.25993200	-3.63635800

H	-0.88644200	0.99813100	-2.44185700
N	0.40927600	-0.41629900	-1.64499000
N	-2.00818100	-1.69304500	-1.97433900
C	1.40033100	0.33099200	-1.00035200
C	2.09018100	-0.56650800	-0.17317900
C	1.73680900	1.68840100	-1.05722800
C	3.17029100	-0.19666800	0.63903300
C	2.79966500	2.12672600	-0.23627000
H	1.18538100	2.36759700	-1.71887900
C	3.48122800	1.18238400	0.57620100
H	4.31428400	1.54450500	1.19308400
C	-2.53718900	-0.88168500	-0.93833700
C	-3.27643500	0.29749900	-1.08797200
C	-2.20600800	-1.34910700	0.35163000
C	-3.67294300	1.02319600	0.06203900
H	-3.53056900	0.65648700	-2.09623300
C	-2.54644400	-0.65397300	1.52139500
C	-3.29819500	0.53461000	1.32983100
H	-3.58686400	1.10233000	2.22082900
O	-1.49509100	-2.54551700	0.31729300
O	1.51300500	-1.82847000	-0.31950500
C	3.24583400	3.60544900	-0.20201900
C	3.07600900	4.15393700	1.23804800
H	3.39058200	5.21817800	1.28837000
H	2.01635000	4.09041600	1.56199700
H	3.68666600	3.58816900	1.97077000
C	2.41159100	4.48654600	-1.15551900
H	2.76245200	5.53773400	-1.10079100
H	2.50848300	4.15967300	-2.21180000
H	1.33484800	4.48306900	-0.88605000
C	4.73361300	3.70458500	-0.62640500
H	5.39826600	3.13638400	0.05568800
H	4.88034700	3.30451200	-1.65113400
H	5.07015100	4.76309900	-0.61667000
C	-2.06703100	-1.13975500	2.90169800
C	-2.63352300	-2.55583200	3.17909800
H	-2.30384900	-3.28119300	2.41081800
H	-2.28897700	-2.92077100	4.17033300
H	-3.74341100	-2.53873500	3.18631300
C	-0.51549100	-1.18059500	2.89488900
H	-0.13230900	-1.85988400	2.11047900
H	-0.09277000	-0.17176700	2.70483700
H	-0.13158700	-1.53634000	3.87459700
C	-2.52491100	-0.20101600	4.03678400
H	-3.63126000	-0.14337100	4.10702400
H	-2.14962500	-0.58395300	5.00840100
H	-2.12975400	0.82842000	3.90991200
C	-4.46584200	2.33605700	-0.12041000
C	-5.77507200	2.04686500	-0.89789100
H	-5.57593700	1.62208500	-1.90299000
H	-6.40884800	1.32180700	-0.34645300
H	-6.35988200	2.98094700	-1.03923800
C	-3.59845700	3.34229700	-0.92071600
H	-4.13920400	4.30272300	-1.06116800
H	-2.64908000	3.55418600	-0.38580400
H	-3.34009200	2.95420500	-1.92784700
C	-4.83936600	2.98749500	1.22755900
H	-3.94055800	3.26149600	1.81778900
H	-5.41698100	3.91812700	1.04882000
H	-5.46980000	2.31685900	1.84734400
P	-0.92003400	-2.92463200	-1.25086100
C	3.94617700	-1.22611400	1.47527800
C	4.54845300	-2.28534000	0.51345900
H	5.25710800	-1.81191100	-0.19727400
H	5.10159400	-3.05533600	1.09161900
H	3.76401800	-2.79716300	-0.07851800

C	5.09221600	-0.57061500	2.27143600
H	5.62951500	-1.34560600	2.85581300
H	5.83449200	-0.08320700	1.60543600
H	4.71752000	0.18794400	2.99020500
C	2.97882300	-1.91238900	2.47252200
H	2.16387000	-2.44755700	1.94874000
H	3.52977500	-2.65302500	3.08985800
H	2.51676700	-1.16882200	3.15405200
C	0.59583100	-1.75335200	-1.32835500
H	-2.29154000	-0.50819600	-3.71696100
H	-1.02089600	-1.76266900	-3.81936900
Cl	1.40800700	-2.74636900	-3.08574500

Sum of electronic and zero-point Energies= -2267.538230
Sum of electronic and thermal Energies= -2267.498785
Sum of electronic and thermal Enthalpies= -2267.497840
Sum of electronic and thermal Free Energies= -2267.608203

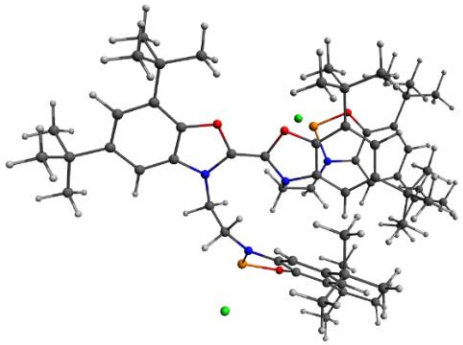
6: In THF

C	-1.35007200	-0.17963300	-3.21617900
C	-0.23347800	0.67475300	-2.56914000
H	0.47104900	1.03076700	-3.34893200
H	-0.64995900	1.55777300	-2.04302300
N	0.54715400	-0.07853200	-1.57289700
N	-1.99258700	-1.06855300	-2.24532300
C	1.64271400	0.44038000	-0.86402600
C	2.16140900	-0.63233100	-0.12707100
C	2.20096000	1.72426500	-0.80374800
C	3.26644500	-0.52766000	0.73260900
C	3.31268500	1.89233300	0.04652700
H	1.77745400	2.54452900	-1.39539100
C	3.80752300	0.77464200	0.78015100
H	4.67643900	0.93833000	1.43086100
C	-2.58354900	-0.44968800	-1.11154600
C	-3.22795800	0.79424300	-1.07488000
C	-2.43700500	-1.20513200	0.07346200
C	-3.71677300	1.29194900	0.15792900
H	-3.33590000	1.38233500	-1.99783800
C	-2.87789200	-0.74416100	1.32550100
C	-3.53003200	0.51638600	1.32132000
H	-3.89257100	0.90696300	2.27840900
O	-1.80624700	-2.41684500	-0.14921200
O	1.37935900	-1.75541300	-0.40407200
C	4.01801800	3.25665800	0.20440600
C	3.96606300	3.68762700	1.69327700
H	4.45983500	4.67347300	1.82357200
H	2.91654300	3.77838400	2.04278900
H	4.48475600	2.96441100	2.35514500
C	3.34783700	4.35725300	-0.64423800
H	3.88179600	5.31840700	-0.49795900
H	3.38030100	4.12243800	-1.72843400
H	2.28909900	4.51809700	-0.35252900
C	5.49454500	3.11907600	-0.24850100
H	6.04885300	2.37720700	0.36163400
H	5.55440400	2.80139700	-1.31017800
H	6.01764500	4.09345400	-0.14871000
C	-2.61223300	-1.55376500	2.60913200
C	-3.30948100	-2.93470300	2.50388900
H	-2.93916500	-3.50895500	1.63275300
H	-3.11799700	-3.53225200	3.42067900
H	-4.40773800	-2.81096900	2.39848000
C	-1.07972900	-1.74561000	2.76899300
H	-0.64779200	-2.28502800	1.90424700
H	-0.56667200	-0.76476200	2.85389800
H	-0.85646200	-2.32974300	3.68696000

C	-3.14446800	-0.83565400	3.86667700
H	-4.24328800	-0.68414100	3.82490400
H	-2.92661000	-1.45145600	4.76374500
H	-2.66367300	0.15360500	4.01613600
C	-4.39736700	2.67856500	0.18590000
C	-5.60384500	2.68451700	-0.78742700
H	-5.29650700	2.47849700	-1.83313400
H	-6.35006800	1.91636600	-0.49529000
H	-6.10577200	3.67534200	-0.77625500
C	-3.36995500	3.75277200	-0.25718000
H	-3.83273300	4.76275200	-0.24794300
H	-2.49544900	3.76748800	0.42673300
H	-2.99394400	3.56502700	-1.28419400
C	-4.91171300	3.05022900	1.59264000
H	-4.08822000	3.10629100	2.33441400
H	-5.39955800	4.04647100	1.56283700
H	-5.66176500	2.32059400	1.96253800
P	-1.03967900	-2.50364300	-1.71107900
C	3.80365400	-1.73027700	1.52074900
C	4.23388500	-2.83231400	0.51635800
H	5.04394200	-2.46593500	-0.14783700
H	4.61345100	-3.71813800	1.06740700
H	3.38962000	-3.16299700	-0.12075900
C	5.01731300	-1.34648900	2.38997900
H	5.37548100	-2.24103200	2.93900100
H	5.86297700	-0.96895000	1.77861800
H	4.75731400	-0.57334100	3.14239100
C	2.67829000	-2.26775700	2.44379000
H	1.79509400	-2.60342100	1.86610500
H	3.05040600	-3.13432800	3.02918300
H	2.34442600	-1.48616800	3.15712700
C	0.45325400	-1.40076200	-1.30788900
H	-2.09738200	0.50286000	-3.66983400
H	-0.92135200	-0.80182800	-4.02353800
Cl	0.95963200	-2.45151700	-3.65574000

Sum of electronic and zero-point Energies= -2267.550455
Sum of electronic and thermal Energies= -2267.510758
Sum of electronic and thermal Enthalpies= -2267.509813
Sum of electronic and thermal Free Energies= -2267.621044

7-cis:



7-cis: In Gas phase

C	2.93497600	2.53008300	-0.09078800
H	2.63713000	1.88575300	0.76073100
H	3.74512800	3.20503300	0.26630400
C	3.44185600	1.59494600	-1.22360100
H	2.62146700	1.43728200	-1.95469200
H	4.27431200	2.05522900	-1.79068100
N	3.89109000	0.31363200	-0.73950500
N	1.74834700	3.27379300	-0.49015800

C	5.21790800	-0.12876300	-0.65422200
C	5.18488100	-1.39820600	-0.03695900
C	6.41685600	0.46219900	-1.06060400
C	6.33861700	-2.15145500	0.20561100
C	7.61727800	-0.26081700	-0.84065200
H	6.41849200	1.45567100	-1.52711600
C	7.54272600	-1.52731200	-0.22653600
H	8.48021200	-2.07858400	-0.05977400
C	0.66265100	3.50262400	0.37313900
C	0.57199900	3.26618500	1.74787400
C	-0.43885100	4.01813000	-0.34371600
C	-0.63700600	3.56362900	2.41480900
H	1.43685500	2.86816800	2.29614700
C	-1.67217600	4.29937500	0.26356700
C	-1.72015800	4.06847500	1.66182300
H	-2.65204100	4.31102600	2.18269600
O	-0.14948800	4.18602400	-1.69929200
O	3.86980000	-1.71491700	0.26769700
C	3.06895400	-0.65202900	-0.12335000
C	6.38834900	-3.53876800	0.87743500
C	8.99682800	0.30361500	-1.24962300
C	7.27783100	-3.45117300	2.14476100
H	6.86015700	-2.72220700	2.86978300
H	7.33246200	-4.44186200	2.64401300
H	8.31495800	-3.13714100	1.90794300
C	7.00348800	-4.55421600	-0.11987200
H	6.38463300	-4.62857500	-1.03789000
H	8.03047400	-4.26797400	-0.42574800
H	7.05786700	-5.56287000	0.34226200
C	4.99572200	-4.05845200	1.30037800
H	4.50630600	-3.38408200	2.03000200
H	4.31194600	-4.16100500	0.43556200
H	5.10469900	-5.05665800	1.77381700
C	9.89305800	0.42699200	0.00911300
H	10.89167700	0.83313300	-0.25991200
H	9.43248700	1.10692700	0.75577300
H	10.05063800	-0.55454500	0.50079100
C	8.88726200	1.69836000	-1.90093900
H	9.89681700	2.06489400	-2.17950200
H	8.27640200	1.67560000	-2.82743400
H	8.44454400	2.44448400	-1.20842700
C	9.66077500	-0.65638900	-2.26950600
H	9.80802700	-1.67036800	-1.84530600
H	9.03343600	-0.76095200	-3.17908800
H	10.65678400	-0.27200800	-2.57721600
C	-2.87143900	4.80700000	-0.55552000
C	-2.50161400	6.14952200	-1.23712800
H	-1.61629700	6.04583100	-1.89291800
H	-3.35134400	6.51319300	-1.85304000
H	-2.27280200	6.92278000	-0.47476300
C	-3.21689800	3.73821300	-1.62490700
H	-2.37196000	3.56285000	-2.31903200
H	-3.46990800	2.77670900	-1.13188800
H	-4.09674600	4.05251300	-2.22447200
C	-4.12099600	5.02925600	0.32174800
H	-3.94649200	5.79303800	1.10765500
H	-4.95778900	5.38979200	-0.31124500
H	-4.45543600	4.09277900	0.81303500
C	-0.71454100	3.34524400	3.94047700
C	-0.38346600	1.86525100	4.26390800
H	-1.05624000	1.17247400	3.72031000
H	0.65454600	1.60124500	3.97532000
H	-0.48431200	1.67478500	5.35322900
C	-2.11177700	3.68065600	4.50269000
H	-2.13944400	3.47935800	5.59341100
H	-2.37024800	4.74989500	4.35529500

H	-2.90551000	3.06619700	4.03258500
C	0.31752500	4.27104000	4.63522300
H	0.10933000	5.33726800	4.40747700
H	0.27825200	4.13702700	5.73724400
H	1.35480600	4.05270000	4.30804600
C	-1.23480600	0.34113200	-1.89752700
H	-1.83592000	1.06736900	-1.31323600
H	-1.32826700	0.64382800	-2.96732900
C	0.24504700	0.47984600	-1.52920200
H	0.86098900	-0.16850000	-2.19255600
H	0.50839700	1.53057600	-1.76395800
N	0.64270600	0.17628700	-0.12295100
N	-1.79057600	-0.98352300	-1.68412500
C	-0.35707300	-0.24257300	0.82114400
C	0.03505600	-1.49592000	1.32920000
C	-1.59304100	0.31742300	1.16783800
C	-0.79513400	-2.30229000	2.12314700
C	-2.47425800	-0.45582400	1.96631000
H	-1.85906700	1.32172600	0.81510800
C	-2.05377000	-1.72956400	2.41434800
H	-2.75115300	-2.31485400	3.02731200
C	-3.17226400	-1.21395000	-1.63704300
C	-4.21825100	-0.29513100	-1.81966700
C	-3.44182800	-2.56651500	-1.34720100
C	-5.54857900	-0.75182800	-1.70060600
H	-3.98869500	0.74991800	-2.05998900
C	-4.74647900	-3.06833500	-1.21121500
C	-5.77581100	-2.11782400	-1.40677300
H	-6.81444400	-2.45970000	-1.31225300
O	-2.27662900	-3.31213900	-1.20007800
O	1.28124700	-1.83764600	0.85774300
C	1.72133500	-0.73590100	0.09643000
C	-0.35336900	-3.70233300	2.57951800
C	-3.88643000	0.03283100	2.36116300
C	-1.43559100	-4.39176000	3.43508400
H	-2.38054900	-4.53092900	2.87004800
H	-1.08149000	-5.39688900	3.74414100
H	-1.66195500	-3.81856900	4.35847600
C	0.94502400	-3.57952100	3.41870000
H	1.76291400	-3.11718400	2.83162700
H	0.77164900	-2.95912000	4.32285100
H	1.28394400	-4.58437800	3.74962600
C	-0.08577900	-4.57802200	1.32696900
H	-1.00201700	-4.66506800	0.70798700
H	0.71488100	-4.14539500	0.69546900
H	0.22775400	-5.59925100	1.63096000
C	-4.93448100	-1.03403800	1.96038000
H	-5.95977000	-0.67466800	2.19016000
H	-4.88262500	-1.25874400	0.87862700
H	-4.78957700	-1.98517000	2.51175000
C	-4.24596200	1.35240300	1.65159600
H	-5.25952000	1.68915400	1.95346800
H	-3.53302300	2.16223000	1.90202200
H	-4.24850200	1.22517400	0.54932900
C	-3.95289500	0.24896500	3.89419300
H	-3.74946700	-0.69248600	4.44485900
H	-3.20818200	0.99728200	4.22833800
H	-4.96101000	0.60705800	4.19456600
C	-5.00248500	-4.53883600	-0.84016400
C	-4.38625300	-5.45903200	-1.92590600
H	-3.29978000	-5.28360700	-2.04335400
H	-4.53932300	-6.52556800	-1.65554400
H	-4.86952900	-5.27979900	-2.90882800
C	-4.34614900	-4.82183100	0.53741200
H	-3.25364400	-4.64686200	0.51101700
H	-4.77740100	-4.16145200	1.31807400

H	-4.51974700	-5.87647400	0.83928400
C	-6.50905800	-4.85084600	-0.73157100
H	-7.03926300	-4.67662100	-1.69098700
H	-6.64809300	-5.91858200	-0.46370400
H	-7.00252100	-4.24309000	0.05537000
C	-6.75739300	0.19648000	-1.86126600
C	-6.32536000	1.64589300	-2.16416400
H	-5.72100600	2.07580500	-1.33968700
H	-5.73449600	1.71870400	-3.10077500
H	-7.22143600	2.28898600	-2.28619700
C	-7.57203200	0.20921900	-0.54242700
H	-8.45247800	0.88020600	-0.63558900
H	-7.94303100	-0.80060200	-0.27354200
H	-6.94606500	0.57124200	0.29818000
C	-7.65069100	-0.30203200	-3.02493900
H	-8.03161100	-1.32756300	-2.84288500
H	-8.52931500	0.36538800	-3.15419200
H	-7.08341200	-0.31749400	-3.97869200
P	1.50948900	4.05951500	-2.01723000
Cl	2.12680500	6.09825300	-1.59390700
P	-0.89410400	-2.46850500	-1.68421900
Cl	-0.87290700	-2.94701000	-3.82107200

Sum of electronic and zero-point Energies= -4535.138459
Sum of electronic and thermal Energies= -4535.057367
Sum of electronic and thermal Enthalpies= -4535.056423
Sum of electronic and thermal Free Energies= -4535.253914

7-cis: In THF

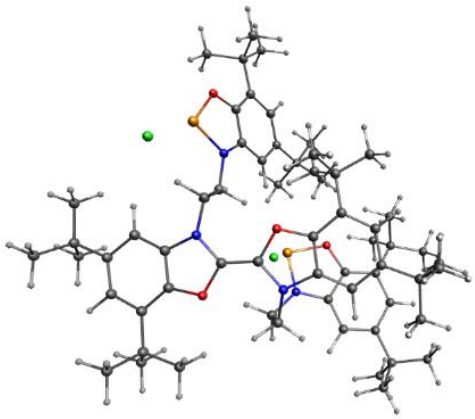
C	2.95409300	2.53268300	-0.10693200
H	2.65491200	1.90038200	0.75249900
H	3.77049100	3.20306500	0.23888000
C	3.44405700	1.58839100	-1.23793700
H	2.62189300	1.42806900	-1.96522400
H	4.27654400	2.03886900	-1.81096600
N	3.88633500	0.30434600	-0.74625000
N	1.76938800	3.28829300	-0.50342600
C	5.21000100	-0.14279600	-0.65762000
C	5.17369800	-1.41232700	-0.03954200
C	6.41218500	0.44516600	-1.06200100
C	6.32477900	-2.16926200	0.20650800
C	7.61025200	-0.28134500	-0.83832400
H	6.41500200	1.43873200	-1.52762500
C	7.53250900	-1.54833500	-0.22325400
H	8.46861000	-2.10119700	-0.05366700
C	0.68439300	3.51638900	0.36174300
C	0.59696500	3.28028400	1.73753200
C	-0.41816900	4.03398700	-0.35295100
C	-0.61186500	3.57784600	2.40552800
H	1.46446200	2.88536500	2.28388700
C	-1.65215300	4.31285900	0.25568300
C	-1.69755900	4.08147200	1.65393000
H	-2.62925100	4.32263500	2.17599300
O	-0.12881900	4.20640300	-1.70698200
O	3.85484800	-1.72415500	0.26224800
C	3.05960900	-0.65663200	-0.13466500
C	6.37199300	-3.55579900	0.88097600
C	8.99231400	0.28082000	-1.24322600
C	7.25189000	-3.46479800	2.15491600
H	6.82636200	-2.73663100	2.87655200
H	7.30477200	-4.45517800	2.65481700
H	8.28970300	-3.14923400	1.92367100
C	6.99624800	-4.57298300	-0.10905700
H	6.38363200	-4.65163000	-1.03127300
H	8.02531200	-4.28580100	-0.40649300

H	7.04841700	-5.57974200	0.35723100
C	4.97742900	-4.07765400	1.29452300
H	4.48419400	-3.40398000	2.02256500
H	4.30127400	-4.18179500	0.42347200
H	5.08505200	-5.07585700	1.76802200
C	9.88295700	0.40630900	0.01953100
H	10.88265500	0.81033800	-0.24812100
H	9.42103500	1.09164900	0.76077900
H	10.03757200	-0.57429500	0.51437400
C	8.88626400	1.67350300	-1.89953100
H	9.89800100	2.03655500	-2.17463700
H	8.27833300	1.64833200	-2.82778700
H	8.44074500	2.42207700	-1.21168600
C	9.66086600	-0.68382000	-2.25600400
H	9.80650400	-1.69614100	-1.82692900
H	9.03931200	-0.78903100	-3.16983700
H	10.65821800	-0.29943400	-2.55881200
C	-2.85544800	4.81464100	-0.56138800
C	-2.49214200	6.15465400	-1.25187500
H	-1.60966500	6.04999800	-1.91158000
H	-3.34596000	6.51137800	-1.86588900
H	-2.26448700	6.93316200	-0.49409600
C	-3.20256300	3.73914300	-1.62350600
H	-2.35862600	3.55403200	-2.31632200
H	-3.45805900	2.78217400	-1.12315100
H	-4.08204300	4.05122500	-2.22446700
C	-4.10196800	5.04077100	0.31926500
H	-3.92471200	5.80745900	1.10168700
H	-4.94023400	5.39769200	-0.31365900
H	-4.43446100	4.10631000	0.81530200
C	-0.68825500	3.36064500	3.93166300
C	-0.36427700	1.87857100	4.25345000
H	-1.04549200	1.19293800	3.71073300
H	0.67208000	1.61046600	3.96209900
H	-0.46474100	1.68885200	5.34288100
C	-2.08272300	3.70309500	4.49647800
H	-2.10791600	3.50238300	5.58730400
H	-2.33668100	4.77320600	4.34807000
H	-2.88057700	3.09268000	4.02801700
C	0.35110100	4.27894800	4.62567200
H	0.14642500	5.34692600	4.40190300
H	0.31194800	4.14247400	5.72730900
H	1.38637400	4.05459200	4.29613800
C	-1.23565500	0.34091600	-1.92301300
H	-1.84826100	1.05533300	-1.33772800
H	-1.32679500	0.64881100	-2.98961500
C	0.23938400	0.49042100	-1.54428000
H	0.87029800	-0.13552900	-2.21324800
H	0.48998900	1.54713400	-1.76159800
N	0.63122300	0.16756200	-0.14071800
N	-1.78828100	-0.99153700	-1.72016800
C	-0.36622200	-0.24578800	0.80468500
C	0.02527000	-1.49755600	1.31967000
C	-1.59946600	0.31912500	1.15549200
C	-0.80075000	-2.29456000	2.12765500
C	-2.47624500	-0.44427000	1.96906100
H	-1.86588400	1.32164100	0.79810300
C	-2.05575700	-1.71505400	2.42628900
H	-2.74863700	-2.29149000	3.05291300
C	-3.17117000	-1.22023500	-1.65347900
C	-4.21736600	-0.30084100	-1.83446100
C	-3.43881900	-2.56852600	-1.34358500
C	-5.54655800	-0.75459400	-1.69610600
H	-3.98848700	0.74105800	-2.08837400
C	-4.74320000	-3.06855100	-1.18946700
C	-5.77261900	-2.11863800	-1.38683800

H	-6.81091900	-2.45790600	-1.27954800
O	-2.27066500	-3.31211500	-1.19743000
O	1.26885100	-1.84561800	0.84173500
C	1.71030300	-0.74221100	0.07632400
C	-0.36042600	-3.69214500	2.59410100
C	-3.88384200	0.05253000	2.37075300
C	-1.44067700	-4.37371800	3.45862200
H	-2.38850400	-4.51328800	2.89873000
H	-1.08685900	-5.37747000	3.77231700
H	-1.66234100	-3.79368900	4.37867200
C	0.94017400	-3.56583800	3.42938000
H	1.75594400	-3.10324000	2.83939200
H	0.76841100	-2.94315700	4.33232400
H	1.28107400	-4.56915800	3.76263500
C	-0.09814600	-4.57886800	1.34813800
H	-1.01605200	-4.66807400	0.73189600
H	0.70055500	-4.15303700	0.70947900
H	0.21343800	-5.59833400	1.65962300
C	-4.93818700	-1.01216300	1.97980700
H	-5.96003300	-0.64700500	2.21515900
H	-4.89477600	-1.23784500	0.89744700
H	-4.79323600	-1.96240500	2.53293000
C	-4.24298200	1.37156800	1.66034500
H	-5.24992600	1.71649800	1.97374000
H	-3.52196300	2.17756500	1.89937100
H	-4.26124800	1.24191900	0.55853800
C	-3.94044100	0.27271100	3.90380000
H	-3.73784600	-0.66809000	4.45613000
H	-3.19256400	1.02126400	4.23062700
H	-4.94582600	0.63537200	4.20712900
C	-4.99928100	-4.53491800	-0.80161400
C	-4.39794200	-5.46623400	-1.88657600
H	-3.31291000	-5.29176200	-2.02098600
H	-4.54667300	-6.52961300	-1.60245400
H	-4.89707000	-5.29849400	-2.86387200
C	-4.32794700	-4.80867200	0.57048300
H	-3.23422500	-4.64382900	0.52945000
H	-4.74438200	-4.13796300	1.35030400
H	-4.50635500	-5.85872900	0.88451500
C	-6.50544800	-4.84163100	-0.67361400
H	-7.04615500	-4.67339400	-1.62811600
H	-6.64328100	-5.90671400	-0.39519600
H	-6.98779100	-4.22543300	0.11342200
C	-6.75537400	0.19399900	-1.85449600
C	-6.32341400	1.64099300	-2.16886000
H	-5.71235700	2.07480800	-1.35135100
H	-5.74004100	1.70865200	-3.11050300
H	-7.22025800	2.28345000	-2.28673300
C	-7.56212100	0.21397300	-0.53074100
H	-8.44106800	0.88639700	-0.62473800
H	-7.93463300	-0.79365300	-0.25542700
H	-6.93155400	0.58091300	0.30425100
C	-7.65633300	-0.31220800	-3.00922100
H	-8.03669800	-1.33639000	-2.81774100
H	-8.53507400	0.35540400	-3.13479700
H	-7.09630200	-0.33036500	-3.96753200
P	1.52830600	4.07256500	-2.02538100
Cl	2.11707400	6.14903100	-1.57507200
P	-0.89843600	-2.47087000	-1.70747000
Cl	-0.94374700	-3.02768300	-3.85954100

Sum of electronic and zero-point Energies= -4535.153324
Sum of electronic and thermal Energies= -4535.072040
Sum of electronic and thermal Enthalpies= -4535.071096
Sum of electronic and thermal Free Energies= -4535.268511

7-trans:



7-trans: In Gas phase

C	-2.61763800	-0.08097100	-0.56713900
H	-1.55942500	-0.25918400	-0.28871700
H	-3.12301700	0.40026300	0.30234500
C	-2.64505400	0.86688200	-1.77644600
H	-2.06536000	0.43430400	-2.61369200
H	-3.69078600	1.01012100	-2.13316300
N	-2.12257400	2.16943700	-1.44526200
N	-3.25219000	-1.35343300	-0.88101800
C	-2.84594700	3.14838000	-0.76040400
C	-1.96175300	4.21853800	-0.50415300
C	-4.18612400	3.17329200	-0.36620400
C	-2.36983700	5.38760600	0.14547300
C	-4.64924300	4.33820900	0.29679300
H	-4.83542500	2.30585300	-0.54734700
C	-3.74480400	5.39512500	0.52383600
H	-4.11563600	6.29113600	1.04378600
C	-3.11710500	-2.47092500	-0.03494900
C	-2.18921800	-2.67867400	0.99288100
C	-4.06498000	-3.46370600	-0.36004200
C	-2.19034000	-3.92288100	1.66483300
H	-1.47334000	-1.88973200	1.26400900
C	-4.12761900	-4.70294200	0.29382900
C	-3.15006700	-4.89362400	1.30149400
H	-3.15142800	-5.84980200	1.83507000
O	-4.89709300	-3.06791600	-1.40774900
O	-0.69965300	3.88386000	-1.00875400
C	-0.77160200	2.56788100	-1.46460300
C	-1.48323100	6.60742300	0.46675800
C	-6.10838700	4.45848400	0.79062600
C	-1.52772500	6.88301500	1.99191000
H	-1.15223600	6.00770800	2.56186100
H	-0.89271600	7.75891100	2.24397800
H	-2.55477500	7.10051600	2.34814900
C	-2.03010000	7.83794700	-0.30129200
H	-2.00115000	7.66397600	-1.39688000
H	-3.07999300	8.06260600	-0.02362300
H	-1.41905200	8.73834000	-0.07695200
C	-0.00635600	6.40006600	0.06499000
H	0.44137000	5.54168800	0.60479200
H	0.10376400	6.21579700	-1.02150500
H	0.57915900	7.30729700	0.32245500
C	-6.11182100	4.61180200	2.33318200
H	-7.15199200	4.70023400	2.71359300
H	-5.64147300	3.73061300	2.81678200
H	-5.55551700	5.51411000	2.66040100
C	-6.94744400	3.21551300	0.42625700
H	-7.98632900	3.34054000	0.79555200
H	-7.00157400	3.05734900	-0.67061300

H	-6.54280800	2.28781900	0.88001700
C	-6.77074700	5.70064500	0.14249200
H	-6.24370900	6.63952100	0.40951400
H	-6.76956900	5.61571900	-0.96411600
H	-7.82431700	5.79995200	0.48063600
C	-5.19829500	-5.75031000	-0.06154300
C	-6.60053000	-5.13892100	0.19776100
H	-6.76505300	-4.22370500	-0.40330400
H	-7.39327400	-5.87182200	-0.06402300
H	-6.71793000	-4.87160400	1.26846500
C	-5.06010900	-6.14637500	-1.55469800
H	-5.20152400	-5.27493200	-2.22248000
H	-4.05756100	-6.57890600	-1.75518100
H	-5.82266500	-6.90940800	-1.81996500
C	-5.05790700	-7.02765200	0.79231000
H	-5.17268900	-6.81833700	1.87616100
H	-5.84915700	-7.75173900	0.50795500
H	-4.07863600	-7.52655300	0.63635900
C	-1.15126100	-4.17216900	2.77766500
C	0.27046500	-3.92705400	2.21381400
H	0.46618800	-4.56512500	1.32704600
H	0.43065600	-2.87260700	1.91537600
H	1.03449200	-4.16262900	2.98213100
C	-1.20923400	-5.61557600	3.32086500
H	-0.43442100	-5.75081300	4.10360100
H	-2.18982800	-5.84789700	3.78589300
H	-1.01550400	-6.36483600	2.52482700
C	-1.41997900	-3.19343500	3.94915200
H	-2.43243200	-3.35690200	4.37388700
H	-0.67398100	-3.34392600	4.75854900
H	-1.34651800	-2.13575500	3.62726800
C	1.79905400	2.82501400	0.69621700
H	2.31061100	3.49076700	1.42599400
H	0.71062000	2.98026400	0.83704100
C	2.19098900	3.21738000	-0.74990200
H	1.77997600	4.22229100	-0.97083100
H	3.29156900	3.27459500	-0.85608500
N	1.71037000	2.25171100	-1.73389400
N	2.09874400	1.42962200	0.97902400
C	2.46612400	1.10566600	-2.06939100
C	1.57180700	0.05107100	-2.32076400
C	3.84859900	0.91467600	-2.16318200
C	1.98168900	-1.25402100	-2.62162000
C	4.32153400	-0.37114800	-2.52248000
H	4.53488100	1.74429200	-1.95340400
C	3.38808400	-1.41128000	-2.72803400
H	3.77203300	-2.40436400	-2.99311700
C	3.39919000	0.93089300	1.15406200
C	4.59921900	1.64311800	1.26513300
C	3.39042200	-0.47952200	1.18836300
C	5.80671400	0.92465000	1.42204700
H	4.58971200	2.74117500	1.24432300
C	4.55357700	-1.23844300	1.38319600
C	5.75137600	-0.48657200	1.47913400
H	6.68627400	-1.03840500	1.62641200
O	2.11142000	-0.99971100	1.02277500
O	0.26602000	0.50823800	-2.16518000
C	0.34873600	1.84113700	-1.74413900
C	0.97503600	-2.40554700	-2.79003900
C	5.82437800	-0.63981900	-2.76201600
C	1.68154500	-3.74765800	-3.06850300
H	2.35905700	-4.03190600	-2.23689100
H	0.92455800	-4.55198900	-3.17306400
H	2.27239600	-3.72021300	-4.00769100
C	0.02438100	-2.08586700	-3.97178900
H	-0.52238000	-1.13641200	-3.80485700

H	0.59143800	-1.99102500	-4.92109500
H	-0.72631900	-2.89535100	-4.09471200
C	0.15017600	-2.55332500	-1.48709800
H	0.80769300	-2.74319200	-0.61607200
H	-0.43259300	-1.63788000	-1.27752700
H	-0.57215600	-3.39234800	-1.56272000
C	6.28230600	-1.90679100	-2.00147100
H	7.36538000	-2.08806000	-2.16740100
H	6.11185300	-1.78339000	-0.91388000
H	5.74376100	-2.81724000	-2.33415900
C	6.69751500	0.53424300	-2.27642000
H	7.77236400	0.29525100	-2.41466200
H	6.49513500	1.46914200	-2.83903200
H	6.52496400	0.72747900	-1.19871000
C	6.04814300	-0.83775600	-4.28315500
H	5.46689200	-1.70148700	-4.66687700
H	5.72766600	0.06193900	-4.84867100
H	7.12222600	-1.02216900	-4.50144800
C	4.49155600	-2.76297000	1.59015400
C	3.75316200	-3.00568800	2.93395900
H	2.74935800	-2.53918300	2.93349900
H	3.63153400	-4.09462200	3.11693800
H	4.32954300	-2.57386000	3.77838300
C	3.72507400	-3.45000600	0.43088700
H	2.68495200	-3.08612500	0.35181200
H	4.22153500	-3.25671400	-0.53988600
H	3.69389600	-4.54752500	0.59593400
C	5.89612800	-3.39548400	1.68252700
H	6.47855200	-2.99889300	2.53970100
H	5.79842400	-4.49061800	1.83046500
H	6.48574500	-3.23511000	0.75628800
C	7.13198500	1.69093300	1.63660000
C	7.20942400	2.94208700	0.72783900
H	7.11485300	2.67065100	-0.34320500
H	6.42090000	3.68527800	0.96474400
H	8.18396900	3.45481600	0.86723500
C	8.36513200	0.80769200	1.34029900
H	9.29298500	1.40730600	1.44499200
H	8.45125100	-0.04401400	2.04548400
H	8.33583500	0.39946800	0.30928600
C	7.18367100	2.14076400	3.12061300
H	7.13663700	1.26440500	3.79966700
H	8.12259600	2.69628100	3.33249500
H	6.32754900	2.80312100	3.36631500
P	-4.70243300	-1.45185200	-1.83002500
Cl	-6.11512900	-0.39271500	-0.47111300
P	0.90289800	0.18094400	1.05413400
Cl	0.38513500	0.10705500	3.18987300

Sum of electronic and zero-point Energies= -4535.161264
Sum of electronic and thermal Energies= -4535.080142
Sum of electronic and thermal Enthalpies= -4535.079198
Sum of electronic and thermal Free Energies= -4535.276444

7-trans: In THF

C	2.62010900	-0.07759000	0.55801500
H	1.55996100	-0.26172900	0.29221400
H	3.10944700	0.40860300	-0.31722000
C	2.65949600	0.86428900	1.77206100
H	2.08775400	0.42985500	2.61333100
H	3.70690400	1.00582700	2.12353900
N	2.13489200	2.16873200	1.44931000
N	3.26641800	-1.34948100	0.85561700
C	2.85388200	3.15005700	0.76524100
C	1.96707100	4.22021300	0.51329800

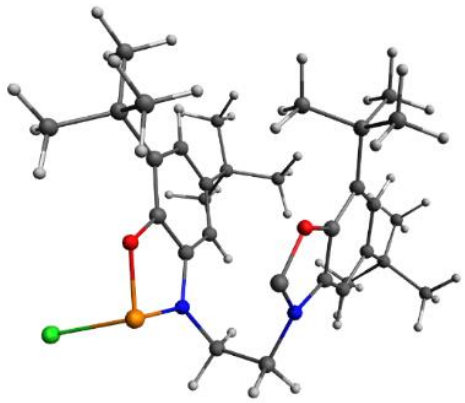
C	4.19371200	3.17901000	0.36758300
C	2.37049700	5.39082900	-0.13743200
C	4.65303100	4.34619500	-0.29604200
H	4.84512500	2.31326900	0.54848900
C	3.74531100	5.40153000	-0.52058100
H	4.11192100	6.29859800	-1.04174800
C	3.11582400	-2.47069800	0.01854300
C	2.18357500	-2.67615500	-1.00676500
C	4.05272000	-3.47257100	0.35071600
C	2.16935400	-3.92662600	-1.66787500
H	1.47578400	-1.88130800	-1.28175900
C	4.09952300	-4.71909700	-0.29180600
C	3.11869800	-4.90607900	-1.29744800
H	3.10789400	-5.86694100	-1.82265500
O	4.89079800	-3.07709900	1.39284500
O	0.70890700	3.88346900	1.02285700
C	0.78329200	2.56720200	1.47680800
C	1.47967100	6.60731000	-0.46065000
C	6.11078300	4.47090900	-0.79389700
C	1.50783900	6.86460100	-1.98967100
H	1.12155900	5.98369000	-2.54384700
H	0.87056700	7.73829200	-2.24277200
H	2.53126600	7.07739800	-2.35956300
C	2.03621800	7.84691800	0.28595700
H	2.01914200	7.68663500	1.38415600
H	3.08158300	8.07151700	-0.00890400
H	1.41971500	8.74236100	0.05800000
C	0.00768700	6.40487500	-0.03962200
H	-0.44921400	5.54465200	-0.56783700
H	-0.09049400	6.23061400	1.04974900
H	-0.57816800	7.31156200	-0.29707800
C	6.10992000	4.61611200	-2.33742800
H	7.14895500	4.70883400	-2.71976900
H	5.64482500	3.72868700	-2.81549600
H	5.54775300	5.51396800	-2.66668500
C	6.95696600	3.23422500	-0.42436400
H	7.99418500	3.36375300	-0.79675500
H	7.01305500	3.08404200	0.67378800
H	6.55530200	2.30231200	-0.87264600
C	6.76979500	5.72008100	-0.15552000
H	6.23690100	6.65431000	-0.42672500
H	6.77522100	5.64074900	0.95177400
H	7.82121400	5.82166900	-0.49936500
C	5.15472500	-5.77888600	0.07328800
C	6.56638400	-5.19090300	-0.19021800
H	6.74424000	-4.27118900	0.40061500
H	7.34667200	-5.93299900	0.08203800
H	6.69018000	-4.94009500	-1.26442300
C	5.00911400	-6.15982400	1.56984500
H	5.16219100	-5.28544700	2.23146200
H	4.00031800	-6.57665900	1.77226900
H	5.76034300	-6.93164700	1.84105600
C	4.99646900	-7.06133000	-0.76977500
H	5.11413100	-6.86296400	-1.85532500
H	5.77766800	-7.79310000	-0.47796500
H	4.01021400	-7.54460800	-0.60966600
C	1.12220700	-4.17759200	-2.77313000
C	-0.29389200	-3.92499700	-2.19852700
H	-0.48413600	-4.55853800	-1.30736400
H	-0.44719100	-2.86856500	-1.90312000
H	-1.06549900	-4.16310200	-2.95826000
C	1.17234200	-5.62308900	-3.31154700
H	0.39254700	-5.75704200	-4.08938200
H	2.14996400	-5.86104200	-3.77986200
H	0.97919800	-6.36843700	-2.51187200
C	1.38387400	-3.20381400	-3.95051800

H	2.39318400	-3.36947000	-4.38235700
H	0.63307400	-3.36036000	-4.75433200
H	1.31052300	-2.14453500	-3.63246800
C	-1.80289300	2.83784300	-0.66926400
H	-2.32274800	3.50343400	-1.39093500
H	-0.71655100	2.99515800	-0.81979100
C	-2.18793400	3.22011000	0.77946000
H	-1.77891100	4.22461600	1.00308600
H	-3.28703000	3.27808800	0.89403400
N	-1.69781600	2.24873000	1.75673900
N	-2.10171400	1.43957700	-0.95818200
C	-2.45046800	1.10334300	2.09715800
C	-1.55368500	0.05058500	2.35081900
C	-3.83345800	0.91005700	2.19182600
C	-1.96084800	-1.25417300	2.65844100
C	-4.30353900	-0.37699900	2.55296400
H	-4.52065100	1.73793200	1.97798600
C	-3.36765500	-1.41464300	2.76654400
H	-3.75015600	-2.40840000	3.03187900
C	-3.40147000	0.94245700	-1.15019300
C	-4.60154300	1.65691000	-1.25143700
C	-3.39038500	-0.46713800	-1.21073800
C	-5.80713000	0.93851500	-1.42234300
H	-4.59262600	2.75390100	-1.20756500
C	-4.55240700	-1.22579500	-1.41906600
C	-5.75007700	-0.47253200	-1.50434900
H	-6.68488200	-1.02202400	-1.66070800
O	-2.10942400	-0.98708400	-1.04840800
O	-0.24910100	0.50864400	2.18745400
C	-0.33589900	1.84016300	1.76154100
C	-0.95252600	-2.40498300	2.82299500
C	-5.80828600	-0.65400900	2.77234600
C	-1.65727200	-3.74786200	3.10233000
H	-2.33826100	-4.03088200	2.27292600
H	-0.89885100	-4.55133400	3.20306600
H	-2.24540100	-3.72176900	4.04312300
C	0.00442800	-2.08598100	3.99982500
H	0.55193600	-1.13725300	3.83056000
H	-0.55797400	-1.99324900	4.95228900
H	0.75478000	-2.89640400	4.11813800
C	-0.13432200	-2.55023500	1.51530700
H	-0.79728300	-2.73562200	0.64719400
H	0.45025300	-1.63588400	1.30550300
H	0.58493400	-3.39236000	1.58721900
C	-6.24918100	-1.91402900	1.98928600
H	-7.33314800	-2.10232000	2.13961000
H	-6.06847800	-1.77558800	0.90485000
H	-5.70844600	-2.82518300	2.31646200
C	-6.68055900	0.52294900	2.29222400
H	-7.75531000	0.27799600	2.41886800
H	-6.48481600	1.45302700	2.86482600
H	-6.50199300	0.72945800	1.21786300
C	-6.05061900	-0.87421700	4.28763200
H	-5.47190500	-1.74161500	4.66737800
H	-5.74460500	0.02033700	4.86968600
H	-7.12679300	-1.06624900	4.48739500
C	-4.49257500	-2.74811600	-1.64439100
C	-3.76458900	-2.97609600	-2.99649400
H	-2.75991200	-2.51040100	-2.99617400
H	-3.64464100	-4.06279000	-3.19265300
H	-4.34777900	-2.53538000	-3.83181100
C	-3.71656100	-3.45099000	-0.50055700
H	-2.66832000	-3.10658600	-0.44223800
H	-4.19227000	-3.25507300	0.48063800
H	-3.70687700	-4.54802300	-0.67036500
C	-5.89884500	-3.37768200	-1.73208200

H	-6.48914100	-2.96932700	-2.57804900
H	-5.80317700	-4.47091600	-1.89423100
H	-6.47890700	-3.22659200	-0.79830300
C	-7.13543600	1.70411400	-1.61921200
C	-7.20530500	2.95005800	-0.70279700
H	-7.09706800	2.67321700	0.36561300
H	-6.42189300	3.69665700	-0.94452200
H	-8.18386100	3.45814500	-0.82928800
C	-8.36382300	0.81567500	-1.31787200
H	-9.29268900	1.41569700	-1.40930200
H	-8.45563500	-0.03121700	-2.02817600
H	-8.32359500	0.40053700	-0.28988200
C	-7.20027000	2.16324800	-3.10010200
H	-7.16263600	1.29104600	-3.78555100
H	-8.14136500	2.72022400	-3.29715800
H	-6.34697300	2.82871200	-3.34776000
P	4.71120800	-1.45709600	1.80332900
Cl	6.15100000	-0.44623600	0.39065900
P	-0.90844400	0.19891200	-1.04355300
Cl	-0.37946300	0.14478700	-3.21360200

Sum of electronic and zero-point Energies= -4535.174227
Sum of electronic and thermal Energies= -4535.092859
Sum of electronic and thermal Enthalpies= -4535.091915
Sum of electronic and thermal Free Energies= -4535.290086

8:



8: In Gas Phase

C	0.77597900	-3.27852400	0.36637600
H	0.01024800	-3.01351800	1.12315100
H	1.26206600	-4.21343100	0.72039100
C	0.09754700	-3.53299300	-1.00974500
H	0.81803500	-3.99239900	-1.71477600
H	-0.76915000	-4.21784700	-0.90264100
N	-0.32352000	-2.27229900	-1.59359800
N	1.74234900	-2.19755200	0.28873300
C	-1.44777900	-1.53880500	-1.17689800
C	-1.26738700	-0.26971900	-1.74008100
C	-2.55892500	-1.85036800	-0.38685200
C	-2.17171600	0.78688400	-1.55028600
C	-3.51618600	-0.83162100	-0.18271400
H	-2.67675000	-2.85214200	0.05062100
C	-3.29950800	0.44244000	-0.77066600
H	-4.04258600	1.22584400	-0.58627900
C	1.49509300	-0.87348800	0.69991000
C	0.48986400	-0.37834700	1.54098800
C	2.44419300	0.00898400	0.13319800
C	0.46837600	1.00269300	1.85065700
H	-0.26186500	-1.06105200	1.96346400
C	2.44921700	1.38860000	0.38597100

C	1.43989200	1.84373500	1.26908700
H	1.41664700	2.91251000	1.50487800
O	3.34557400	-0.63775400	-0.70007200
O	-0.06713600	-0.29289400	-2.44686000
C	-1.89673400	2.19248900	-2.10361500
C	-4.78183800	-1.13688900	0.65060300
C	-3.03385700	3.17689700	-1.76558900
H	-3.16982500	3.29343600	-0.67000600
H	-2.79305400	4.17845700	-2.17759000
H	-4.00242800	2.85841500	-2.20466300
C	-1.74026100	2.11559800	-3.64378800
H	-0.90532900	1.44789800	-3.93253400
H	-2.66993900	1.73616800	-4.11700100
H	-1.53105900	3.12518400	-4.05638500
C	-0.58015600	2.71047100	-1.46660300
H	-0.66933000	2.77767500	-0.36353600
H	0.27176400	2.03624800	-1.68027500
H	-0.33223900	3.71931100	-1.85924300
C	-5.56866100	0.14350300	1.00497700
H	-6.44151900	-0.11432000	1.63940300
H	-4.94083800	0.86425600	1.56876400
H	-5.96137500	0.65593800	0.10291000
C	-4.39793800	-1.84120100	1.97686400
H	-5.30699600	-2.04115000	2.58206300
H	-3.89979800	-2.81738200	1.80809400
H	-3.71570900	-1.20920300	2.58166400
C	-5.69824200	-2.07206800	-0.18022400
H	-5.99504500	-1.58841400	-1.13388100
H	-5.18420500	-3.02309700	-0.43132500
H	-6.62162900	-2.32122100	0.38520900
C	3.50020500	2.31676400	-0.24917400
C	4.90725600	1.88781100	0.24449600
H	5.12708500	0.83491800	-0.01849400
H	5.68799800	2.53151300	-0.21408400
H	4.98176600	1.98774400	1.34743500
C	3.42440200	2.20946700	-1.79482700
H	3.59961300	1.17446100	-2.14393800
H	2.42843500	2.53113100	-2.16261400
H	4.19010000	2.86673700	-2.25916600
C	3.26933500	3.79159600	0.14049800
H	3.34719000	3.95140000	1.23605600
H	4.03934000	4.42781800	-0.34273200
H	2.27556700	4.15579100	-0.19560600
C	-0.60159400	1.54101700	2.82717700
C	-0.50126300	0.77553300	4.17171400
H	-0.69113300	-0.31027900	4.04673900
H	0.50791900	0.89051300	4.61884400
H	-1.24873800	1.16278900	4.89684800
C	-2.00564100	1.32726200	2.21588800
H	-2.79940400	1.64796600	2.92451400
H	-2.12217700	1.90603200	1.27785700
H	-2.18588900	0.26631300	1.95459900
C	-0.42722900	3.04669000	3.11718500
H	-0.52432000	3.65821400	2.19599600
H	-1.21290900	3.38627800	3.82356400
H	0.55734700	3.26875400	3.57816000
P	3.21000900	-2.31623600	-0.64975000
Cl	4.64944700	-2.74935800	0.93942400
C	0.53423200	-1.51898800	-2.35434200

Sum of electronic and zero-point Energies= -2267.533776
Sum of electronic and thermal Energies= -2267.494044
Sum of electronic and thermal Enthalpies= -2267.493100
Sum of electronic and thermal Free Energies= -2267.603160

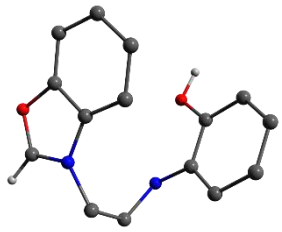
8: In THF

C	0.80550700	-3.30537800	0.21700600
H	0.04585200	-3.08357300	0.99195400
H	1.28336400	-4.26386400	0.50699500
C	0.12840000	-3.46452400	-1.17019400
H	0.84419000	-3.88331000	-1.90378600
H	-0.73906300	-4.15132900	-1.10411500
N	-0.29388400	-2.16602600	-1.67401700
N	1.78617800	-2.22424500	0.20870300
C	-1.42824600	-1.46845400	-1.22121000
C	-1.27511000	-0.17329800	-1.73047100
C	-2.53220500	-1.83886800	-0.44634100
C	-2.19931600	0.85738900	-1.49369700
C	-3.50954500	-0.84958300	-0.19985100
H	-2.62893700	-2.86115000	-0.05569000
C	-3.31828200	0.45510500	-0.72873500
H	-4.07753200	1.21376500	-0.50945300
C	1.52696800	-0.91630600	0.66747700
C	0.52343900	-0.46597900	1.53630900
C	2.45725800	-0.00180200	0.12066600
C	0.47853500	0.90609800	1.88162200
H	-0.20601200	-1.17614700	1.95140500
C	2.43277300	1.37277800	0.40193500
C	1.42314500	1.78328400	1.30599400
H	1.37621500	2.84580900	1.56557200
O	3.36809400	-0.61330100	-0.73194600
O	-0.08010000	-0.14793700	-2.44945700
C	-1.95923800	2.29199500	-1.98696500
C	-4.77184900	-1.21899700	0.61152600
C	-3.10964800	3.23751200	-1.58878100
H	-3.23140200	3.29863300	-0.48718900
H	-2.89217700	4.26108800	-1.95683200
H	-4.07799600	2.92059900	-2.02894700
C	-1.82525400	2.28662500	-3.53127600
H	-0.98353300	1.64737000	-3.86292900
H	-2.75577300	1.91163000	-4.00637600
H	-1.64059700	3.31702200	-3.90174000
C	-0.64463600	2.81055800	-1.34673400
H	-0.71927200	2.82873700	-0.24050400
H	0.21809200	2.16537200	-1.60265000
H	-0.42407800	3.84068200	-1.69762300
C	-5.57425100	0.02872100	1.04079700
H	-6.44152700	-0.27894000	1.66029000
H	-4.95429900	0.72327900	1.64497700
H	-5.97645400	0.58822700	0.17129400
C	-4.38320400	-2.00037800	1.89235000
H	-5.29377500	-2.24806000	2.47685500
H	-3.87127600	-2.95775500	1.66644000
H	-3.71312400	-1.39785400	2.53940200
C	-5.67384600	-2.11229900	-0.27944800
H	-5.97484700	-1.57349400	-1.20202900
H	-5.14664200	-3.04027400	-0.58385300
H	-6.59535300	-2.40491100	0.26764800
C	3.44988200	2.34232300	-0.22681000
C	4.87415200	1.94925200	0.24687600
H	5.12252300	0.90647400	-0.03226800
H	5.63045400	2.62186300	-0.21086100
H	4.95698800	2.03912100	1.35027200
C	3.36339000	2.25859600	-1.77342100
H	3.57379500	1.23671500	-2.14215100
H	2.35299300	2.55197700	-2.12564400
H	4.10045100	2.95097200	-2.23253400
C	3.17754800	3.80328000	0.18789300
H	3.26279900	3.94888200	1.28468300
H	3.92152600	4.47017600	-0.29460100

H	2.16845900	4.13928400	-0.13098500
C	-0.58567400	1.39660600	2.88937400
C	-0.43905300	0.60274400	4.21312100
H	-0.60402800	-0.48428300	4.06590000
H	0.57440200	0.73693600	4.64599000
H	-1.18305500	0.95476400	4.95902900
C	-1.99573100	1.16111400	2.29992900
H	-2.78131000	1.44955900	3.03047300
H	-2.14476400	1.75753000	1.37785200
H	-2.15886100	0.10112600	2.02315900
C	-0.44219700	2.89952500	3.20928000
H	-0.57391500	3.52907100	2.30467500
H	-1.22244800	3.20139500	3.93818500
H	0.54524900	3.13704200	3.65665500
P	3.25132900	-2.29405100	-0.71500900
Cl	4.73247500	-2.69367000	0.89188500
C	0.53673400	-1.37183800	-2.41412600

Sum of electronic and zero-point Energies= -2267.546700
Sum of electronic and thermal Energies= -2267.506836
Sum of electronic and thermal Enthalpies= -2267.505892
Sum of electronic and thermal Free Energies= -2267.616577

Gas phase:

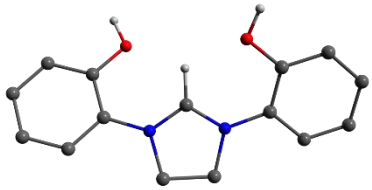


C	-1.77970	0.51006	1.09213
C	-2.63592	1.48933	0.57096
C	-3.43171	1.21126	-0.55805
H	-4.09908	1.98775	-0.96048
C	-3.37372	-0.05875	-1.15358
C	-2.52937	-1.05365	-0.62307
H	-2.51773	-2.05361	-1.08301
C	-1.72129	-0.78706	0.50314
C	-0.24512	-2.78279	0.30428
H	-1.01494	-3.48923	-0.08056
H	0.40240	-3.37597	0.98272
C	0.58891	-2.32569	-0.93344
H	1.12130	-3.17847	-1.39895
H	-0.06408	-1.86441	-1.69834
N	1.57715	-1.30072	-0.55436
C	1.38165	0.09748	-0.58663
C	0.36901	0.91954	-1.10876
H	-0.53345	0.52100	-1.59285
C	0.56741	2.29843	-0.94359
C	1.71783	2.83142	-0.30735
H	1.81803	3.92331	-0.21178
C	2.74222	2.01018	0.19556
C	2.52667	0.64296	0.02911
O	3.35595	-0.41049	0.40582
C	2.74465	-1.52813	0.04518
H	3.21045	-2.50271	0.24075
O	-0.91357	0.71537	2.13765
H	-1.10133	1.57526	2.55944
N	-0.82730	-1.70735	1.05441
H	-0.31566	-1.36053	1.86757
H	-2.66600	2.48568	1.04290
H	-3.99955	-0.28996	-2.02863

H	-0.20380	2.98633	-1.32048
H	3.64642	2.40548	0.67827

Sum of electronic and zero-point Energies= -839.510907
Sum of electronic and thermal Energies= -839.495115
Sum of electronic and thermal Enthalpies= -839.494171
Sum of electronic and thermal Free Energies= -839.554748

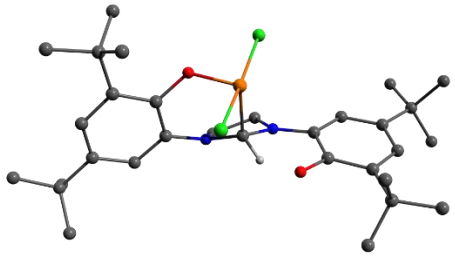
Gas phase:



C	0.00000	-0.02132	0.00010
H	0.00001	-1.11509	0.00004
C	-0.75869	2.15200	-0.13922
H	-1.33555	2.74341	0.59741
H	-1.00089	2.51862	-1.15864
N	-1.11882	0.71406	-0.03549
C	-2.46882	0.26309	-0.05397
C	-2.82383	-1.04178	0.39542
C	-4.17734	-1.42485	0.39599
C	-5.17785	-0.54150	-0.03390
H	-6.22961	-0.86422	-0.02232
C	-4.83195	0.74645	-0.47560
C	-3.48792	1.14291	-0.48223
H	-3.23417	2.15272	-0.83376
C	0.75870	2.15201	0.13936
H	1.00092	2.51868	1.15876
H	1.33558	2.74333	-0.59732
N	1.11882	0.71403	0.03571
C	2.46883	0.26306	0.05401
C	2.82378	-1.04184	-0.39534
C	4.17729	-1.42487	-0.39613
C	5.17787	-0.54151	0.03359
H	6.22963	-0.86422	0.02184
C	4.83202	0.74643	0.47534
C	3.48799	1.14289	0.48212
H	3.23429	2.15270	0.83369
O	1.82701	-1.87686	-0.81315
H	2.21580	-2.70102	-1.16634
O	-1.82711	-1.87682	0.81334
H	-2.21597	-2.70084	1.16678
H	4.44080	-2.43696	-0.74573
H	5.60753	1.44782	0.81588
H	-4.44089	-2.43694	0.74553
H	-5.60741	1.44782	-0.81624

Sum of electronic and zero-point Energies= -839.530579
Sum of electronic and thermal Energies= -839.514449
Sum of electronic and thermal Enthalpies= -839.513505
Sum of electronic and thermal Free Energies= -839.574933

TS2':

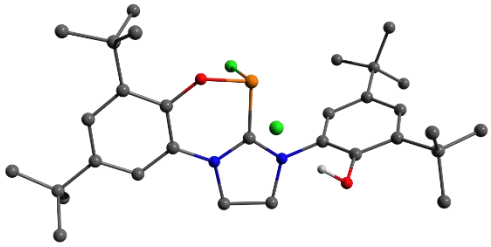


P	-0.28552	-1.24155	1.06161
Cl	0.50706	-0.02665	2.97983
O	-1.83728	-0.75079	1.49081
C	-2.77692	-0.23781	0.62711
C	-4.14285	-0.57434	0.77554
C	-5.05330	0.09815	-0.06970
H	-6.11456	-0.15570	0.02120
C	-4.67658	1.07764	-1.01588
C	-3.30981	1.39461	-1.11966
H	-2.95287	2.14818	-1.83709
C	-2.35925	0.74233	-0.31589
C	-4.61233	-1.59833	1.83393
C	-4.20241	-1.10807	3.24914
H	-4.55996	-1.82932	4.01429
H	-4.66283	-0.12166	3.46774
H	-3.10563	-1.00939	3.35385
C	-3.98393	-2.98451	1.54017
H	-4.31252	-3.71755	2.30711
H	-2.87950	-2.95363	1.53742
H	-4.30578	-3.35697	0.54560
C	-6.14813	-1.76546	1.82197
H	-6.43969	-2.50789	2.59289
H	-6.52028	-2.13931	0.84560
H	-6.67466	-0.81744	2.05834
C	-5.69643	1.78520	-1.93260
C	-5.37141	1.43863	-3.40862
H	-6.09269	1.93736	-4.09016
H	-5.43439	0.34376	-3.57964
H	-4.35233	1.76951	-3.69618
C	-5.59513	3.31807	-1.72439
H	-6.32814	3.84337	-2.37238
H	-4.58780	3.70676	-1.97861
H	-5.80938	3.58985	-0.66974
C	-7.14707	1.34909	-1.63737
H	-7.84338	1.88786	-2.31243
H	-7.44569	1.58273	-0.59417
H	-7.29602	0.26263	-1.80667
N	-1.00926	1.14108	-0.35284
C	-0.59130	2.55567	-0.18306
H	-1.34780	3.10833	0.40390
H	-0.47650	3.04234	-1.17600
C	0.74704	2.41721	0.55548
H	1.48612	3.18589	0.26771
H	0.63112	2.38837	1.66391
N	1.18733	1.07157	0.13765
C	2.48885	0.63572	0.05562
C	3.54064	1.35775	0.66879
H	3.28475	2.17235	1.35724
C	4.86692	1.00692	0.42692
C	5.11948	-0.06494	-0.48998
H	6.16850	-0.33583	-0.66982
C	4.13319	-0.79147	-1.15521
C	2.74989	-0.50142	-0.83166
C	6.05430	1.71934	1.09686

C	5.59432	2.84043	2.05118
H	6.47835	3.32739	2.51135
H	4.96433	2.44660	2.87572
H	5.02124	3.62782	1.51867
C	6.87083	0.68361	1.91399
H	7.73152	1.18002	2.40994
H	7.27569	-0.12652	1.27366
H	6.24121	0.21672	2.69960
C	6.95556	2.34398	-0.00058
H	7.82222	2.85977	0.46424
H	6.39082	3.08837	-0.59965
H	7.35649	1.57913	-0.69685
C	4.46141	-1.93500	-2.13581
C	3.89765	-3.27520	-1.59155
H	4.14878	-4.10234	-2.28888
H	2.79731	-3.23611	-1.47895
H	4.34339	-3.51333	-0.60293
C	3.83157	-1.61404	-3.51730
H	4.05581	-2.43050	-4.23607
H	4.24888	-0.67104	-3.92870
H	2.73243	-1.51016	-3.44313
C	5.98384	-2.10215	-2.32779
H	6.17464	-2.91452	-3.05869
H	6.49476	-2.38064	-1.38252
H	6.45876	-1.17949	-2.72235
O	1.76680	-1.19147	-1.31384
H	0.54170	-0.47460	-1.05607
C	0.08940	0.29575	-0.21913
Cl	-1.09615	-2.57232	-0.70859

Sum of electronic and zero-point Energies= -2728.234683
Sum of electronic and thermal Energies= -2728.192536
Sum of electronic and thermal Enthalpies= -2728.191592
Sum of electronic and thermal Free Energies= -2728.308102

5:



P	-0.01700	0.75018	1.44950
Cl	0.95365	-0.14173	3.18212
O	1.34220	1.30141	0.63038
C	2.46250	0.53518	0.34288
C	3.73202	1.15677	0.32212
C	4.83462	0.34107	-0.02017
H	5.82554	0.80605	-0.03786
C	4.73161	-1.03096	-0.32736
C	3.45228	-1.61578	-0.28672
H	3.32084	-2.68305	-0.51227
C	2.32538	-0.84742	0.04575
C	3.90851	2.65266	0.67115
C	3.45916	2.89441	2.13680
H	3.59183	3.96481	2.40115
H	4.07116	2.28873	2.83715
H	2.39784	2.63106	2.29791
C	3.07870	3.52733	-0.30595
H	3.23133	4.60182	-0.07079
H	1.99647	3.31096	-0.24045
H	3.40433	3.35684	-1.35335
C	5.38433	3.09505	0.55498

H	5.46249	4.17121	0.81243
H	5.77711	2.97065	-0.47537
H	6.04580	2.54028	1.25220
C	5.95248	-1.89774	-0.69909
C	5.75767	-2.45253	-2.13379
H	6.62326	-3.08509	-2.42336
H	5.67267	-1.62502	-2.86857
H	4.84385	-3.07597	-2.21692
C	6.06829	-3.07400	0.30404
H	6.94727	-3.70521	0.05518
H	5.17260	-3.72837	0.28592
H	6.19476	-2.69857	1.34088
C	7.26955	-1.09465	-0.66059
H	8.11767	-1.75682	-0.93050
H	7.47492	-0.68527	0.35031
H	7.26251	-0.25239	-1.38305
N	1.04288	-1.43163	0.02596
C	0.70011	-2.66250	-0.73235
H	1.13946	-3.54498	-0.22691
H	1.10245	-2.56003	-1.75867
C	-0.84707	-2.66483	-0.71170
H	-1.26568	-2.43843	-1.71249
H	-1.27596	-3.60170	-0.30873
N	-1.17979	-1.51865	0.18147
C	-2.45434	-0.87300	0.13297
C	-3.61488	-1.58591	0.47627
H	-3.50174	-2.61051	0.85494
C	-4.87458	-0.98083	0.33912
C	-4.91008	0.34220	-0.16462
H	-5.89323	0.81715	-0.28021
C	-3.77068	1.08443	-0.53168
C	-2.50165	0.45974	-0.36715
C	-6.19072	-1.69384	0.71140
C	-5.94505	-3.12119	1.24243
H	-6.91359	-3.59852	1.49748
H	-5.32309	-3.11922	2.16182
H	-5.44699	-3.76354	0.48654
C	-6.91687	-0.87885	1.81257
H	-7.86564	-1.37936	2.10021
H	-7.16896	0.14606	1.47109
H	-6.28395	-0.78955	2.72004
C	-7.09322	-1.78650	-0.54588
H	-8.04972	-2.29395	-0.29863
H	-6.59265	-2.36512	-1.35001
H	-7.34055	-0.78408	-0.95158
C	-3.87461	2.50078	-1.13763
C	-3.08261	3.51242	-0.26815
H	-3.18597	4.53490	-0.68958
H	-2.00772	3.25795	-0.22828
H	-3.47850	3.52890	0.76918
C	-3.30878	2.46649	-2.58338
H	-3.32815	3.48591	-3.02442
H	-3.92806	1.80462	-3.22482
H	-2.26818	2.09110	-2.61827
C	-5.33789	2.98979	-1.21283
H	-5.36172	4.00406	-1.66179
H	-5.80631	3.05843	-0.20877
H	-5.96824	2.33312	-1.84788
O	-1.33743	1.11379	-0.64018
H	-0.81948	0.65332	-1.50352
C	-0.06338	-0.86517	0.51519
Cl	-0.09551	-0.13658	-2.82421

Sum of electronic and zero-point Energies= -2728.290586
Sum of electronic and thermal Energies= -2728.248514
Sum of electronic and thermal Enthalpies= -2728.247570

Sum of electronic and thermal Free Energies= -2728.363989

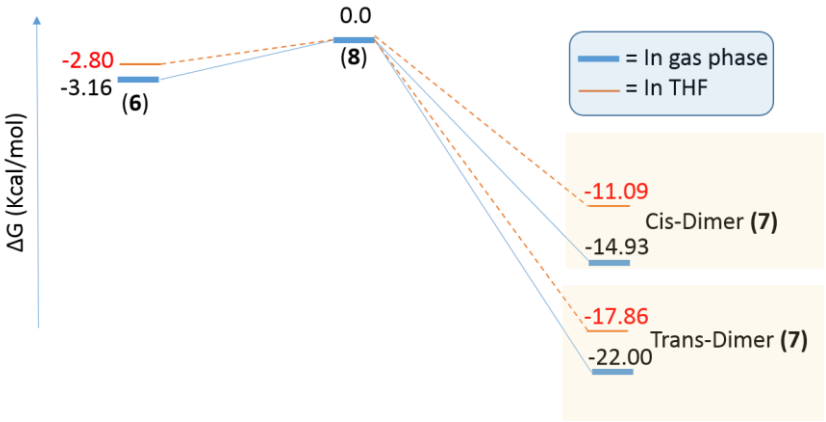


Figure S44. DFT calculated (BP86-D3/def2-SVP) Gibbs free energies of **6**, **7** and **8** in gas phase (blue color) and in THF (red color) (CPCM).

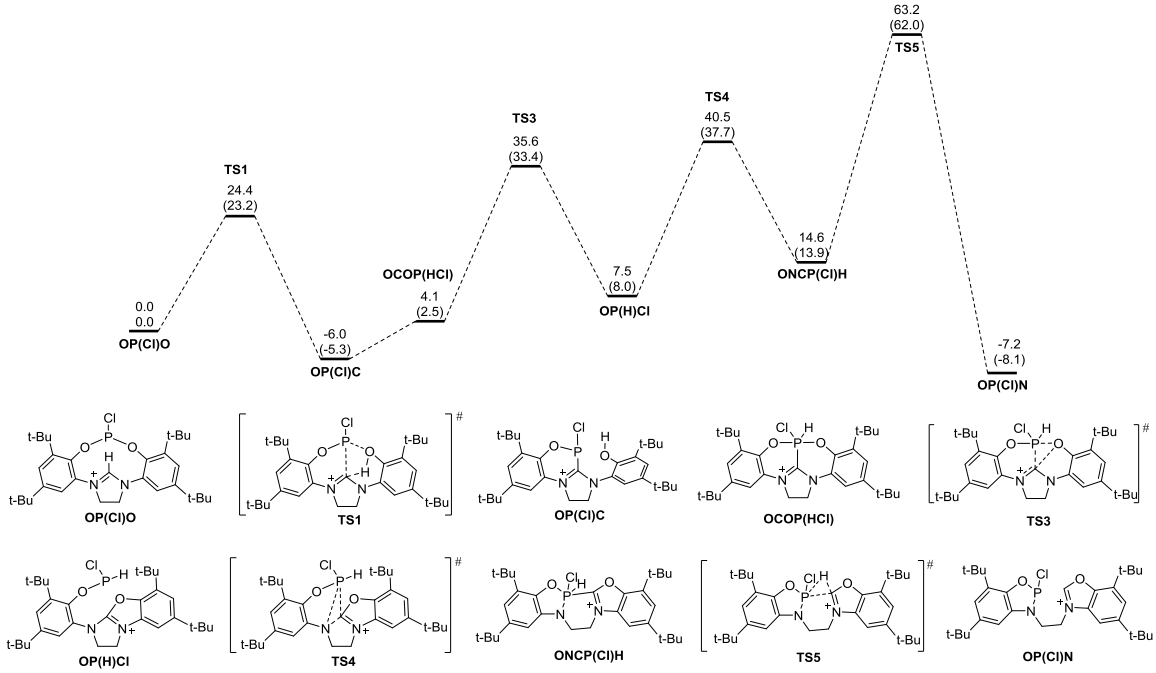


Figure S45. DFT calculated (BP86-D3/def2-SVP) Gibbs free energies (enthalpies) of PES for the rearrangement of **4** to **3** in gas phase without the Cl^- counter anion.

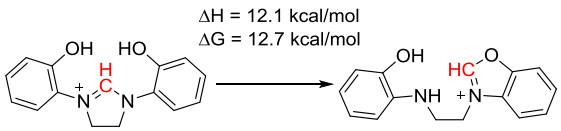


Figure S46. DFT calculated (BP86-D3/def2-SVP) Gibbs free energies (enthalpies) of difference in energy between **1a** and **1a-R** in gas phase without the Cl^- counter anion.

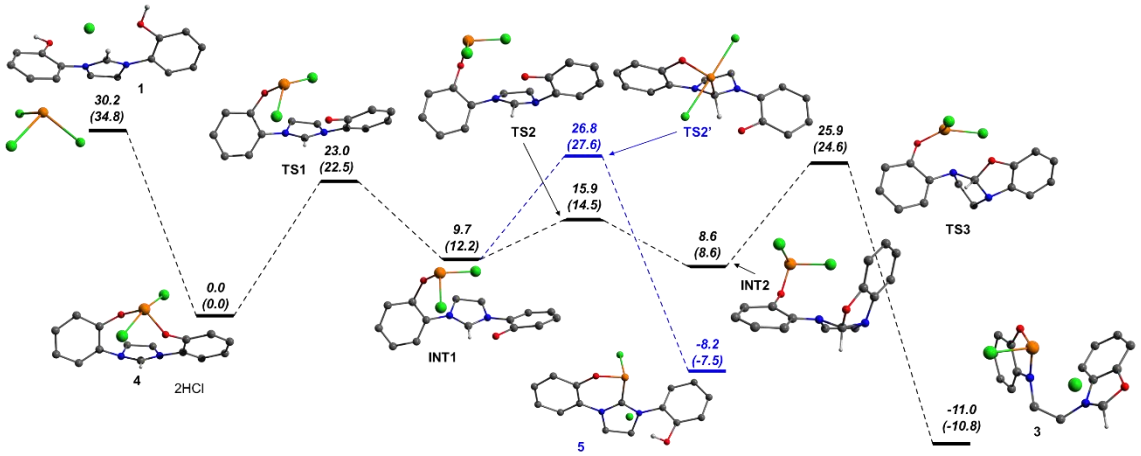


Figure S47. DFT calculated (BP86-D3/def2-SVP) Gibbs free energies (enthalpies) of difference in energy between **1a** and **1a-R** in gas phase without the Cl^- counter anion.

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