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Influence of *N*-Heterocyclic Carbenes (NHCs) on the Hydrolysis of a Diphosphene, A Phosphorus-Analogue of an Alkene

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Experimental section

All experiments were carried out under argon atmosphere using standard Schlenk techniques or in a PL-HE-2GB Innovative Technology GloveBox or in MBraun Unilab GloveBox. *n*-Hexane, diethyl ether, THF, and toluene were dried by PS-MD-5 Innovative Technology solvent purification system. Benzene was refluxed over sodium/benzophenone, then distilled and stored under argon. Starting compounds **1**[S1], **NHC^{Me_4}**,[S2] **NHC^{Me_2iPr_2}**,[S2] **NHC^{Me_2}**,[S3] **NHC^{iPrMe}**,[S3] **NHC^{iPr_2}**,[S4] **NHC^{tBu_2}**,[S5] **NHC^{Dip_2}**,[S6] and **NHC^{Mes_2}**[S6] were prepared according to known literature procedures. Tol-d8, C_6D_6, and THF-d8 were dried and distilled over potassium under argon. NMR spectra were recorded with Bruker NanoBay 300 MHz NMR spectrometer. ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to the peaks of residual protons of the deuterated solvent (^{1}H) or the deuterated solvent itself. ^{31}P NMR and ^{31}P{^{1}H} spectra were referenced to the peaks of H_3PO_4. UV/vis spectra were acquired using a Jasco V-670 spectrometer using quartz cells with a path length of 0.1 cm. Elemental analyses were performed on a Leco CHN-900 analyzer. Mass spectrometry was performed on an Agilent 6210 ESI-TOF in positive mode, using HPLC grade solvents. Melting points were determined in closed NMR tubes under argon atmosphere and are uncorrected.

Synthesis of 1·NHC^{Me_2}

5 mL of toluene were added to a Schlenk flask containing **1** (0.205 g, 0.295 mmol) and **NHC^{Me_2}** (0.029 g, 0.300 mmol) at room temperature. The reaction mixture was kept at −35 °C refrigerator for two days. After two days bright red crystals of **1·NHC^{Me_2}** were obtained along with **1**. From that we were able to selectively measured the solid state molecular structure of **1·NHC^{Me_2}**. In solution compound **1·NHC^{Me_2}** is in equilibrium with **1** and **NHC^{Me_2}**. NMR data from 1:1 stoichiometric ratio of **1** and **NHC^{Me_2}** in Tol-d8 at RT (almost 20% of **1** and **NHC^{Me_2}** and 80% of **1 NHC^{Me_2}**). We were unable to assign the ^{1}H NMR of **1·NHC^{Me_2}** due to broadening of the peaks and presence of **1** and **NHC^{Me_2}**. ^{31}P NMR (121.5 MHz, Tol-d8,

298 K): δ = −7.2 (d, $^{1}J_{(P,\ P)}$ = 420 Hz, **NHC^{Me_2}** *P*–P), −103.8 (d, $^{1}J_{(P,\ P)}$ = 420 Hz, **NHC^{Me_2}** P–*P*) ppm. UV/vis (THF): λ_{max} = 458, 371, 326 nm.

Synthesis of 1·NHC$^{i\text{PrMe}}$

5 mL of toluene were added to a Schlenk flask containing **1** (0.200 g, 0.290 mmol) and **NHC$^{i\text{PrMe}}$** (0.038 g, 0.305 mmol) at room temperature. In solution below 273 K the compound **1·NHC$^{i\text{PrMe}}$** was in equilibrium with **1** and **NHC$^{i\text{PrMe}}$**. We assigned ^{31}P resonances of **1·NHC$^{i\text{PrMe}}$** unambiguously, but were unable to assign the ^{1}H NMR due to broadening of the peaks and presence of **1** and **NHC$^{i\text{PrMe}}$**. ^{31}P NMR (121.5 MHz, Tol-d8, 223 K): δ = 19.1 (d, $^{1}J_{(P,\ P)}$ = 405 Hz, **NHC$^{i\text{PrMe}}$***P*–P), −87.6 $^{1}J_{(P,\ P)}$ = 405 Hz, **NHC$^{i\text{PrMe}}$** P–*P*) ppm for major isomer. δ = 1.1 (d, $^{1}J_{(P,\ P)}$ = 430 Hz, **NHC$^{i\text{PrMe}}$***P*–P), −92.6 $^{1}J_{(P,\ P)}$ = 430 Hz, **NHC$^{i\text{PrMe}}$**P–*P*) ppm for minor isomer. UV/vis (THF): λ_{max} = 442, 366, 325 nm.

Synthesis of 1·NHC$^{i\text{Pr}_2}$

5 mL of toluene were added to Schlenk flask containing **1** (0.200 g, 0.290 mmol) and **NHC$^{i\text{Pr}_2}$** (0.038 g, 0.305 mmol) at room temperature. In solution below 233 K compound **1·NHC$^{i\text{Pr}_2}$** is in equilibrium with **1** and **NHC$^{i\text{Pr}_2}$**. We have assigned ^{31}P resonances of **1·NHC$^{i\text{Pr}_2}$** unambiguously but could not able to assign the ^{1}H NMR due to broadening of the peaks and presence of **1** and **NHC$^{i\text{Pr}_2}$**. ^{31}P NMR (121.5 MHz, Tol-d_8, 223 K): δ = 28.7 (d, $^{1}J_{(P,\ P)}$ = 404 Hz, NHC$^{i\text{Pr}_2}$*P*–P), −74.2 (d, $^{1}J_{(P,\ P)}$ = 404 Hz, NHC$^{i\text{Pr}_2}$P–*P*) ppm. UV/vis (THF): λ_{max} = 430, 372, 322 nm.

Reaction of 1 and H_2O in presence of stoichiometric amount of coordinated NHCs

Variable temperature ^{31}P NMR study of the reaction of 1 and H_2O in presence of stoichiometric amount of NHC^{Me_4}

In a 50 mL Schlenk flask, 0.230 g (0.333 mmol) of **1** and 0.042 g (0.338 mmol) of **NHC^{Me_4}** were dissolved in 10 mL of THF. Subsequently, degassed water (6 µL, 0.338 mmol) was added at −78 °C and allowed the reaction mixture to stir at that temperature for 30 minutes. After that 0.4 mL of reaction aliquot has been transferred to a precooled NMR tube at −78 °C which contained two drops of Tol-d8. Subsequently, measured the ^{31}P NMR at 193 K. On rising temperature to 223 K, two new doublet at δ = 110.8 and −34.2 ppm ($^1J_{(P,\ P)}$ = 340 Hz) appeared in $^{31}P\{^1H\}$ NMR spectrum, which we assigned for **2·NHC^{Me_4}**. In ^{31}P spectrum resonance at δ = 110.8 ppm remained as doublet however resonance at δ = −34.2 ppm became doublet of a doublet ($^1J_{(P,\ P)}$ = 340 Hz, $^1J_{(P,\ H)}$ = 209 Hz) for **2·NHC^{Me_4}**. At above 273 K we observed the peak for the formation of **3** and **4·NHC^{Me_4}**. ^{31}P NMR for **2·NHC^{Me_4}** (121.5 MHz, THF/Tol-d8, 263 K): δ = 111.0 (d, $^1J_{(P,\ P)}$ = 338 Hz) and −34.2 ppm (dd, 1P, $^1J_{(P,\ P)}$ = 338 Hz, $^1J_{(P,\ H)}$ = 209 Hz) ppm. $^{31}P\{^1H\}$ NMR for **2·NHC^{Me_4}** (121.5 MHz, THF/Tol-d_8, 263K): δ = 111.0 (d, ^1J(P, P) = 338 Hz), −34.2 (d, $^1J_{(P,\ P)}$ = 338 Hz) ppm.

Reaction of 1 with 2 equivalent H_2O in the presence of 2 equivalent of NHC^{Me_4}

In a 50 mL Schlenk flask, 0.050 g (0.072 mmol) of **1** and 0.019 g (0.150 mmol) of **NHC^{Me_4}** were dissolved in 10 mL of THF at −78 °C and the reaction mixture was stirred for 10 minutes. Subsequently, degassed water (35 µL, from stock solution of 2 mL water in 20 mL THF) was added at −78 °C and brought at room temperature within one hour. Subsequent ^{31}P NMR shows that formation of mostly **4·NHC^{Me_4}** along with very small amount of **3**.

Reaction of 1 and H_2O in presence of stoichiometric amount of NHC^{Me_2}

In a 50 mL Schlenk flask, 0.245 g (0.355 mmol) of **1** and 0.035 g (0.364 mmol) of **NHC^{Me_2}** were dissolved in 10 mL of THF at −78 °C. The reaction mixture was stirred for 10 minutes. Subsequently, degassed water (6.6 µL, 0.364 mmol) was added at −78 °C and brought at room temperature within one hour. The reaction mixture was stirred at room temperature for another 1.5 hrs. The red color of the solution slowly changed to an orange color solution. The ^{31}P NMR showed complete consumption of **1** and the formation of mixture of **3** and **4·NHC^{Me_2}** (75:25). Also the presence of **NHC^{Me_2}** has been observed in the reaction mixture. The reaction mixture was then evaporated and extracted with boiling toluene (10 mL). Crystallization happened upon cooling the extract at room temperature. Isolated crude yield: 0.190 g. In the crystalline compounds mostly the presence of compound **3** along with very small amount of **4·NHC^{Me_2}** were observed. Selected NMR data of **4·NHC^{Me_2}:** ^1H NMR (300 MHz, C_6D_6, 298 K): (selected resonances) δ = 1.18 (s, 6H, Mes−CH_3), 1.84 (s, 6H, Mes−CH_3), 1.90 (s, 6H, Mes−CH_3), 2.01(s, 6H, Mes−CH_3), 2.21 (s, 6H, Mes−CH_3), 2.22 (s, 6H, Mes−CH_3) 6.91 (d, $^1J_{(P,H)}$ = 464 Hz, 1H, P–*H*) ppm. $^{31}P\{^1H\}$ NMR (121.5 MHz, C_6D_6, 298 K): δ = 29.7 (d, $^1J_{(P,P)}$ = 464 Hz, P–*P*–O), −47.8 (d, $^1J_{(P,P)}$ = 464 Hz, *P*–P–O) ppm. **^{31}P NMR (121.5 MHz, C_6D_6, 298 K):** 29.7 (*t*, 1P, $^1J_{(P,P)}$ = $^1J_{(P,H)}$ 464 Hz, P–*P*–O), −47.8 (d, $^1J_{(P,P)}$ = 464 Hz, *P*–P–O) ppm.

Reaction of 1 and H_2O in presence of stoichiometric amount of NHC^{iPrMe}

In a 50 mL Schlenk flask, 0.302 g (0.438 mmol) of **1** and 0.055 g (0.442 mmol) of **NHC^{iPrMe}** were dissolved in 15 mL of THF at −78 °C. The reaction mixture was stirred for 10 minutes. Subsequently, degassed water (8 µL, 0. 442 mmol) was added at −78 °C and brought at room temperature within one hour. The reaction mixture was stirred at room temperature for another 2 hrs and the red colour of the solution slowly changed to an orange color solution. The ^{31}P NMR measurement showed the complete

consumption of **1** and the formation of mixture of compound **3** and **4·NHC^{iPrMe}** (60:40). The reaction mixture was then evaporated and extracted with boiling toluene (7 mL). Crystallization happened upon cooling at room temperature. Isolated crude yield: 0.260 g. Selected NMR data of **4·NHC^{iPrMe}:** ^{1}H NMR (300 MHz, C_6D_6, 298 K): δ = 1.50 (d, $^{3}J_{(H,H)}$ = 6.75 Hz, 6H, CH(CH_3)$_2$), 1.80 (s, 6H, Mes–CH_3), 1.85 (s, 6H, Mes–CH_3), 1.90 (s, 6H, Mes–CH_3), 2.01 (s, 6H, Mes–CH_3), 2.23 (s, 6H, Mes–CH_3), 2.25 (s, 6H, Mes–CH_3), 3.48 (3H, N-CH_3), 4.50 (sep, $^{3}J_{(H, H)}$ = 6.65 Hz, CH(CH$_3$)$_2$), 6.82 (d, $^{1}J_{(P, H)}$ = 462 Hz, 1H, P–*H*), 11.01 (s, br, 1H, N–C*H*–N) ppm. ^{31}P{^{1}H} NMR (121.5 MHz, C_6D_6, 298 K): δ = 28.6 (d, $^{1}J_{(P, P)}$ = 462 Hz, P–*P*–O), −46.4 (d, $^{1}J_{(P, P)}$ = 462 Hz, *P*–P–O) ppm. ^{31}P NMR (121.5 MHz, C_6D_6, 298 K): δ = 28.6 (*t*, 1P, $^{1}J_{(P, P)}$ = $^{1}J_{(P, H)}$ 462 Hz, P–*P*–O), −46.4 (d, $^{1}J_{(P, P)}$ = 462 Hz, *P*–P–O) ppm.

Reaction of 1 and H_2O in presence of stoichiometric amount of NHC^{iPr_2}

In a 50 mL Schlenk flask, 0.300 g (0.435 mmol) of **1** and 0.680 g (0.435 mmol) of **NHC^{iPr_2}** were dissolved in 15 mL of THF at −78 °C. Then water (8 μL, 0.435 mmol) was added at −78 °C and brought to room temperature within one hour. Subsequently, the reaction mixture was stirred at room temperature for 2 hrs. The measurement of ^{31}P NMR showed complete consumption of starting diphosphene and the formation of mixture of **3** and **4·NHC^{iPr_2}** (60:40) along with the presence of NHC^{iPr_2} in the reaction mixture. The reaction mixture was then evaporated and extracted with boiling toluene (10 mL). Crystallization happened upon cooling at room temperature. Isolated crude yield: 0.270 g. Selected NMR data of **4·NHC^{iPr_2}**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): δ = 2.03 (s, 6H, Mes–CH_3), 2.09 (s, 6H, Mes–CH_3), 2.12 (s, 6H, Mes–CH_3), 2.22 (s, 6H, Mes–CH_3), 2.47 (s, 6H, Mes–CH_3), 2.53 (s, 6H, Mes–CH_3) 7.13 (d, $^{1}J_{(P, H)}$ = 464 Hz, 1H, P–*H*) ppm. ^{31}P{^{1}H} NMR (121.5 MHz, C_6D_6, 298 K): δ = 29.5 (d, $^{1}J_{(P, P)}$ = 464 Hz, P–*P*–O), −47.8 (d, $^{1}J_{(P, P)}$ = 464 Hz, *P*–P–O) ppm. ^{31}P NMR (121.5 MHz, C_6D_6, 298 K): δ = 29.5 (*t*, 1P, $^{1}J_{(P, P)}$ = $^{1}J_{(P, H)}$ 464 Hz, P–*P*–O), −46.4 (d, $^{1}J_{(P, P)}$ = 464 Hz, *P*–P–O) ppm.

Catalytic hydrolysis of 1 with various coordinated NHCs

General procedure: Compound **1** and 10 mol% of **NHC** were dissolved in about 10 mL of THF (10 mL) and cooled down to−78 °C. Subsequently, equivalent amount of degassed water was added and the reaction mixture was allowed warming to room temperature. Subsequently, ^{31}P NMR spectra were recorded to detect the TON.

Reaction of 1 and H_2O in presence of catalytic amount of NHC^{Me_4}

0.277 g (0.402 mmol) of 1 and 0.005 g (0.040 mmol) of **NHC^{Me_4}** were dissolved in about 10 mL of THF and cooled down to −78 °C. Subsequently, 8 μL (0.450 mmol) of water were added and the reaction mixture allowed to warm to room temperature. Subsequent measurement of $^{31}P\{^1H\}$ NMR spectrum of crude reaction mixture showed the formation of **3** in an about 95%.

Reaction of 1 and H_2O in presence of catalytic amount of NHC^{Me_2}

0.230 g (0.334 mmol) of **1** and 0.003 g (0.033 mmol) of **NHC^{Me_2}** were dissolved in about 10 mL of THF and cooled down to −78 °C. Subsequently, 6 μL (0.334 mmol) of water were added portion wise and the reaction mixture allowed to warm to room temperature. Subsequent measurement of $^{31}P\{^1H\}$ NMR spectrum of crude reaction mixture showed the formation of **3** in an about 77%.

Reaction of 1 and H_2O in presence of catalytic amount of NHC^{iPrMe}

0.220 g (0.319 mmol) of **1** and 0.004 g (0.032 mmol) of **NHC^{iPrMe}** were dissolved in about 10 mL of THF (10 mL) and cooled down to −78 °C. Subsequently, 6 μL (0.334 mmol) of water were added portion wise and the reaction mixture allowed to warm to room temperature. Subsequent measurement of $^{31}P\{^1H\}$ NMR spectrum of crude reaction mixture showed the formation of **3** in an about 85 %.

Reaction of 1 and H_2O in presence of catalytic amount of NHC^{iPr_2}

0.200 g (0.290 mmol) of **1** and 0.004 g (0.029 mmol) of **NHC^{iPr_2}** were dissolved in about 10 mL of THF (10 mL) and cooled down to −78 °C. Subsequently, 5.5 µL (0.300 mmol) of water were added portion wise and the reaction mixture allowed to warm to room temperature. Subsequent measurement of $^{31}P\{^1H\}$ NMR spectrum of crude reaction mixture showed the formation of **3** in an about 70 %.

Reaction of 1 and H_2O in presence of stoichiometric amount of non-coordinated NHCs

Reaction of 1 and H_2O in presence of stoichiometric amount of $NHC^{iPr_2Me_2}$

In a 50 mL Schlenk flask, 0.340 g (0.493 mmol) of **1** and 0.089 g (0.493 mmol) of **$NHC^{iPr_2Me_2}$** were dissolved in 20 mL of THF at room temperature. Subsequently, degassed water (9 µL, 0.500 mmol) was added at −78 °C and brought at room temperature within an hour. The reaction mixture was stirred at room temperature for 2 hrs. The ^{31}P NMR showed complete consumption of **1** and the formation of **2·$NHC^{Me_2iPr_2}$** along with **3** and **4·$NHC^{Me_2iPr_2}$**. The reaction mixture was then evaporated and extracted with boiling toluene (10 mL). Crystallization happened upon cooling at room temperature and ^{31}P NMR of the obtained crystals showed **4·$NHC^{Me_2iPr_2}$** as the major product (90 %) along with **3** (7 %) and **2·$NHC^{Me_2iPr_2}$** (3 %). Isolated crude yield: 0.300 g. Selected NMR data of **2·$NHC^{Me_2iPr_2}$**: ^1H NMR (300 MHz, C_6D_6, 298 K): 1.15 (s, br, 12H), 1.29 (s, br, 6H), 2.14 (s, 6H), 2.20 (s, 12H), 2.33 (s, 6H), 2.47 (s, 6H), 2.48 (s, 6H), 3.34 (dd, $^1J_{(P,\,H)}$ = 221.89 Hz, $^2J_{(P,\,H)}$ = 22.78 Hz, *H*–P–P–O), 3.85 (sep, $^3J_{(H,\,H)}$ = 6.73 Hz, 2H), 6.86–6.88 (m, 6H), 6.91(s, 1H), 6.95–6.97 (m, 4H), 7.02–7.04 (m, 3H). $^{31}P\{^1H\}$ NMR (121.5 MHz, C_6D_6, 298 K): δ = 122.3 (d, $^1J_{(P,\,P)}$ = 320 Hz, P–*P*–O), −41.8 (d, $^1J_{(P,\,P)}$ = 320 Hz, *P*–P–O) ppm. ^{31}P NMR (121.5 MHz, C_6D_6, 298 K): 122.3 (*dd*, 1P, $^1J_{(P,\,P)}$ = 320, $^2J_{(P,\,H)}$ = 23 Hz, H–P–*P*–O), −41.8 (d, $^1J_{(P,\,P)}$ = 320 Hz, $^1J_{(P,\,H)}$ = 222 Hz, H–*P*–P–O) ppm.

NMR data for **4·NHC^{iPr_2Me_2}**: ^{1}H NMR (300 MHz, THF-d$_8$, 298 K): δ = 1.38 (d, $^{3}J_{(H,H)}$ = 6.75 Hz, 6H, CH(CH_3)$_2$, from coordinated carbene), 1.80 (s, 6H,CH_3–Mes) 1.85 (s, 6H,CH_3–Mes), 1.88 (s, 6H,CH_3–Mes), 2.01 (s, 6H,CH_3–Mes), 2.25 (s, br, 9H, 3H from CH_3–Mes, 6H from coordinated carbene), 2.30 (s, 3H, CH_3–Mes), 2.35 (s, 6H,CH_3–Mes), 4.52 (sep, $^{3}J_{(H, H)}$ = 6.76 Hz CH(CH$_3$)$_2$), 6.32 (d, $^{3}J_{(H, H)}$ = 7.10 Hz, 1H,Ar–H), 6.44–6.47 (m, 3H, Ar–H), 6.53–6.65 (m, 3H, Ar–H), 6.73 (s, 2H, Ar–H), 6.81–6.85 (m, 1H, Ar–H), 7.04 (d, $^{3}J_{(P, H)}$ = 461 Hz, 1H, P–H), ppm. ^{13}C{^{1}H} NMR (75.43 MHz, THF-d8, 298 K): δ = 8.8 (2C, C–CH$_3$ of NHC), 20.8 (1C, CH$_3$), 21.2 (1C, CH$_3$), 21.3 (1C, CH$_3$), 21.4 (1C, CH$_3$), 21.5 (1C, CH$_3$), 21.6 (2C, CH$_3$), 21.8 (1C, CH$_3$), 22.1 (1C, CH$_3$), 22.4 (1C, CH$_3$), 22.9 (1C, CH$_3$), 23.0 (1C, CH$_3$), 23.4 (4C, CH$_3$), 51.4 (2C, CH–(CH$_3$)$_2$ of NHC), 120.5 (1C, Ar–CH), 126.2 (1C, Ar–CH), 127.6 (1C, Ar–CH), 127.9 (1C, Ar–CH), 128.1 (1C, Ar–CH), 128.5 (1C, Ar–CH), 128.7 (1C, Ar–CH), 129.1 (1C , Ar–CH), 129.2 (1C, Ar–CH), 129.4 (1C, Ar–CH), 129.4 (1C, Ar–CH), 129.8 (1C, Ar–CH), 130.1 (1C, Ar–CH), 130.3 (1C, Ar–CH), 134.0 (2C, Ar–C), 134.7 (2C, Ar–C), 136.3 (2C, Ar–C), 136.9 (2C, Ar–C), 140.0 (2C, Ar–C), 137.3 (2C, Ar–C), 138.1 (2C, Ar–C), 138.6 (2C, Ar–C), 141.7 (2C, Ar–C), 143.5 (2C, Ar–C), 143.5 (2C, Ar–C), 145.6 (2C, Ar–C), 158.4 (1C, N–C–N of NHC) ppm. ^{31}P{^{1}H} NMR (121.5 MHz, THF-d8, 298 K): δ = 27.3 (d, $^{1}J_{(P, P)}$ = 469.28 Hz, P–P–O), −50.5 (d, $^{1}J_{(P, P)}$ = 469.28 Hz, P–P–O) ppm. ^{31}P NMR (121.5 MHz, THF-d8, 298 K): 28.6 (*dd*, 1P, $^{1}J_{(P, P)}$ = 469.28, $^{1}J_{(P, H)}$ = 461 Hz, P–P–O), −46.4 (d, $^{1}J_{(P, P)}$ = 469.28 Hz, P–P–O) ppm. HRMS (ESI-TOF) m/z M+ Calcd for $C_{11}H_{21}N_2$: 181.1704; Found : 181.177.

Variable temperature NMR study of the reaction of 1 with water in presence of stoichiometric amount of NHC^{iPr_2Me_2}

In a 50 mL Schlenk flask, 0.263 g (0.381 mmol) of **1** and 0.042 g (0.383 mmol) of **NHC^{iPr_2Me_2}**, were dissolved in 10 mL of THF. Subsequently, degassed water (7 µL, 0.400 mmol) was added at −78 °C and allowed the reaction mixture to stir at that temperature for 30 minutes. After that 0.4 mL of reaction aliquot has been transferred to a precooled NMR tube at −78 °C which contained two drops of Tol-d8. Subsequently, the ^{31}P NMR was measured at 203. At 203 K ^{31}P{^{1}H} NMR showed the presence of two new doublet at δ = 123.2 and −47.7 ppm ($^{1}J_{(P, P)}$ = 308 Hz) for **2·NHC^{iPr_2Me_2}** along with a singlet resonance

of **1**. On rising temperature, the intensity of two doublets increased whereas singlet resonance for **1** decreased. After three days at room temperature the initially formed hydrolysis product converted to **3** and **4·NHC^{iPr_2Me_2}**. $^{31}P\{^1H\}$ NMR (121.5 MHz, THF/Tol-d8, 203 K) for **2·NHC^{iPr_2Me_2}**: δ = 123.2 (d, $^1J_{(P,\,P)}$ = 308 Hz), −47.8 (d, $^1J_{(P,\,P)}$ = 308 Hz) ppm. ^{31}P NMR (121.5 MHz, THF/Tol-d8, 263 K) for **2·NHC^{iPr_2Me_2}**: δ = 123.2 (dd, $^1J_{(P,\,P)}$ = 308 Hz, $^2J_{(P,\,H)}$ = 18 Hz) and −47.8 ppm (*dd*, $^1J_{(P,\,P)}$ = 308 Hz, $^1J_{(P,\,H)}$ = 222 Hz) ppm.

Reaction of 2·NHC^{iPr_2Me_2} with BPh_3

First we have reacted **1** (0.100 g, 0.145 mmol), **NHC^{iPr_2Me_2}** (0.031 g, 0.174 mmol), and H_2O (3.5 µL, 0.194 mmol) in THF at −78 °C and warm up to room temperature in 1 hr to get **2·NHC^{iPr_2Me_2}**. Then we reacted BPh_3 (0.047 g, 0.194 mmol) with it immediately at room temperature. Subsequent measurement of $^{31}P\{^1H\}$ and ^{31}P NMR spectra showed the formation of two new compounds and these are two conformational isomers of **2** in a 7:10 ratio along with **NHC^{iPr_2Me_2}·BPh_3**. After 24 hrs, these two conformational isomers leads to compound 3 within 24 hrs of time at room temperature. $^{31}P\{^1H\}$ NMR (121.5 MHz, THF/Tol-d8, 298K): δ = 115.4 (d, $^1J_{(P,\,P)}$ = 191 Hz), −65.4 (d, $^1J_{(P,\,P)}$ = 191 Hz) ppm for minor diastereomer and δ = 109.1 (d, $^1J_{(P,\,P)}$ = 317 Hz), −44.9 (d, $^1J_{(P,\,P)}$ = 317 Hz) ppm for major diastereomer. ^{31}P NMR (121.5 MHz, THF/Tol-d8, 263K): δ = 115.4 (dd, $^1J_{(P,\,P)}$ = 191 Hz, $^2J_{(P,\,H)}$ = 13 Hz) and −65.4 ppm (*dd*, $^1J_{(P,\,P)}$ = 191 Hz, $^1J_{(P,\,H)}$ = 221 Hz) ppm for minor diastereomer and δ = 109.1 (dd, $^1J_{(P,\,P)}$ = 317 Hz, $^2J_{(P,\,H)}$ = 18 Hz) and −44.9 ppm (*dd*, $^1J_{(P,\,P)}$ = 316 Hz, $^1J_{(P,\,H)}$ = 217 Hz) ppm for major diastereomer.

Hydrolysis of NHC^{Me_4}

In a Schlenk flask 0.100 g (0.805 mmol) of **NHC^{Me_4}** was taken and dissolved in 5 mL of dry THF. 15 µL (0.833 mmol) of water was added to it at **−**78 °C and brought it at room temperature within one hour. All the volatiles were removed to get dense liquid product which contains mixture of products type of

type **A** (60%) and **B** (40%). A: **^{1}H NMR (300 MHz, C_6D_6, 298 K):** δ = 1.13 (d, $^3J_{(H, H)}$ = 6.95 Hz, 3H, NHCH_3), 1.35 (s, 3H, CH_3C–CH_3), 2.11 (s, 3H, CH_3–NCHO), 2.86 (s, 3H, CH_3C–CH_3), 5.14 (q, $^3J_{(H, H)}$ = 6.95 Hz., 1H, N–*H*), 7.87 (s, 1H, C*H*O). **B**: **^{1}H NMR (300 MHz, C_6D_6, 298 K):** δ = 1.07 (d, $^3J_{(H, H)}$ = 6.82 Hz, 3H, NHCH_3), 1.16 (s, 3H, CH_3C–CH_3), 2.47 (s, 3H, CH_3–NCHO), 2.84 (s, 3H, CH_3C–CH_3), 3.46 (q, $^3J_{(H, H)}$ = 6.82 Hz., 1H, C*H*–NCHO), 8.04 (s, 1H, C*H*O) ppm.

Hydrolysis of NHC^{iPr_2Me_2}

In a Schlenk flask 0.090 g (0.500 mmol) of **NHC^{iPr_2Me_2}** was taken and dissolved in 5 mL of dry THF. 9 µL (0.5 mmol) of water was added to it at −78 °C and brought it at room temperature. It was then allowed to stir for a month. The volatile were removed and ^{1}H NMR spectrum suggested that about 60% of **NHC^{iPr_2Me_2}** hydrolyzed and gave products type of **A** (46%) and B (54%). **A**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected peaks, δ = 8.09 (s, br, NH), 8.10 (s, 1H, C*H*O) ppm. **B**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected peaks, δ = 5.17 (q, $^3J_{(H, H)}$ = 6.94 Hz, 1H, C*H*–NCHO), 8.32 (s, 1H, C*H*O) ppm.

Hydrolysis of NHC^{Me_2}

In a Schlenk flask 0.085 g (0.884 mmol) of **NHC^{Me_2}** was taken and dissolved in 5 mL of dry THF. 16 µL (0.888 mmol) of water was added to it at −78 °C and brought it to room temperature. It was then allowed to stir for another 1 hour. Subsequently, all the volatiles were removed under vacuum and the resulting sticky solid which did not lead any conclusive ^{1}H NMR spectrum.

Hydrolysis of NHC^{iPrMe}

In a Schlenk flask 0.105 g (0.845 mmol) of **NHC^{iPrMe}** was taken and dissolved in 5 mL of dry THF. 15 µL (0.833 mmol) of water was added to it at −78 °C and brought to room temperature. It was then allowed

to stir for another 1 hour. Subsequently, all the volatiles were removed under vacuum and the resulting dense liquid which did not lead any conclusive ^{1}H NMR spectrum.

Hydrolysis of NHC^{iPr_2}

In a Schlenk flask 0.100 g (0.656 mmol) of **NHC^{iPr_2}** was taken and dissolved in 5 mL of dry THF. 12 µL (0.666 mmol) of water was added to it at −78 °C and brought it to room temperature. It was then allowed to stir for another 1 hr. Subsequently, all the volatiles were removed under vacuum and the resulting liquid showed the formation of **A** type hydrolyzed product in ^{1}H NMR spectrum. ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected peak, δ = 8.77 (s, 1H, CHO) ppm.

Hydrolysis of NHC^{tBu_2}

In a Schlenk flask 0.132 g (0.732 mmol) of **NHC^{tBu_2}** was taken and dissolved in 7 mL of dry THF. 13 µL (0.722 mmol) of water was added to it at −78 °C and brought it to room temperature. It was then allowed to stair for another 5 days. Subsequently, all the volatiles were removed under vacuum and the ^{1}H NMR spectrum of the resulting solid showed about 1 % of **NHC^{tBu_2}** hydrolyzed and it leads to the formation of only **B** type of product. ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected peaks, δ = 4.12 (d, $^{3}J_{(H, H)}$ = 4.15 Hz, C*H*$_2$N, 2H), 7.49 (t, $^{3}J_{(H, H)}$ = 4.15 Hz, C*H*=N,1H), 8.40 (s, 1H, C*H*O) ppm.

Hydrolysis of NHC^{Dip_2}

In a Schlenk flask 0.145 g (0.373 mmol) of **NHC^{Dip_2}** was taken and dissolved in 10 mL of dry THF. 6.7 µL (0.372 mmol) of water was added to it at room temperature and allowed to stair for 10 days. Subsequently, all the volatiles were removed under vacuum and ^{1}H NMR spectrum showed the formation of **A** (25%) and **B** (75%) types of both hydrolyzed product (57%) along with unreacted **NHC^{Dip_2}**

(43%). **A**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected peaks, δ = 3.20 (sep, $^{3}J_{(H, H)}$ = 6.89 Hz, 2H, C*H*$(CH_3)_2$,), 3.72 (sep, $^{3}J_{(H, H)}$ = 6.82 Hz, 2H, C*H*$(CH_3)_2$,), 5.55, (dd, $^{1}J_{(H, H)}$ = 9.04 Hz & 6.65, 1H, Hz, =C*H*–NH), 4.67 (d, $^{1}J_{(H, H)}$ = 6.65 Hz, =C*H*–NH CHO, 1H), 6.73 (d, 1H, $^{1}J_{(H, H)}$ = 9.04 Hz, N*H*), 8.02 (s, C*H*O) ppm. **B**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected speaks δ = 0.94 (d, $^{3}J_{(H, H)}$ = 6.90 Hz, 6H,CH(CH_3)$_3$), 0.98 (d, $^{3}J_{(H, H)}$ = 6.90 Hz, 6H, CH(CH_3)$_2$), 1.18 (d, 12H, CH(CH_3)$_2$), 2.88–3.06 (m, 4H, C*H*$(CH_3)_2$ along with C*H*$(CH_3)_2$ of free carbene), 4.50 (d, $^{3}J_{(H, H)}$ = 4.04 Hz, 2H, NCH_2), 7.80 (t, 1H, $^{3}J_{(H, H)}$ = 4.04 Hz, 1H, C*H*=N), 8.19 (s, 1H, C*H*O) ppm.

Hydrolysis of NHC^{Mes_2}

In a Schlenk flask 0.135 g (0.443 mmol) of **NHC^{Mes_2}** was taken and dissolved in 10 mL of dry THF. 8 µL (0.444 mmol) of water was added to it at room temperature and allowed to stair for 5 days. Subsequently, all the volatiles were removed under vacuum and ^{1}H NMR spectrum showed the formation of **A** (60%) and **B** (40%) types of both hydrolyzed product (95%) along with unreacted **NHC^{Mes_2}** (5%). **A**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected peaks, δ = 5.49 (dd, $^{1}J_{(H, H)}$ = 9.30 Hz & 6.70 Hz, 1H, =C*H*–NH), 4.75 (d, $^{1}J_{(H, H)}$ = 6.70 Hz, =C*H*–N–CHO, 1H), 6.30 (d, $^{3}J_{(H, H)}$ = 9.30 Hz, $^{1}J_{(H, H)}$ = 9.04 Hz, N*H*), 7.80 (s, C*H*O) ppm. **B**: ^{1}H NMR (300 MHz, C_6D_6, 298 K): Selected speaks δ = 4.36 (d, $^{3}J_{(H, H)}$ = 4.14 Hz, 2H, NCH_2), 7.75 (t, 1H, $^{3}J_{(H, H)}$ = 4.14 Hz, 1H, C*H*=N), 7.92 (s, 1H, C*H*O) ppm.

Table S1. ^{31}P NMR data at 223 K for the adducts between NHCs and 1.

Sl. No.	**Compounds**	**δ^{31}P (ppm)**		**$^{1}J_{(31P,31P)}$ (Hz)**
		NHC*P*–P	NHCP–*P*	
1	**1·NHC^{Me_4}**	−7.1 (d)	−98.4 (d)	416
2	**1·NHC^{Me_2}**	−7.2 (d)	−103.8 (d)	420
3#	**1·NHC^{iPrMe}**	+19.1 (d) +1.1 (d)	−87.6 (d) −92.6 (d)	405 430 (major isomer)
4	**1·NHC^{iPr_2}**	+28.7 (d)	−74.2 (d)	404

[#]Two isomers due to two different *N*-substitution in **NHC^{iPrMe}**.

Thermodynamic data of equilibrium between 1 and NHC

Thermodynamic data of equilibrium between 1 and 1·NHC^{Me_2}

In a NMR tube 0.5 mL Tol-d_8 solution of **1** (0.0830 M) and **NHC^{Me_2}** (0.0830 M) were taken. Then ^{31}P and ^{1}H spectra was measured 10 or 5 K interval starting at 298 K up to 253 K. The Integration of ^{31}P resonance of **1** alone and adduct, **1·NHC^{Me_2}** allowed the concentration of both the component to be measured. The equilibrium constants were calculated.

Table S2. Concentrations for 1, NHC^{Me_2}, and 1·NHC^{Me_2} determined via ^{31}P NMR spectroscopy at a range of temperatures.

Sl. No.	T/K	[1]/mM	[NHC^{Me_2}]/mM	[1·NHC^{Me_4}]/mM	*K*/M	ln*K*	ΔG/kJ mol^{-1}
1	253	21.58	21.58	61.41	131.86	4.88	10.264
2	263	26.56	26.56	56.44	80.01	4.38	9.577
3	273	36.52	36.52	46.48	34.85	3.55	8.057
4	283	52.29	52.29	30.71	11.23	2.42	5.693
5	293	60.59	60.59	22.41	6.10	1.81	4.409
6	298	66.40	66.40	16.63	3.77	1.32	3.270

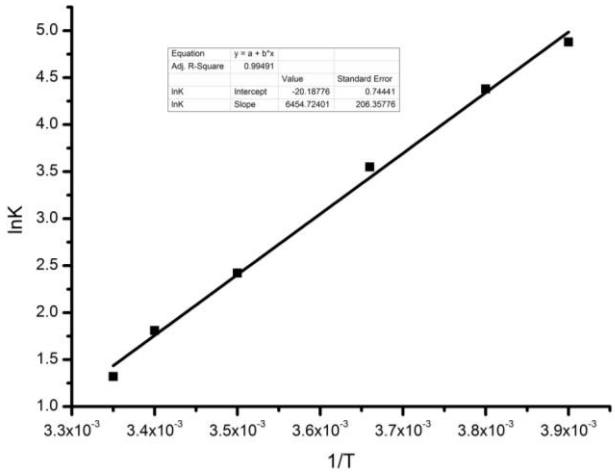


Figure S1. The linear regression of 1/T *vs* ln*K* allowed to determine the value of $\Delta H = -53.664 \pm 1.715$ kJmol^{-1}, $\Delta G_{298} = -3.64 \pm 1.25$ kJmol^{-1}, $\Delta S = -167.840 \pm 6.189$ Jmol^{-1}K^{-1}.

Thermodynamic data of equilibrium between 1 and 1·NHC^{iPrMe}

In a NMR tube 0.5 mL Tol-d_8 solution of **1** (0.0638 M) and **NHC^{iPrMe}** (0.0638 M) were taken. Then ^{31}P and ^{1}H spectra was measured 10 K interval starting at 263 K up to 213 K. The integration of ^{31}P resonance of **1** alone and adduct, **1·NHC^{iPrMe}** allowed the concentration of both the component to be measured. The equilibrium constants were calculated. In room temperature there is no indication of adducts formation. We observed the adduct formation at 273 K. Due to two different *N*-substitution in **NHC^{iPrMe}** we observed the formation of two magnetically non-equivalent adduct formation.

Table S3. Concentrations for 1, NHC^{MeiPr}, and 1·NHC^{MeiPr} determined via ^{31}P NMR spectroscopy at a range of temperatures.

Sl. No.	T/K	[1]/mM	[NHC^{iPrMe}]/mM	[1·NHC^{MeiPr}]/Mm	*K*/M	ln*K*	ΔG/kJ mol^{-1}
1	203	11.85	11.85	72.830	518.60	6.25	10.548
2	213	19.47	19.47	65.21	172.02	5.14	9.102
3	223	26.25	26.25	58.43	84.79	4.44	8.231
4	233	40.64	40.64	44.04	26.66	3.28	6.354
5	243	64.35	64.35	20.33	4.91	1.60	3.244
6	253	71.97	71.97	12.71	2.45	0.89	1.884

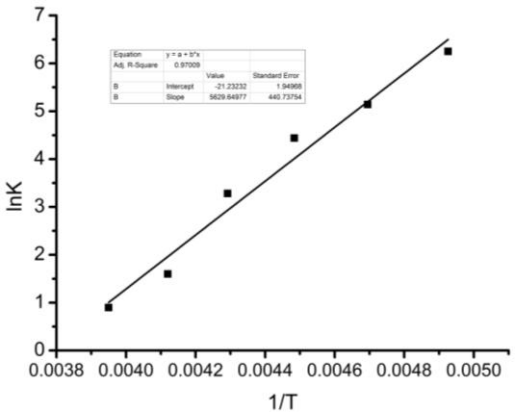


Figure S2. The linear regression of 1/T *vs* ln*K* allowed to determine the value of $\Delta H = -46.805 \pm 3.604$ kJmol^{-1}, $\Delta G_{298} = 5.78 \pm 3.516$ kJmol^{-1}, $\Delta S = -176.52 \pm 16.20$ Jmol^{-1}K^{-1}.

Thermodynamic data of equilibrium between 1 and 1·NHC$^{iPr}{}_2$

In a NMR tube 0.5 mL Tol-d_8 solution of **1** (0.0784 M) and **NHC^{iPr_2}** (0.0784 M) were taken. Then ^{31}P and ^{1}H spectra was measured 10 K interval starting at 233 K up to 203 K. The Integration of ^{31}P resonance of **1** alone and adduct, **1·NHC^{iPr_2}** allowed the concentration of both the component to be measured. The equilibrium constants were calculated.

Table 4. Concentrations for 1, NHC^{iPr_2}, and 1·NHC^{iPr_2} determined via ^{31}P NMR spectroscopy at a range of temperatures.

SI. No.	T/K	[1]/mM	[NHC^{iPr_2}]/mM	[1·NHC^{iPr_2}]/mM	*K*/M	ln*K*	ΔG/kJ mol^{-1}
1	203	56.44	56.44	21.95	6.89	1.93	3.257
2	213	64.08	64.08	14.31	3.48	1.24	2.195
3	223	72.90	72.90	5.49	1.03	0.03	0.055
4	233	75.25	75.25	3.13	0.55	−0.59	−1.142

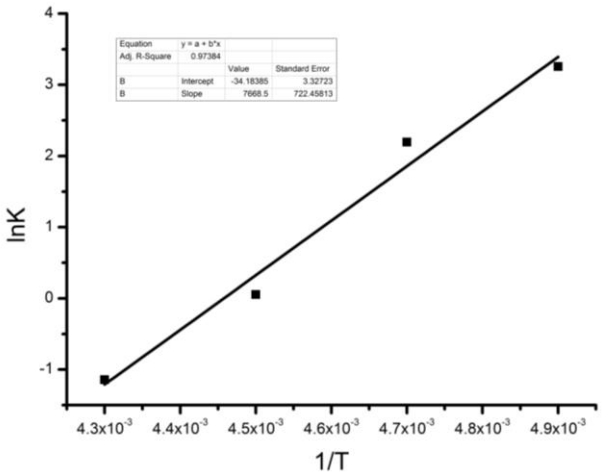


Figure S3. The linear regression of 1/T *vs* ln*K* allowed determining the value of ΔH = −63.75 ± 6.00 kJmol^{-1}, ΔG_{298} = 20.93 ± 7.81 kJmol^{-1}, ΔS = −284.20 ± 27.66 Jmol^{-1}K^{-1}.

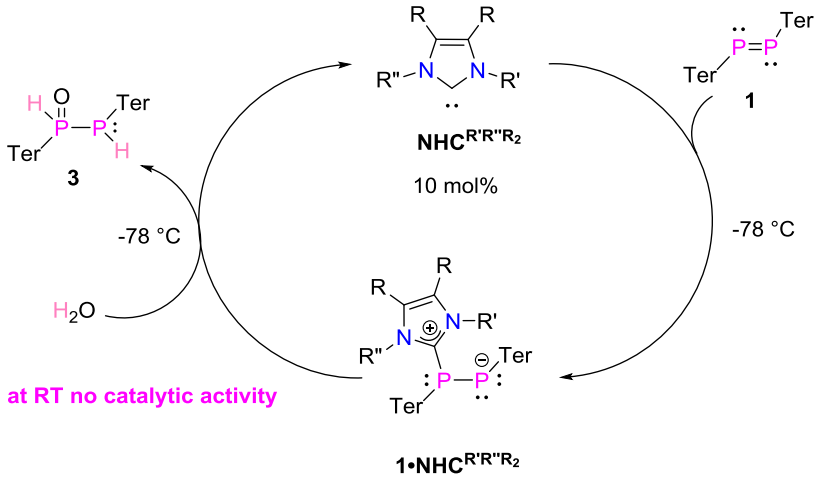
Table S5. Thermodynamic parameters and equilibrium constants for the adduct formation between NHCs and 1.

Sl. No.	1+ $NHC^{R'R''}$	ΔG_{298} (kJ mol^{-1})	ΔH (kJmol^{-1})	ΔS_{298} (J$mol^{-1}K^{-1}$)	K_{298} / M
1	**1+NHC^{Me_4}**	−11.2±1.07	−50.7±1.09	−132.8±2.56	90
2	**1+NHC^{Me_2}**	−3.6±1.25	−53.7±1.71	−167.8±6.189	3.77
3	**1+NHC^{iPrMe}**	+5.8±3.51	−46.8±3.60	−176.5±16.20	0.01
4	**1+NHC^{iPr_2}**	+20.9±7.81	−63.7±6.00	−284.2±27.66	0.0002

Table S6. Hydrolysis reaction of 1 in presence of equivalent amount of coordinated NHC.

Sl. No.	*N*-Heterocyclic Carbenes	Yield of Products#	
		3 (%)	**4·NHC (%)**
1	**NHC^{Me_4}**	5	95
2	**NHC^{Me_2}**	75	25
3	**NHC^{iPrMe}**	60	40
4	**NHC^{iPr_2}**	40	60

[#]Yields are calculated from the crude reaction mixture based on ^{31}P NMR.



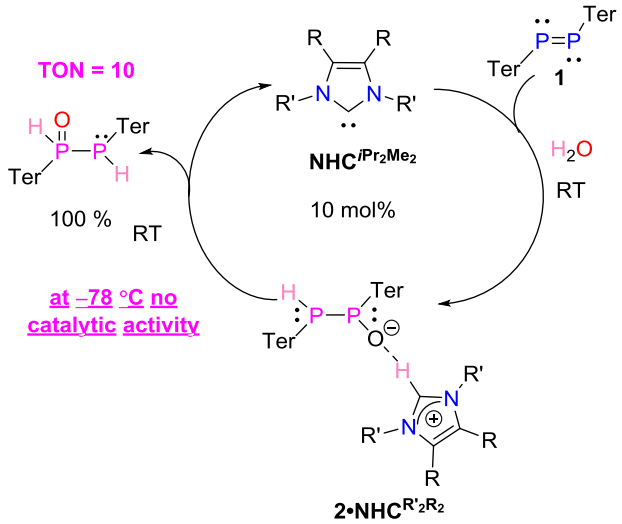
Scheme S1. Catalytic reaction of **H_2O** with **1** in presence of 10 mol% of **$NHC^{R'R''R_2}$**.

Table S7. Hydrolysis reaction of 1 in presence of 10 mol % of coordinated NHC.

Sl. No.	N-Heterocyclic Carbenes	Yield (%) of 3	Remarks
1	**NHC^{Me_4}**	95	Work up at −78 °C.
2	**NHC^{Me_2}**	77	Work up at −78 °C and water added portion wise (about 9 mol %) every 30 minutes interval.
3	**NHC^{iPrMe}**	85	Work up at −78 °C and water added portion wise (about 9 mol %) every 30 minutes interval.
4	**NHC^{iPr_2}**	70	Work up at −78 °C and water added portion wise (about 9 mol %) every 30 minutes interval

Table S8. Hydrolysis reaction of 1 in presence of equivalent amounts of non-coordinated NHC.

Sl. No.	*N*-heterocyclic carbenes	Product(s)	Remarks
1	**NHC^{iPr_2Me_2}**	**3**:**4**·**NHC^{iPr_2Me_2}**:**2**· **NHC^{iPr_2Me_2}** (5:2:93 in the crude reaction mixture and 15:80:5 after crystallization)	3 hrs at RT
2	**NHC^{tBu_2}**	**3**:**4**·**NHC^{tBu_2}**:**2**·**NHC^{tBu_2}** (90:5:5 in the crude reaction mixture)	Over night at RT
3	**NHC^{Dip_2}**	After 2 days only about 20 % **3** formed.	
4	**NHC^{Mes_2}**	No reaction of compound **1** even after 5 days.	



Scheme S2. Catalytic reaction of H_2O with 1 in presence of 10 mol % of NHC^{Me_2iPr_2}.

Table S9. Hydrolysis reaction of 1 in presence of 10 mol% of non-coordinated NHC.

SI. No.	*N*-heterocyclic carbenes	Yield (%) of 3	Remarks
1	**NHC^{iPr_2Me_2}**	95	Work at RT; 2 days
2	**NHC^{tBu_2}**	100	Work at RT; 4 days

NMR Spectra

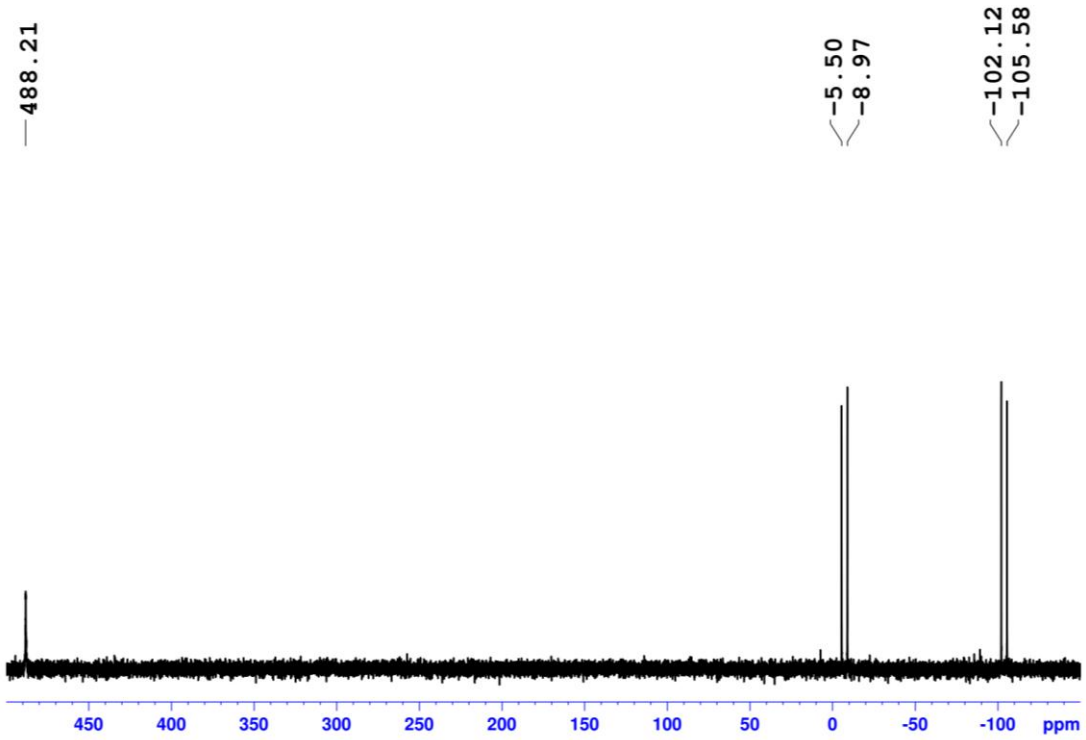


Figure S4. $^{31}P\{^{1}H\}$ NMR of 1:1 of **1** and **NHC^{Me_2}** in tol-d_8 at 223 K.

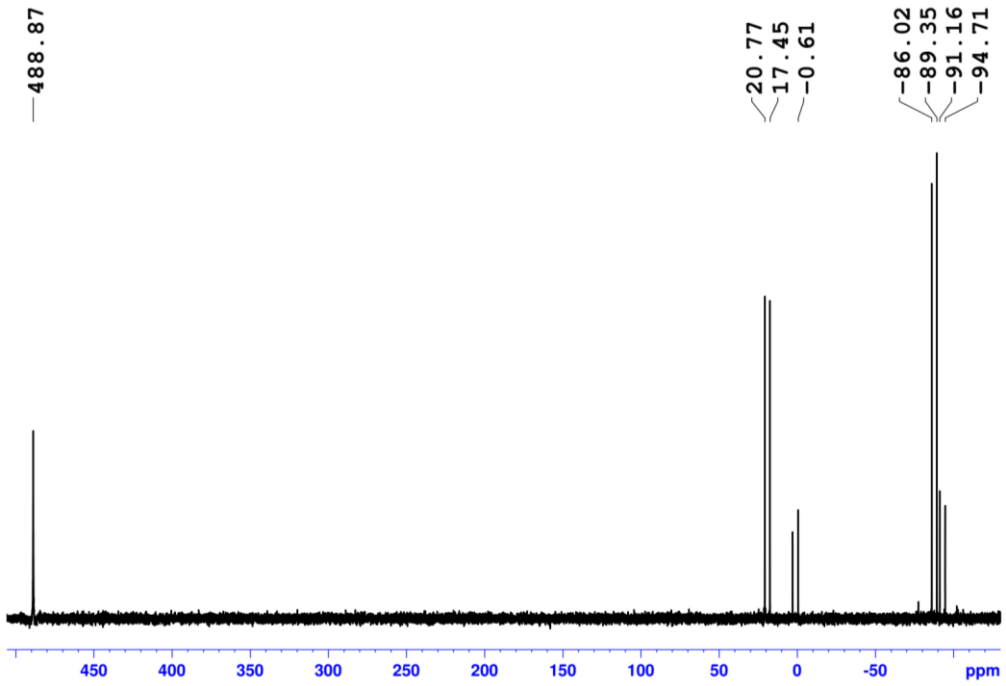


Figure S5. $^{31}P\{^{1}H\}$ NMR of 1:1 of **1** and **NHC^{iPrMe}** in tol-d_8 at 223 K.

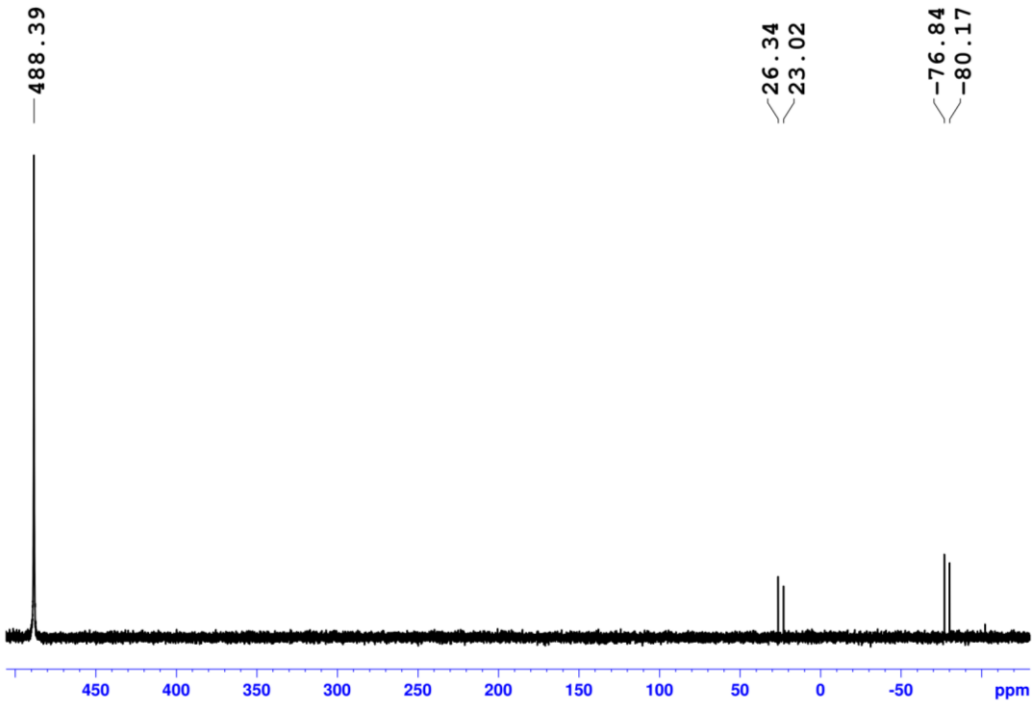


Figure S6. $^{31}P\{^{1}H\}$ NMR of 1:1 of **1** and **NHC^{iPr_2}** in tol-d_8 at 223 K.

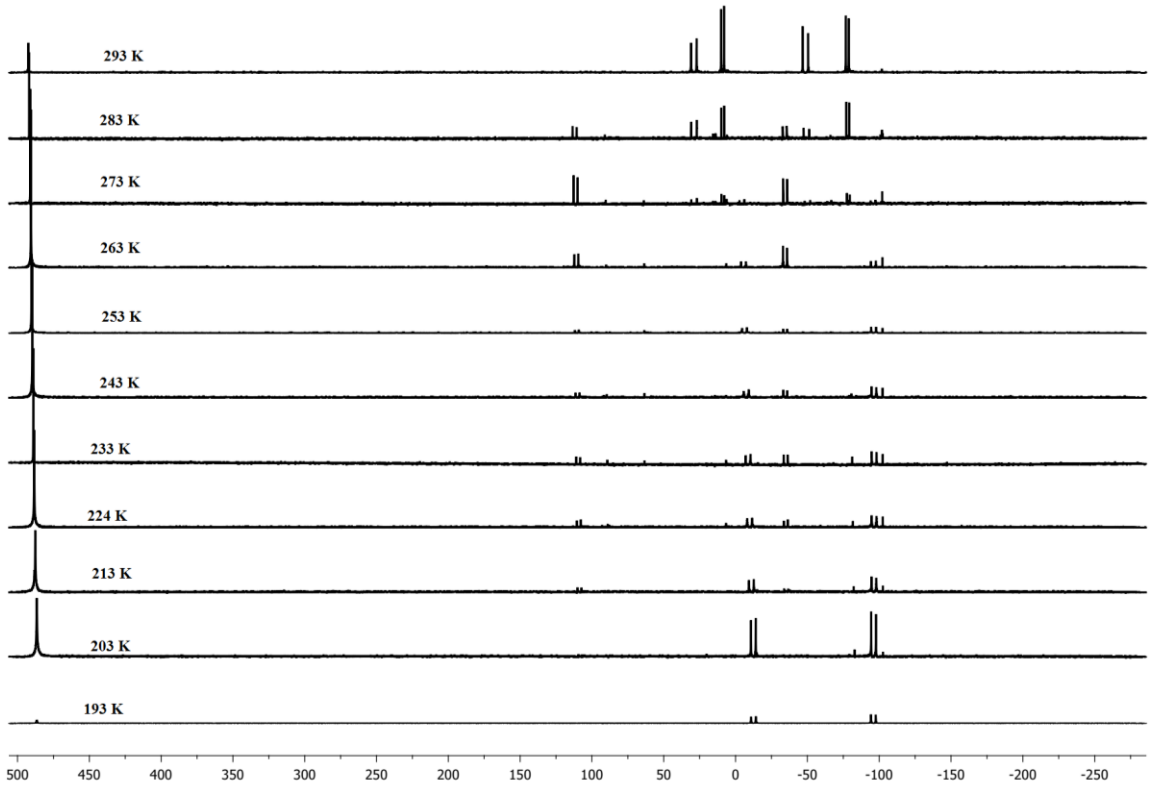


Figure S7. Variable temperature $^{31}P\{^{1}H\}$ NMR spectra from the 1:1:1 reaction mixture of **1**, **NHC^{Me_4}**, and **H_2O** in Tol-d_8.

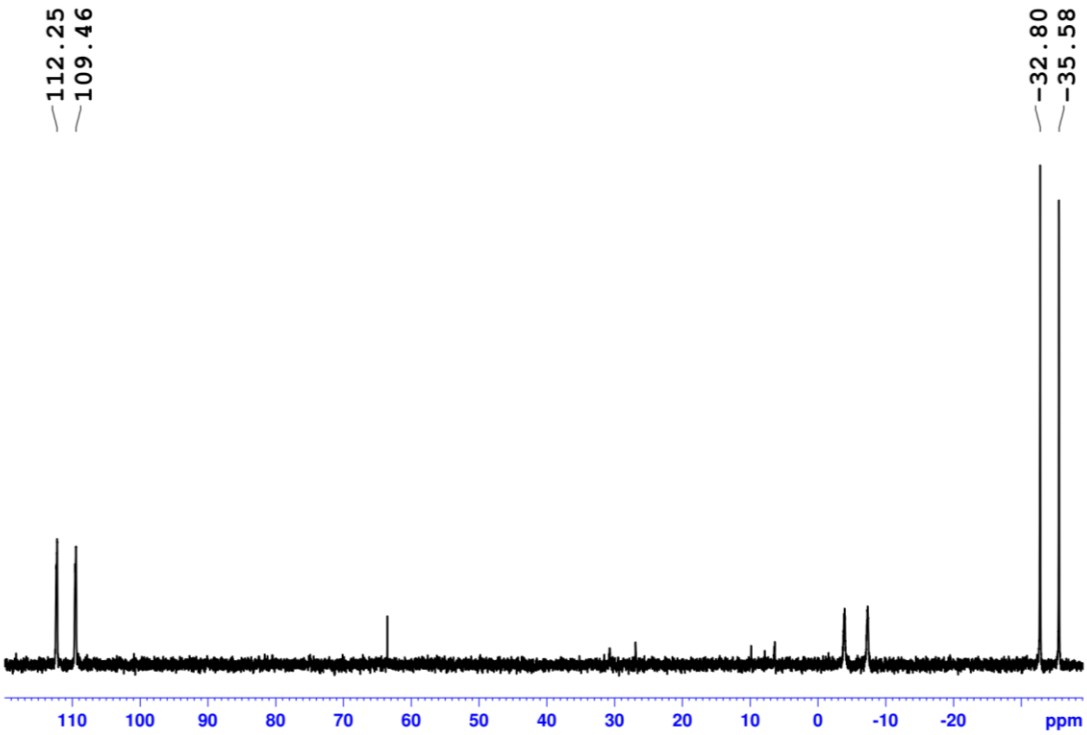


Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Me4}**, and **H_2O** at 263 K in Tol-d_8.

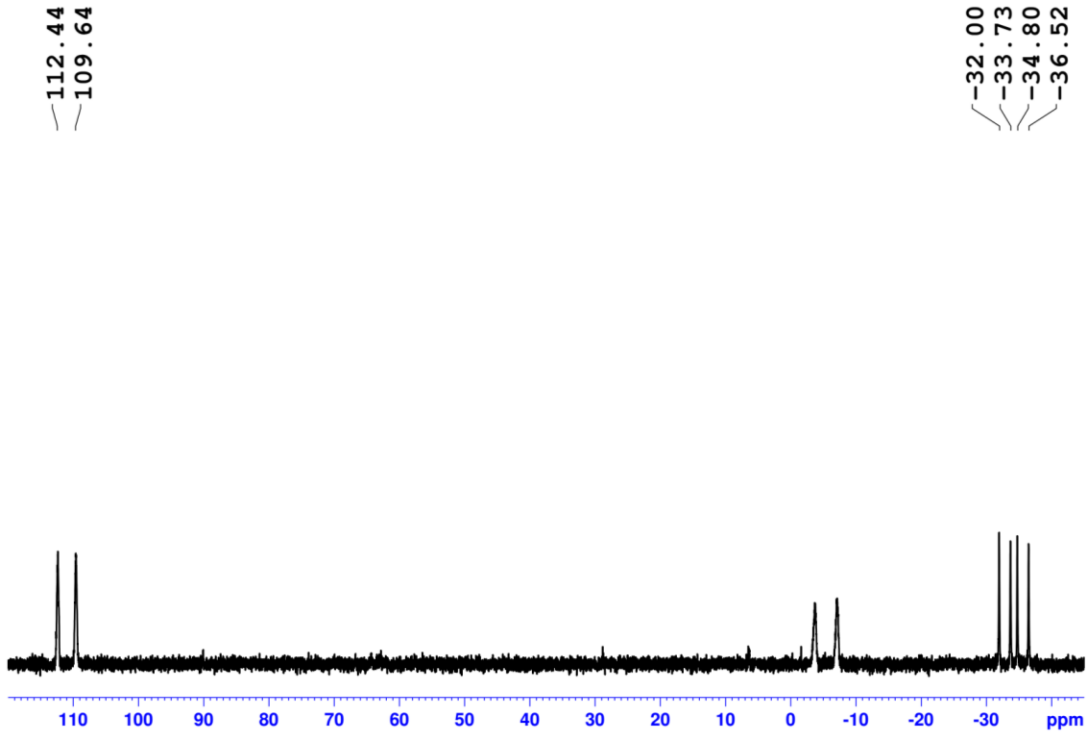


Figure S9. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Me4}**, and **H_2O** at 263 K in Tol-d_8.

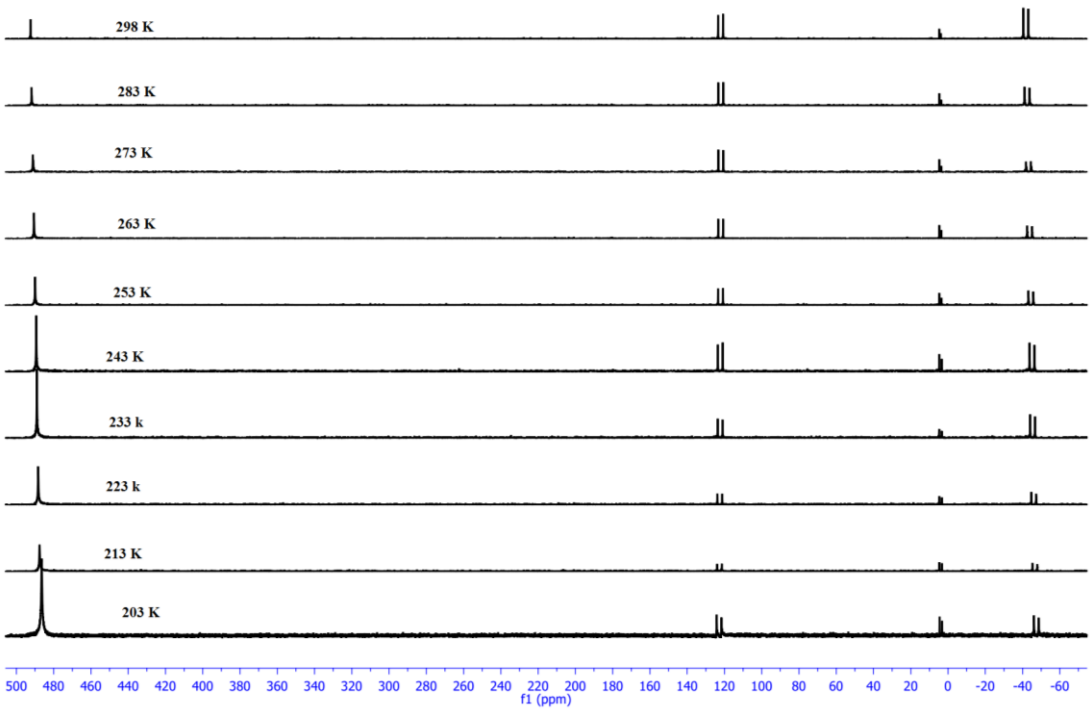


Figure S10. Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in Tol-d_8.

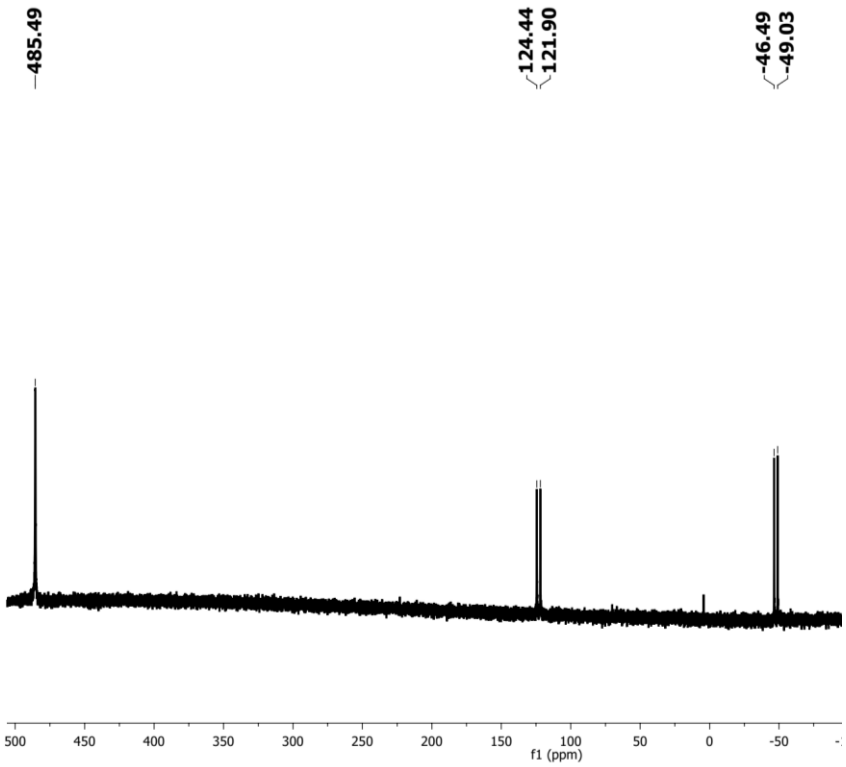


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** at 203 K in Tol-d_8.

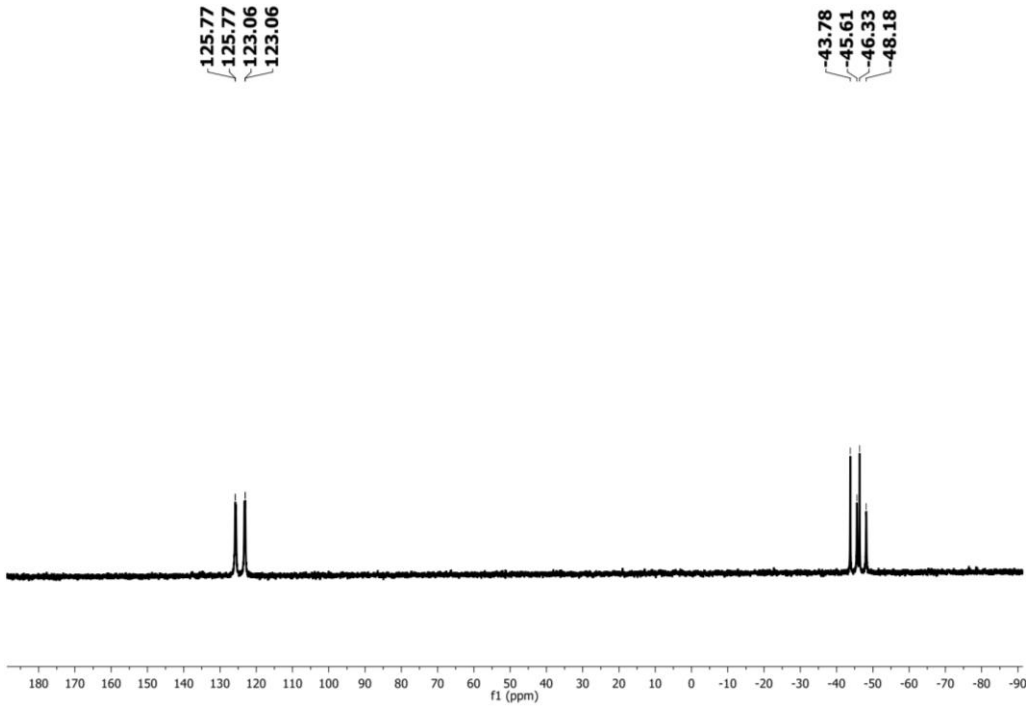


Figure S12. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** at 203 K in Tol-d_8.

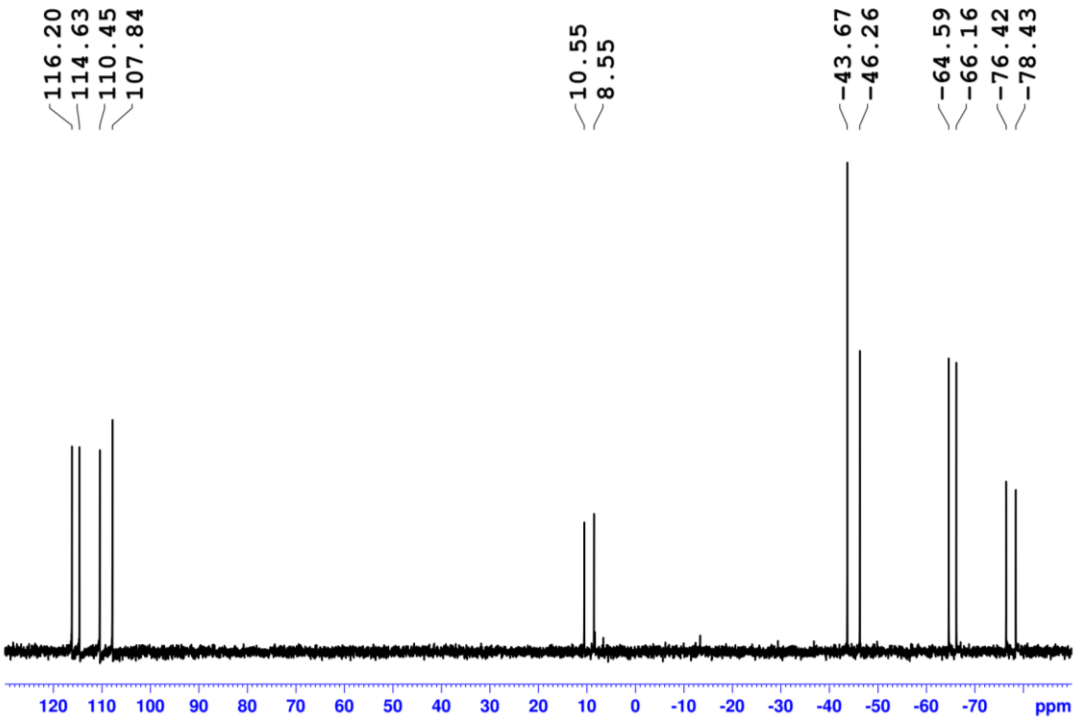


Figure S13. ^{31}P{^{1}H} NMR spectrum of reaction mixture of 1:1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, **H_2O** and **BPh_3** at RT in Tol-d_8.

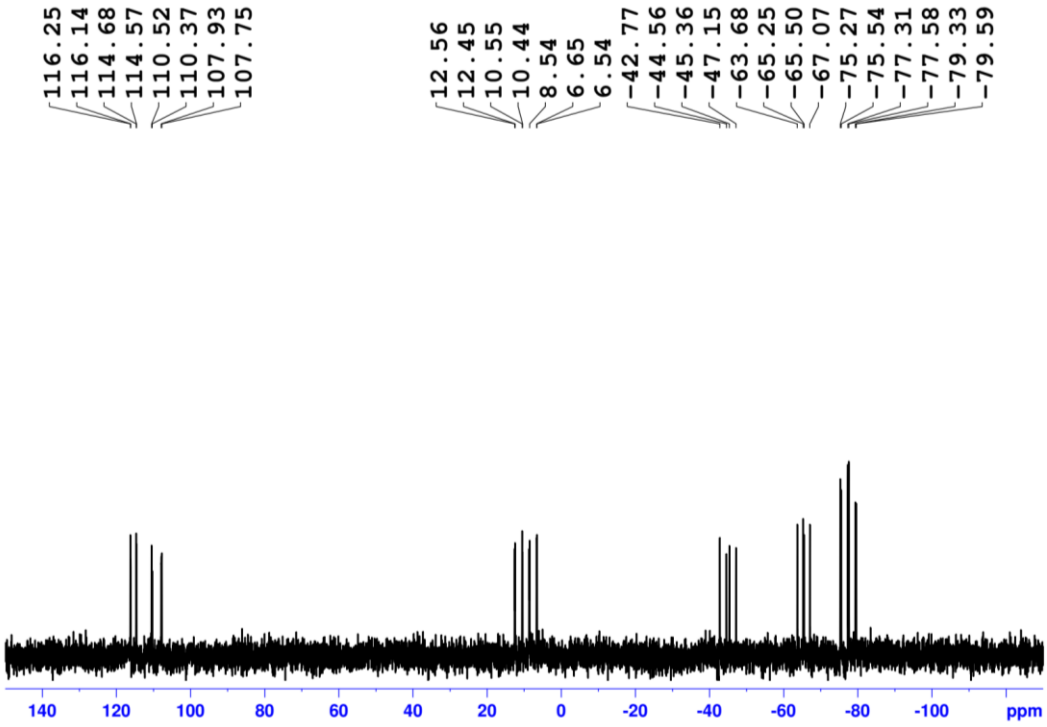


Figure S14. ^{31}P NMR spectrum of reaction mixture of 1:1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, **H_2O,** and **BPh_3** at RT in Tol-d_8.

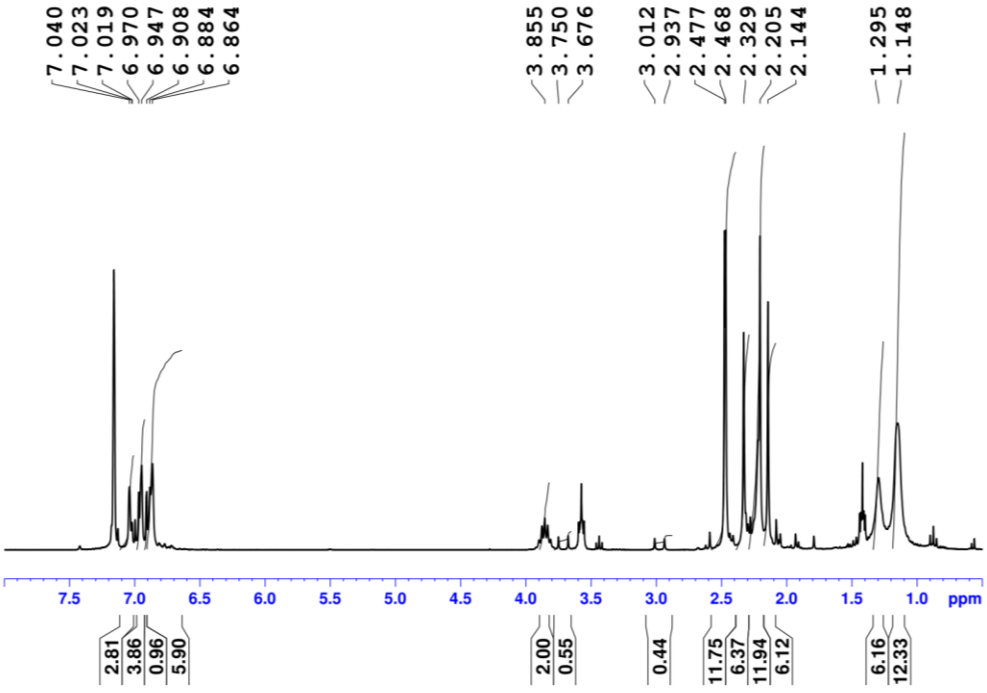


Figure S15. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in C_6D_6 at RT.

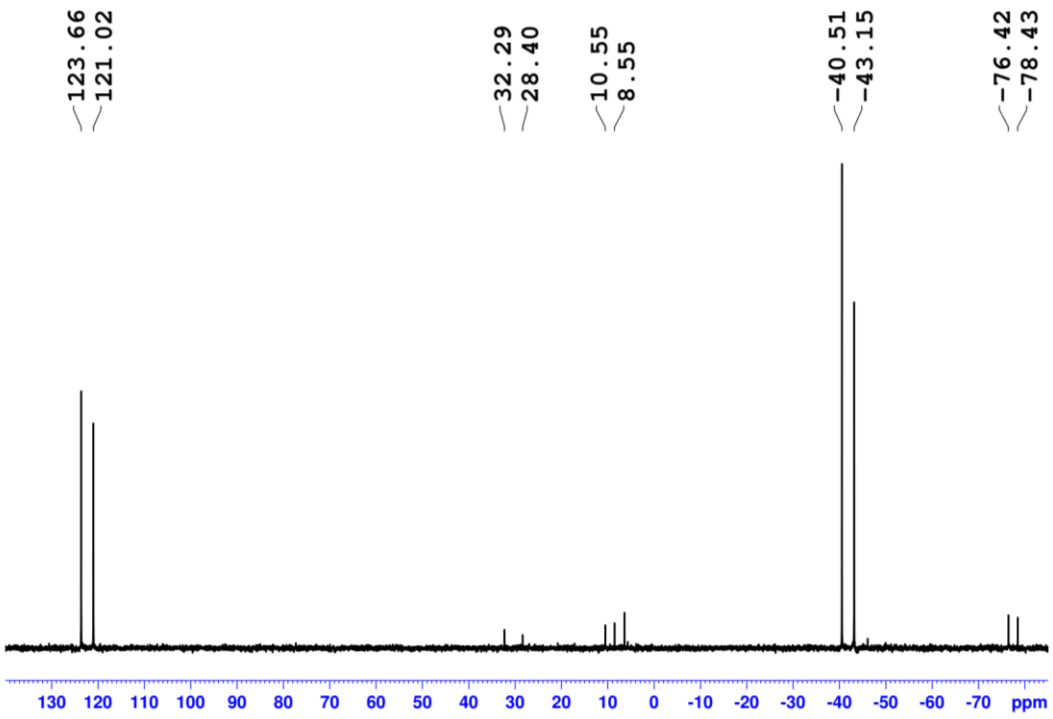


Figure S16. $^{31}P\{^{1}H\}$ NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in C_6D_6 at RT.

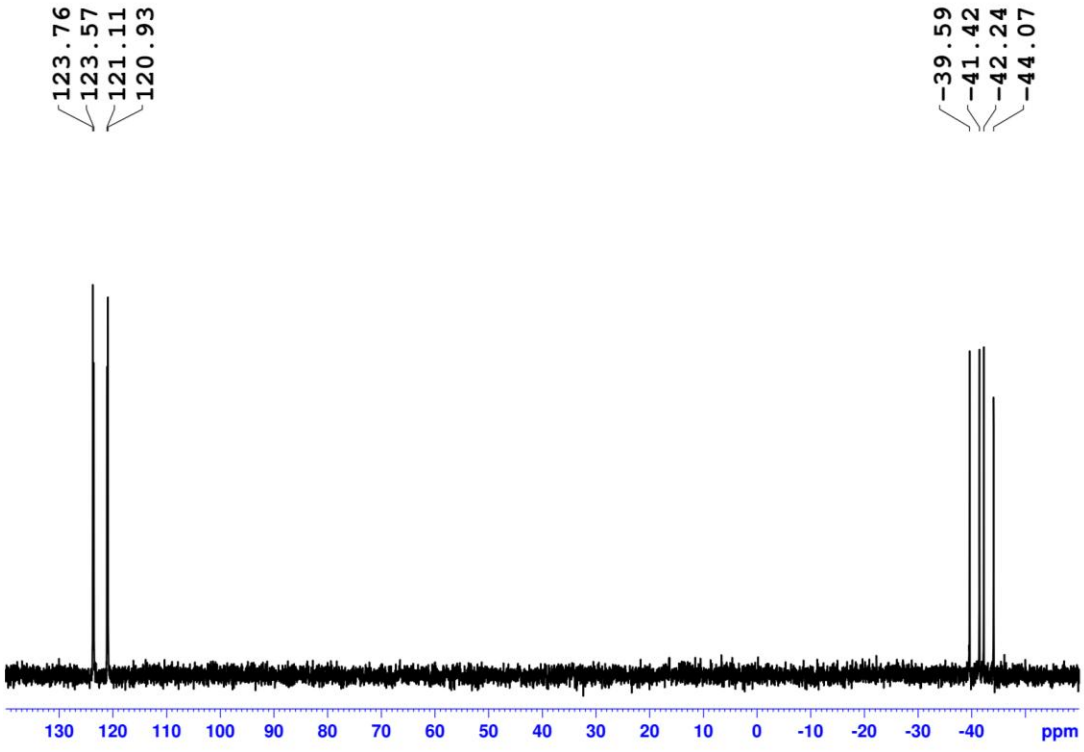


Figure S17. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in C_6D_6 at RT.

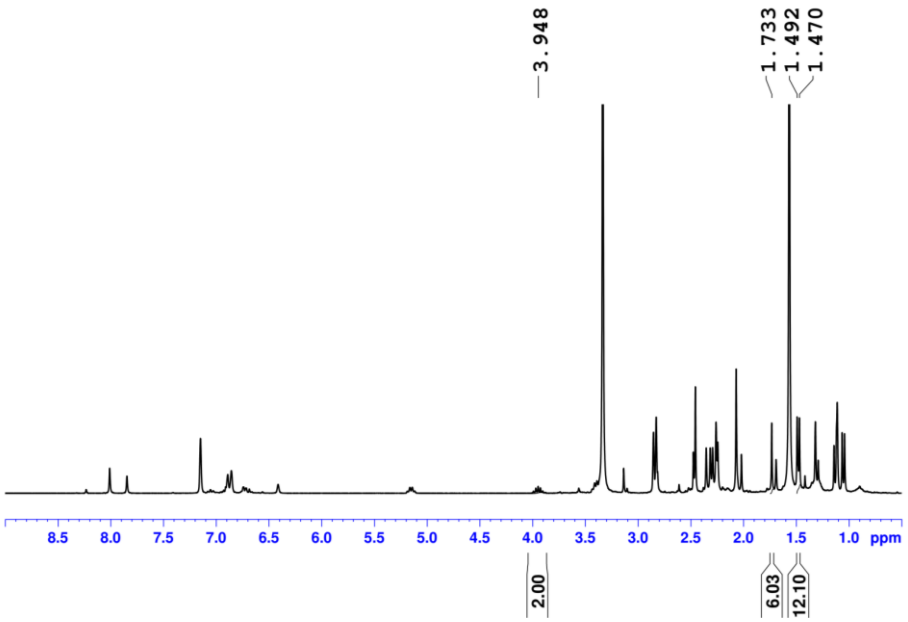


Figure S18. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** and excess **NHC ^{Me_4}** (10 equivalent) in C_6D_6 at RT.

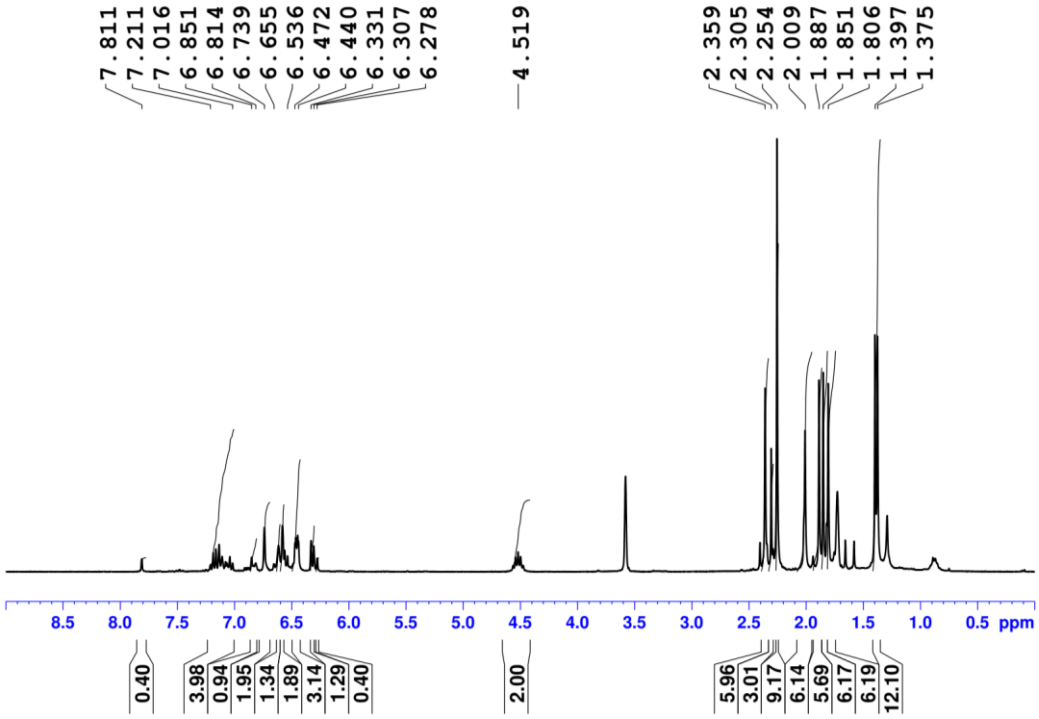


Figure S19. ^{1}H NMR of spectrum crystalline products, **4·NHC^{iPr_2Me_2}** (mostly contained **4·NHC^{iPr_2Me_2}** along with small amounts of **2·NHC^{iPr_2Me_2}** and **3**) obtained from the 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in THF-d_8 at RT.

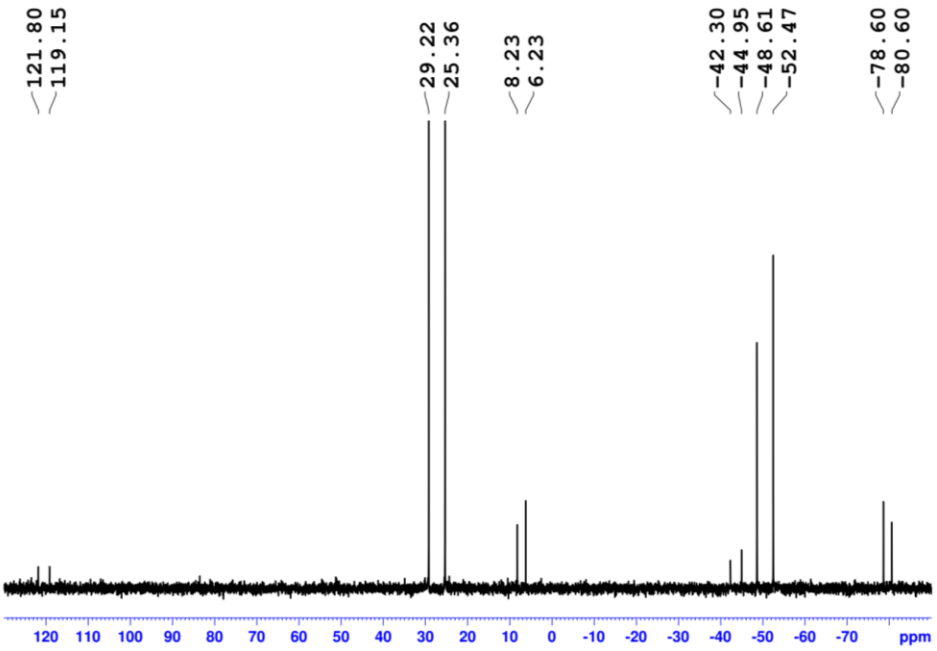


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of crystalline products **4·NHC^{iPr_2Me_2}** (mostly contained **4·NHC^{iPr_2Me_2}** along with small amounts of **2· NHC^{iPr_2Me_2}** and **3**) obtained from the 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in THF-d_8 at RT.

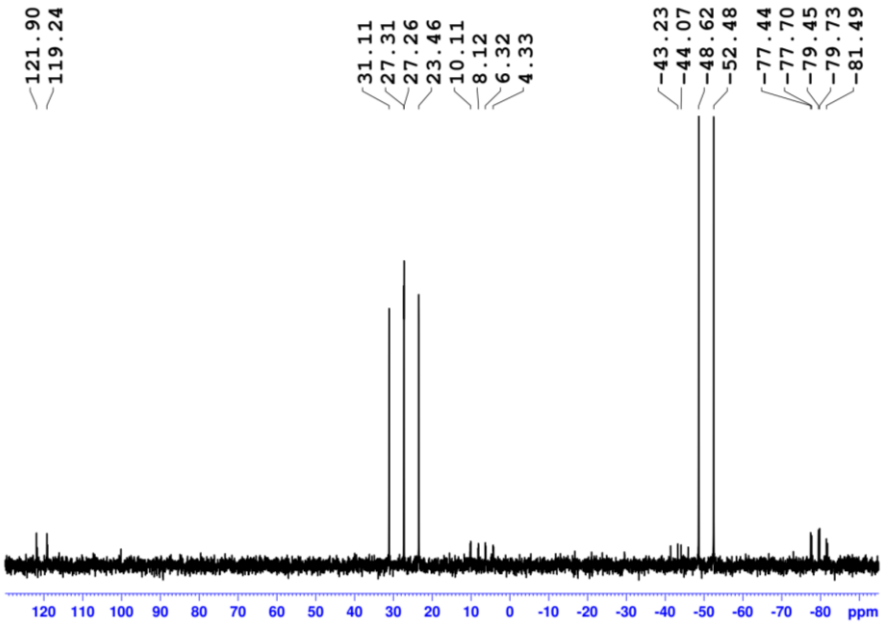


Figure S21. ^{31}P NMR spectrum of crystalline products **4·NHC^{iPr_2Me_2}** (mostly contained **4·NHC^{iPr_2Me_2}** along with small amounts of **2·NHC^{Me_2iPr_2}** and **23**) obtained from the 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in THF-d_8 at RT.

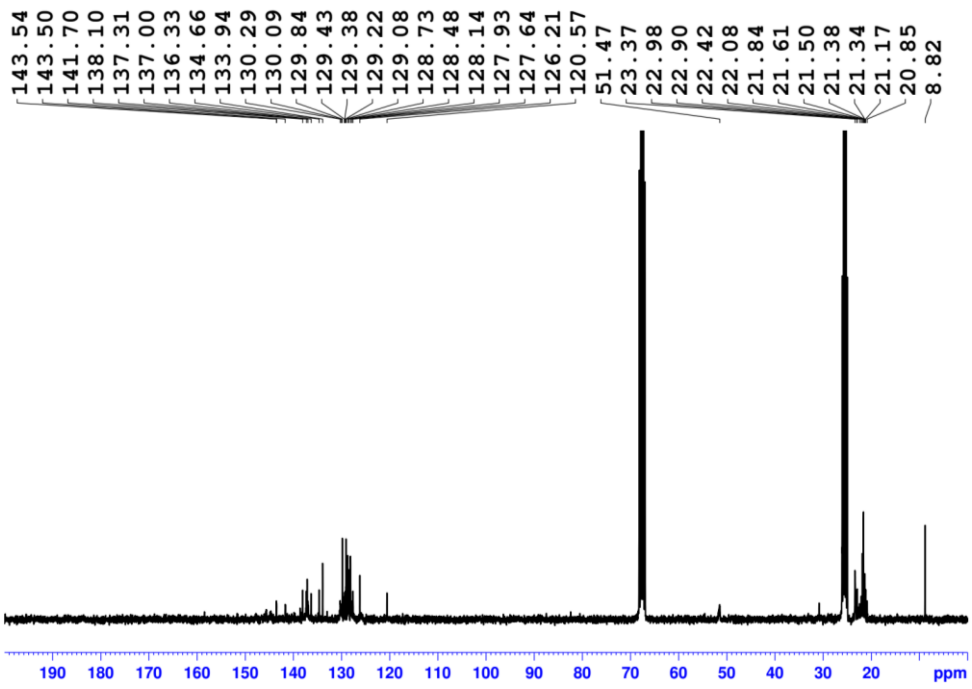


Figure S22. $^{13}C\{H\}$ NMR spectrum of crystalline products **4·NHC^{iPr_2Me_2}** (mostly contained **4·NHC^{iPr_2Me}** along with small amounts of **2· NHC^{iPr_2Me}** and **3**) obtained from the 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in THF-d_8 at RT.

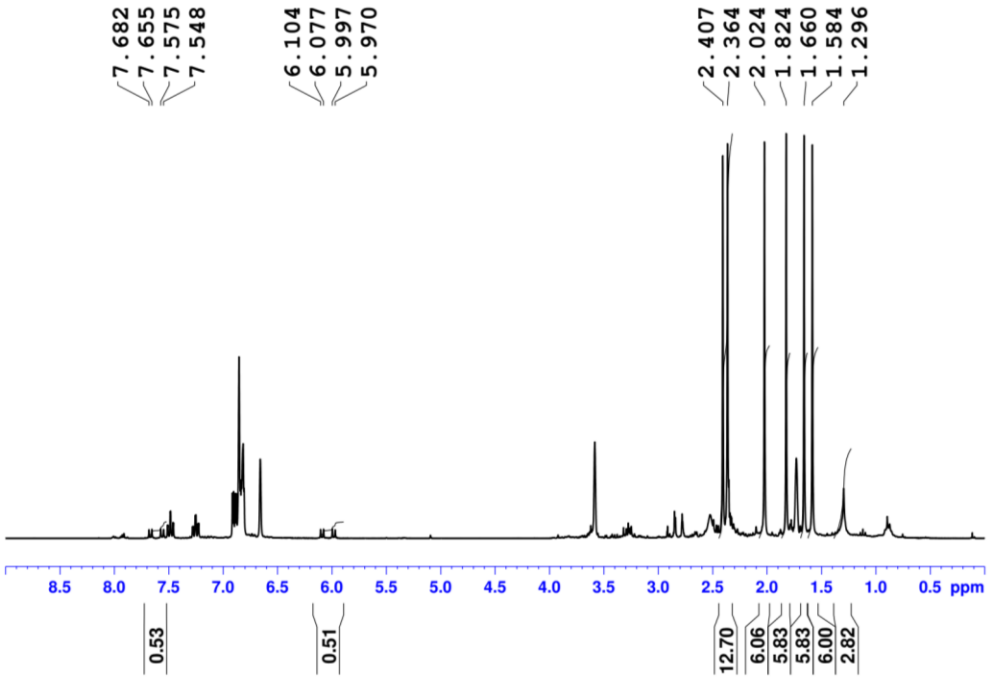


Figure S23. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Me_2}**, and **H_2O** in THF-d_8 at RT.

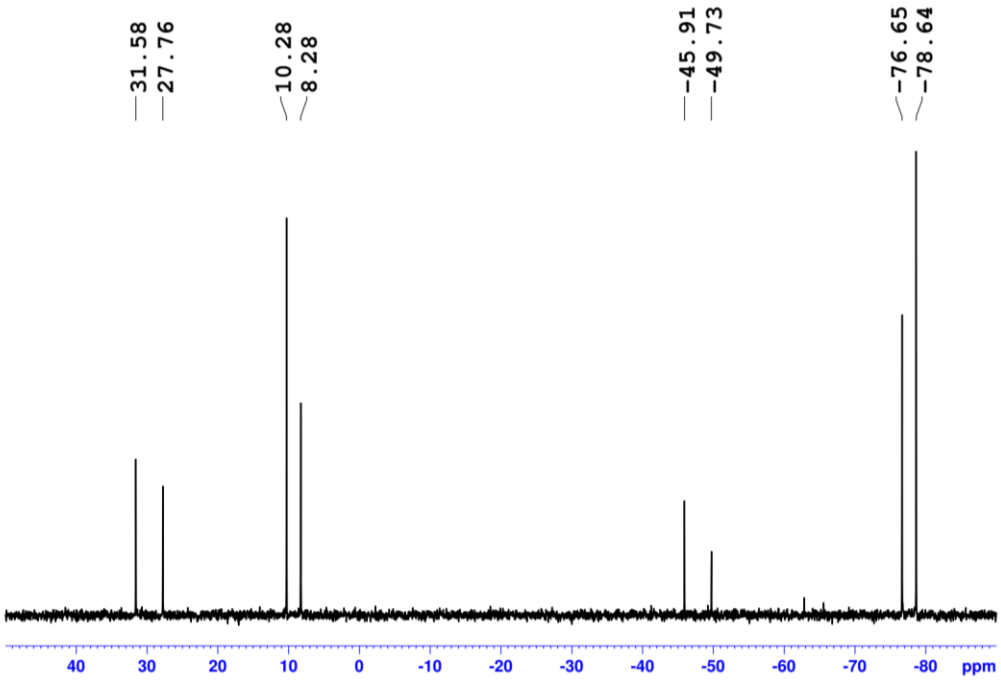


Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Me_2}**, and **H_2O** in THF-d_8 at RT.

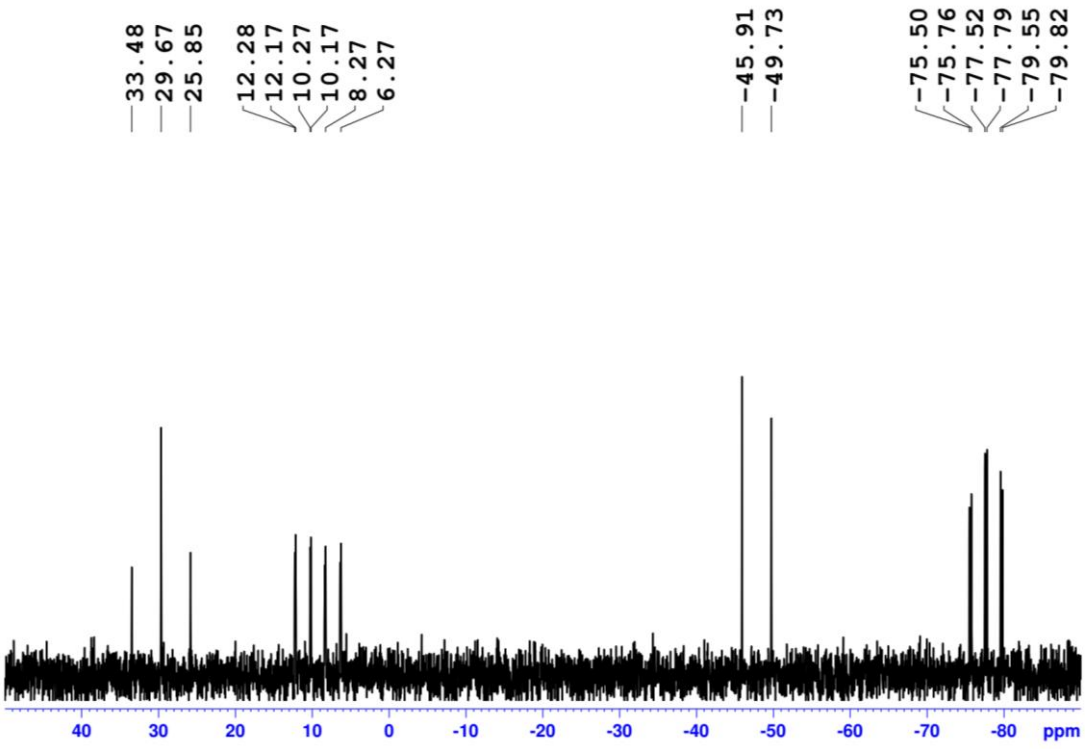


Figure S25. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Me_2}**, and **H_2O** in THF-d_8 at RT.

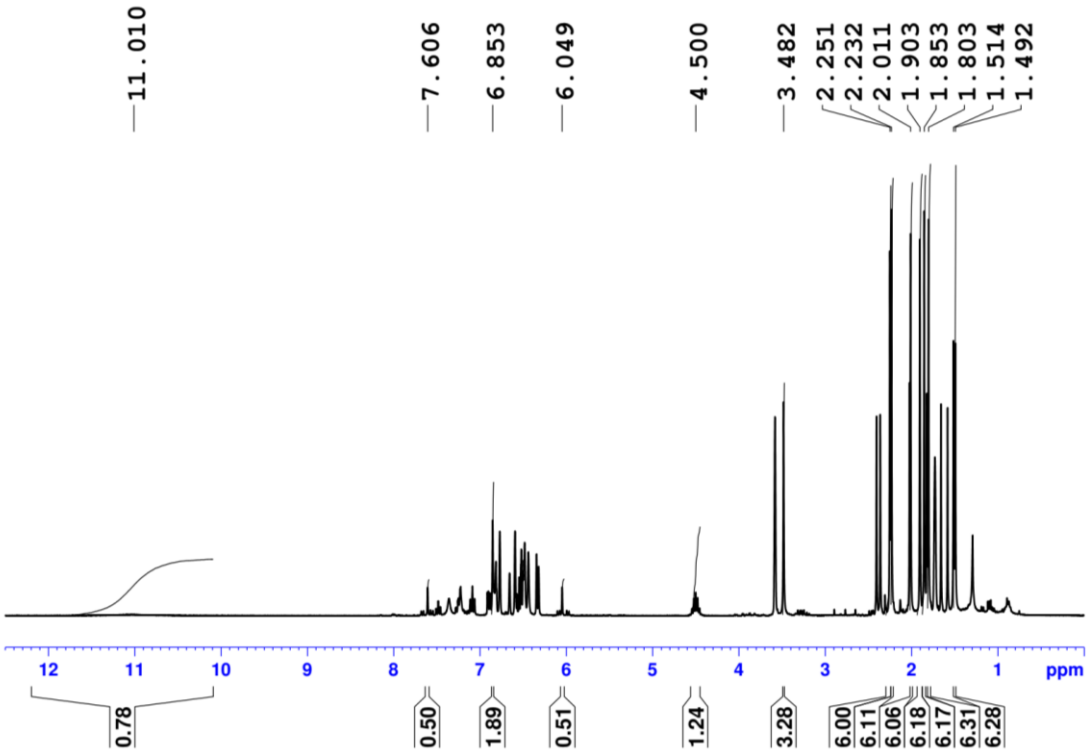


Figure S26. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPrMe}**, and **H_2O** in THF-d_8 at RT.

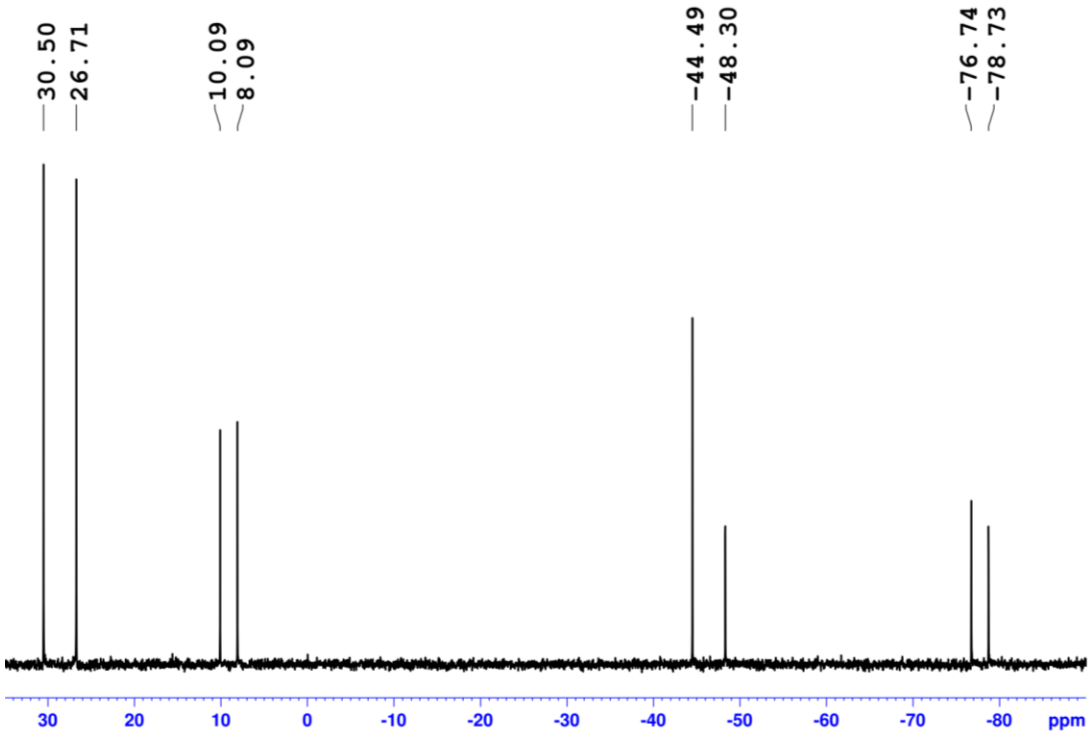


Figure S27. ^{31}P{^{1}H} NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPrMe}**, and **H_2O** in THF-d_8 at RT.

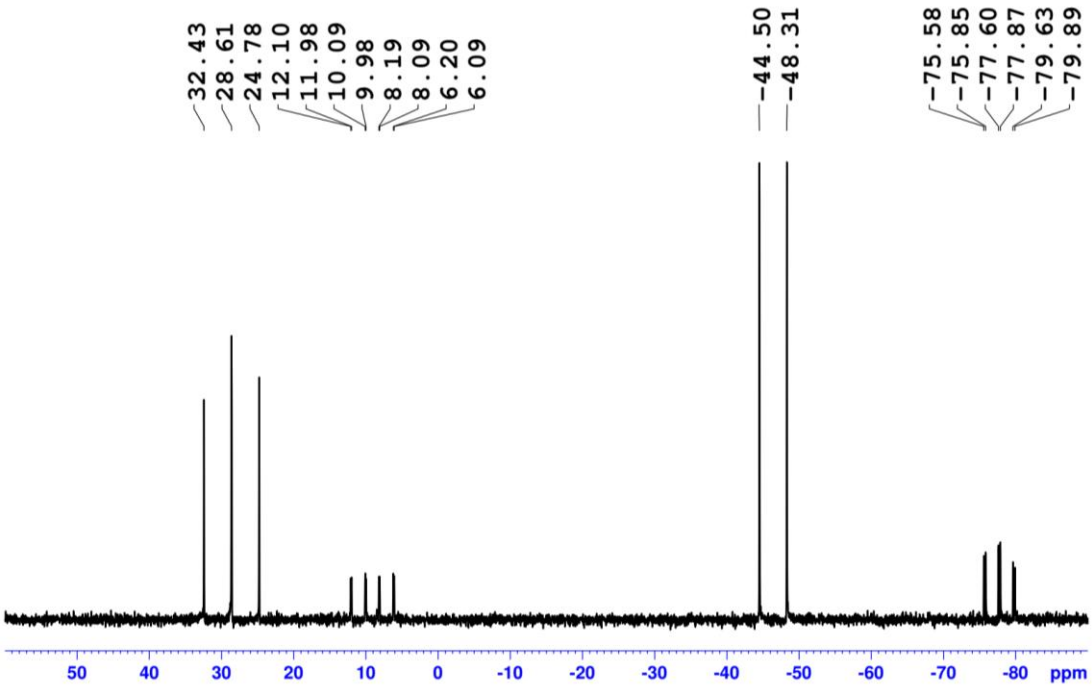


Figure S28. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPrMe}**, and **H_2O** in THF-d_8 at RT.

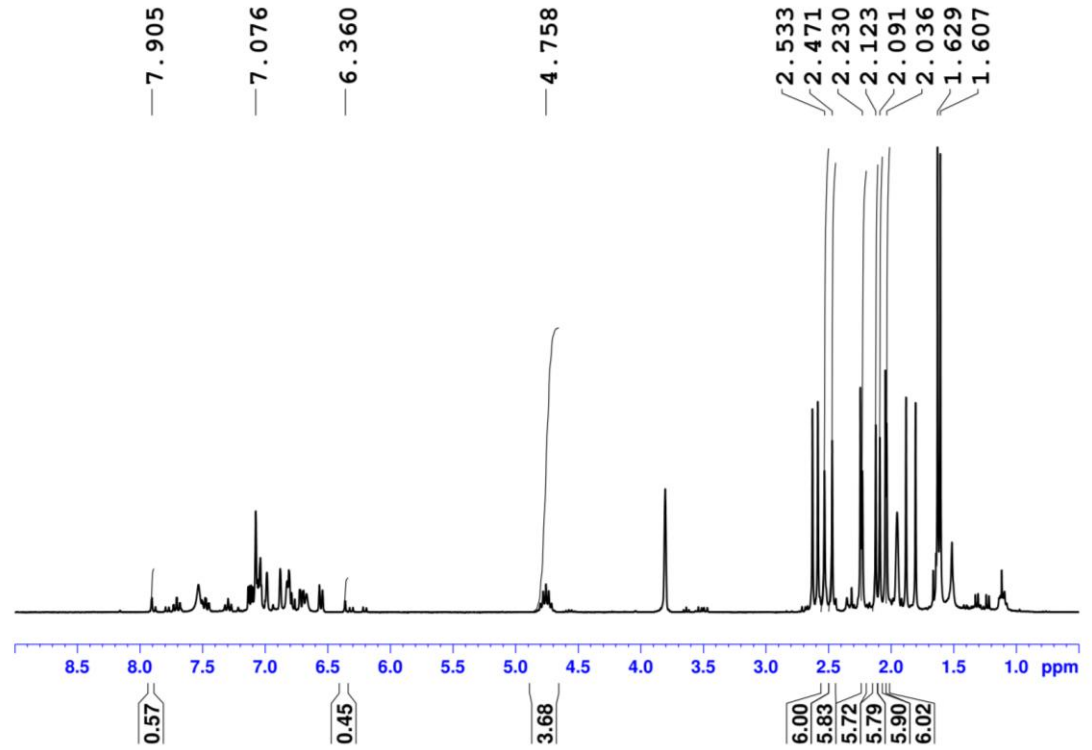


Figure S29. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr2}**, and **H_2O** in THF-d_8 at RT.

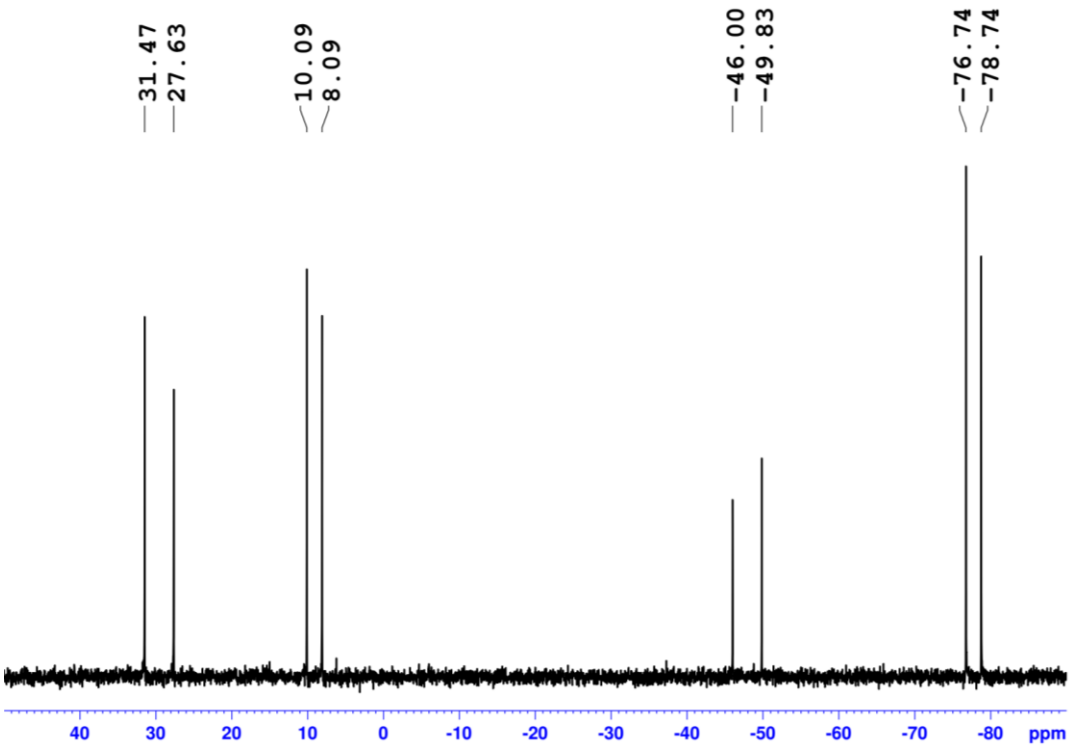


Figure S30. $^{31}P\{^{1}H\}$ NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2}**, and **H_2O** in THF-d_8 at RT.

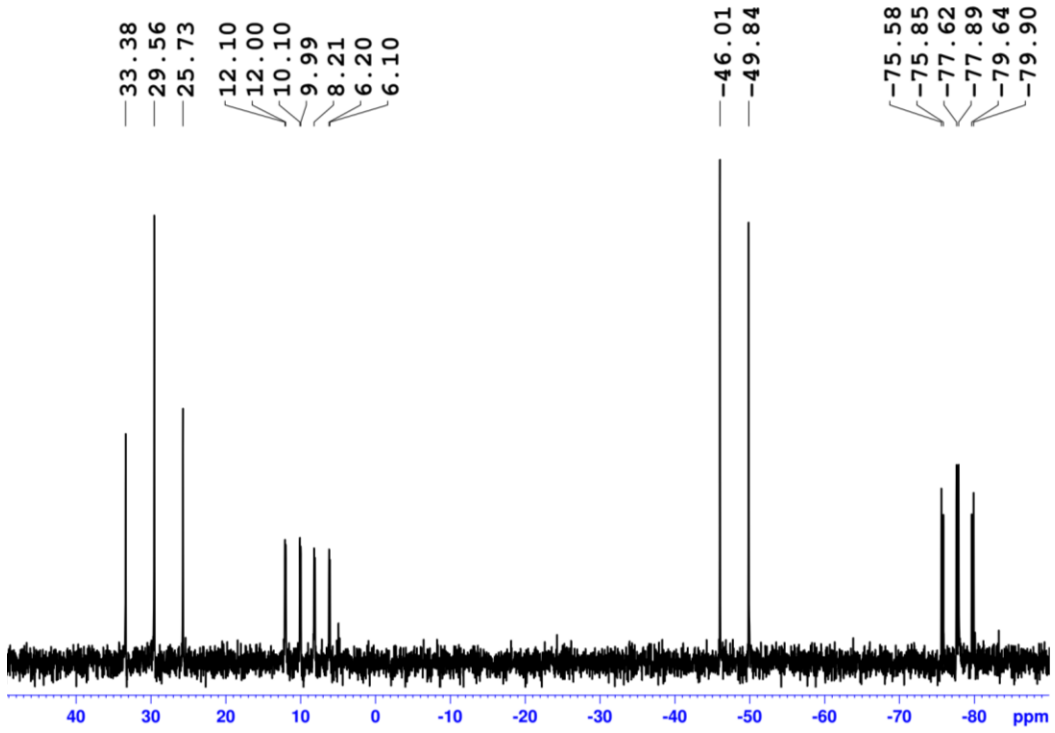


Figure S31. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{iPr_2}**, and **H_2O** in THF-d_8 at RT.

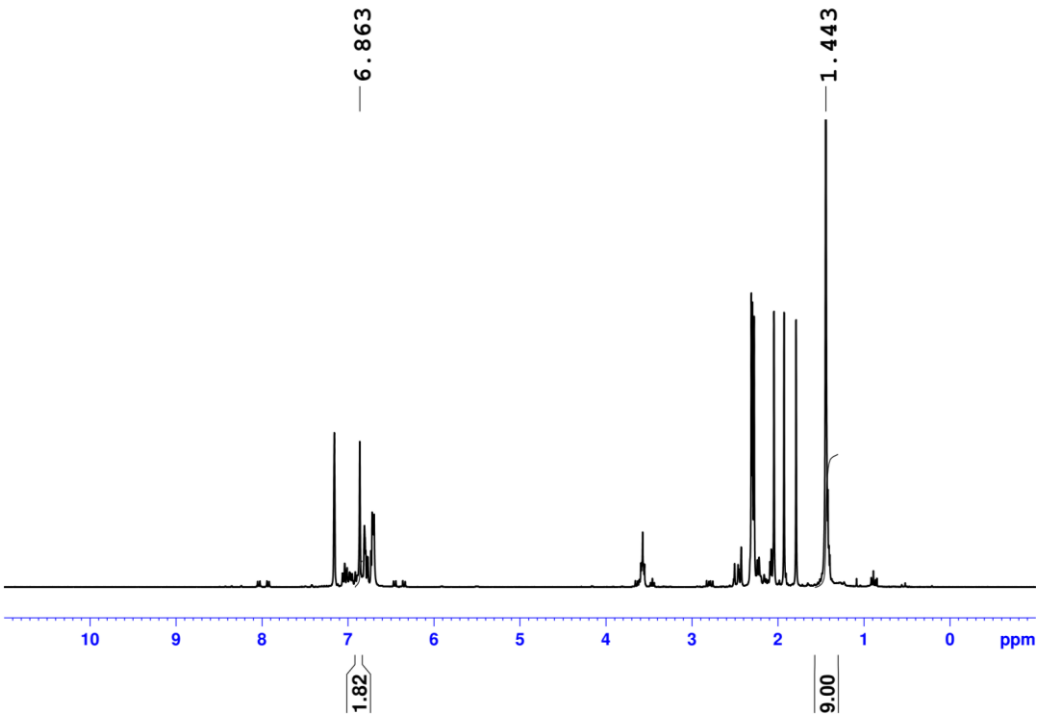


Figure S32. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{tBu2}**, and **H_2O** in C_6D_6 at RT.

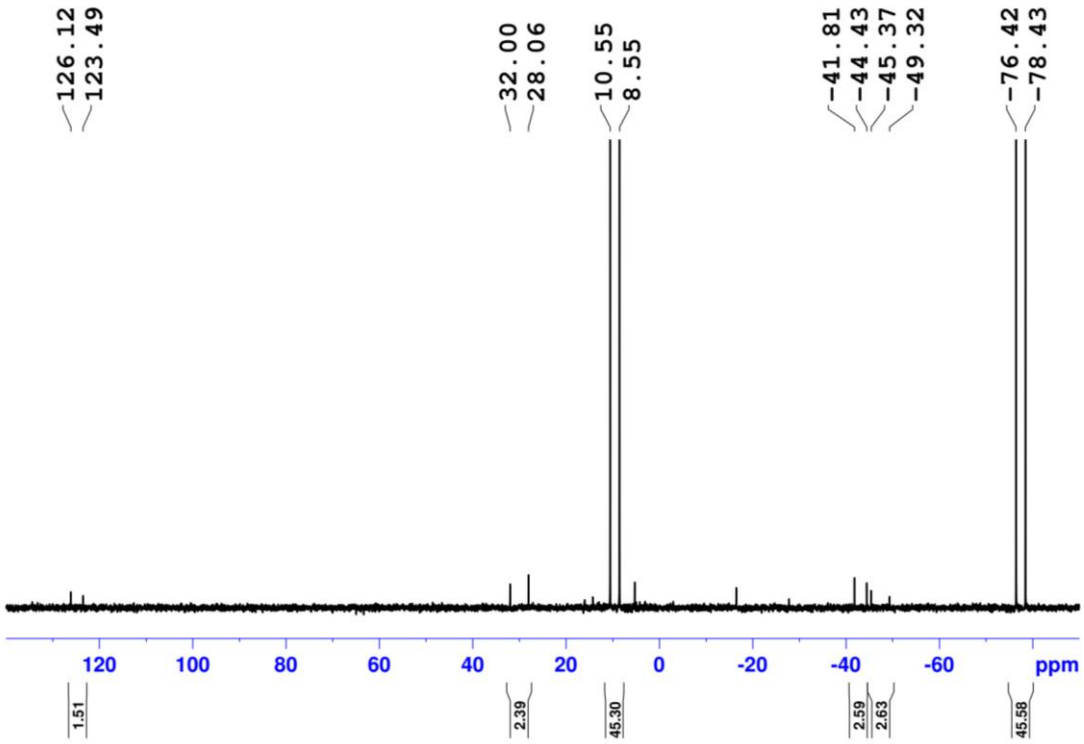


Figure S33. ^{31}P{^{1}H} NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{tBu2}**, and **H_2O** in C_6D_6 at RT.

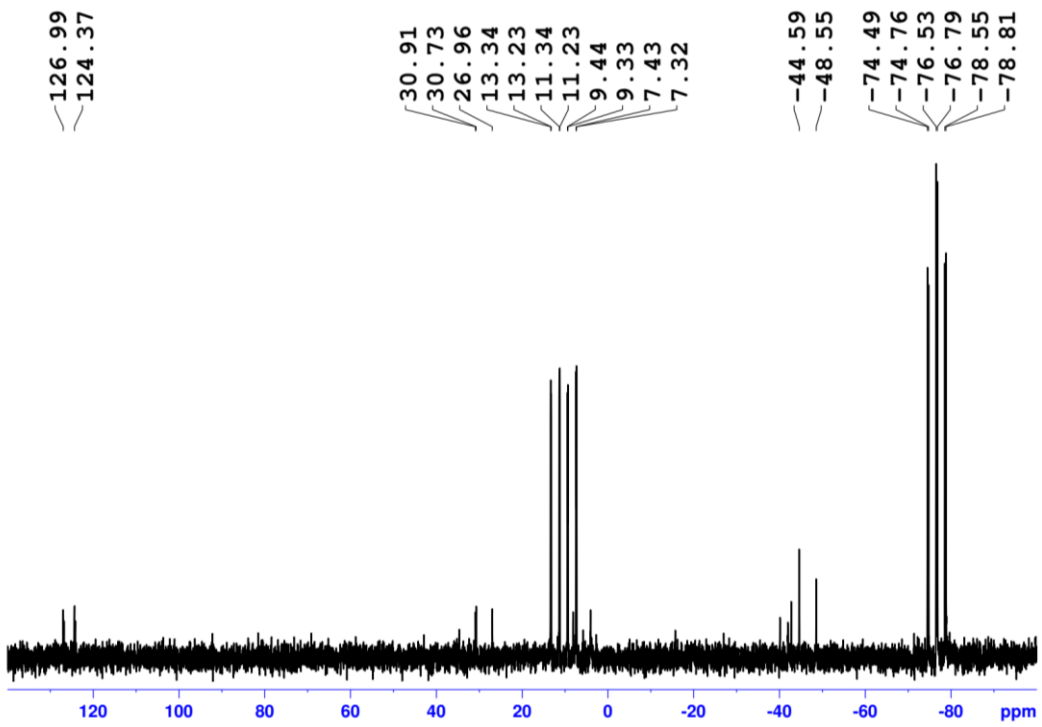


Figure S34. ^{31}P NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{tBu2}**, and **H_2O** in C_6D_6 at RT.

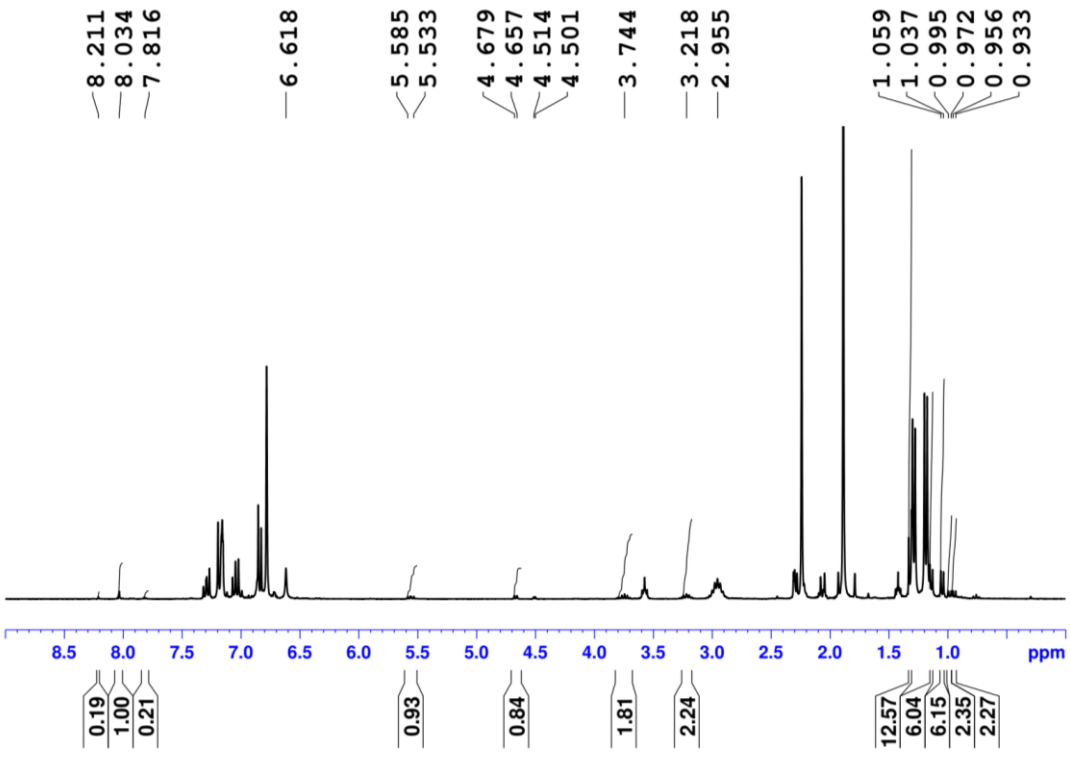


Figure S35. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Dip2}**, and **H_2O** in C_6D_6 at RT.

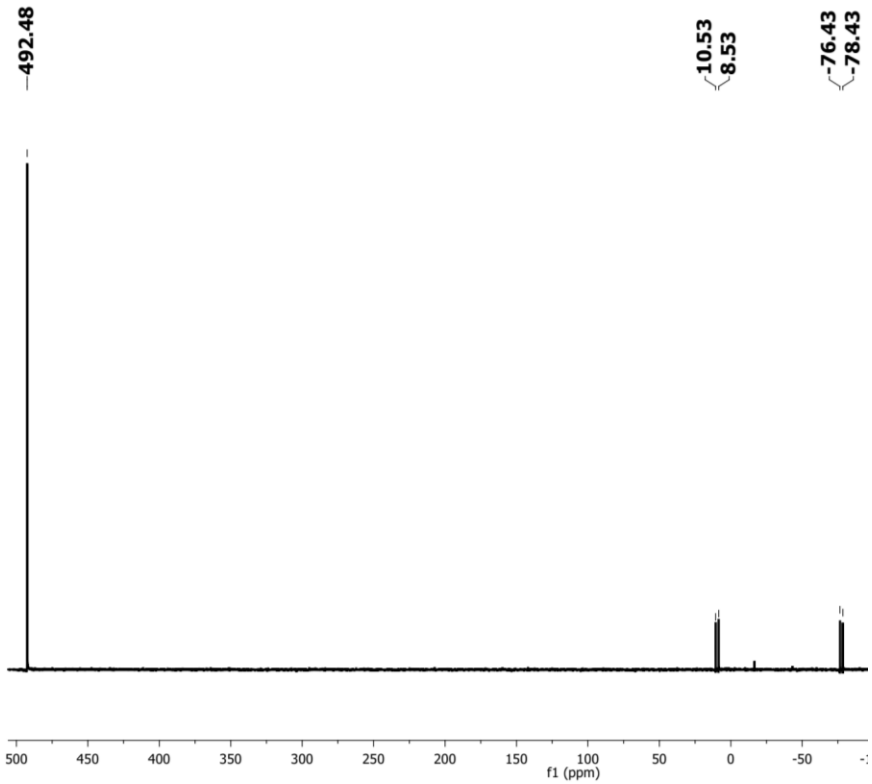


Figure S36. $^{31}P\{^{1}H\}$ NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Dip2}**, and **H_2O** in C_6D_6 at RT.

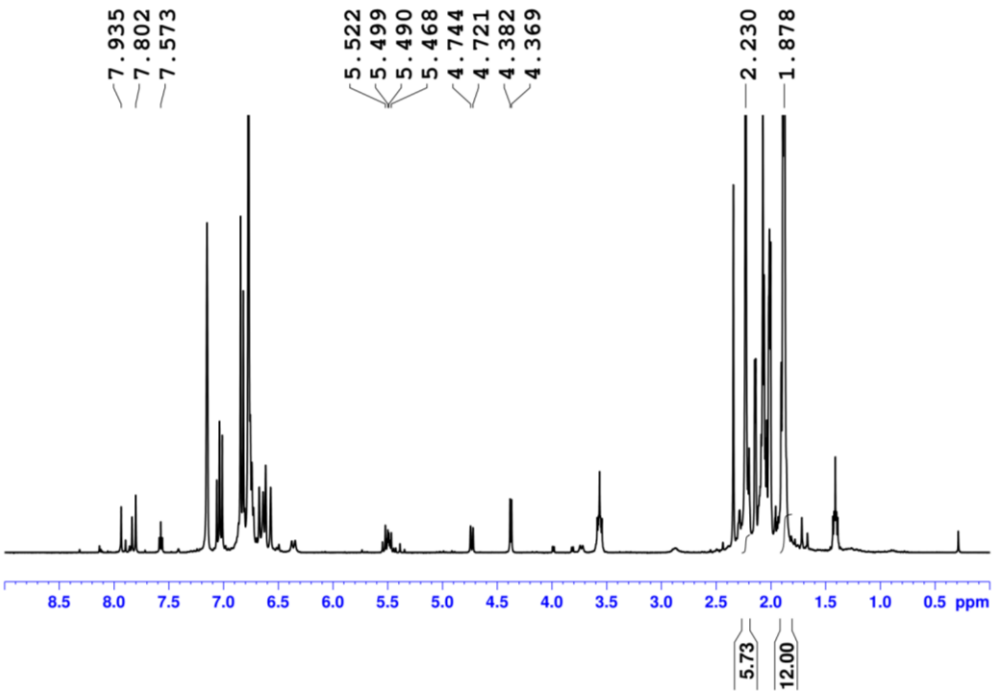


Figure S37. ^{1}H NMR spectrum of 1:1:1 reaction mixture of **1**, **NHC^{Mes2}**, and **H_2O** in C_6D_6 at RT.

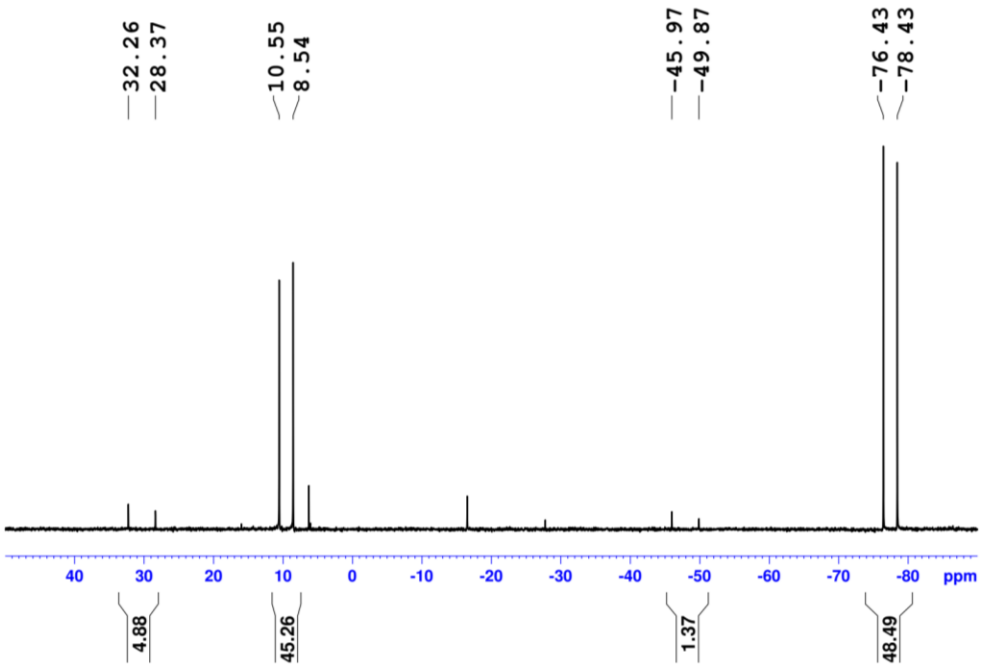


Figure S38. $^{31}P\{^{1}H\}$ NMR spectrum from the 1:1 reaction mixture of **1** and **H_2O** in presence of 10 mol% of **$NHC^{iPr_2Me_2}$** in THF/C_6D_6 at RT.

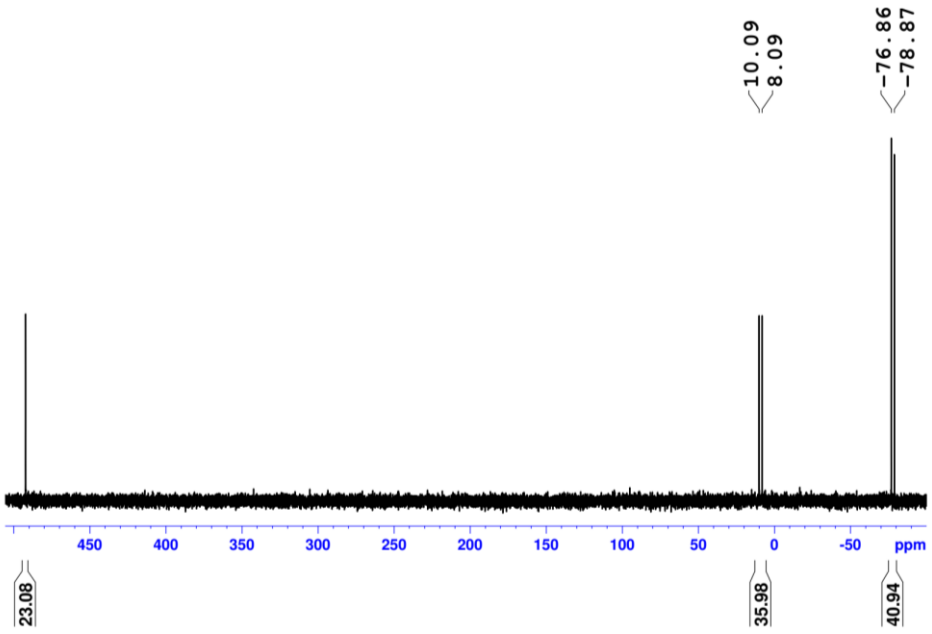


Figure S39. $^{31}P\{^{1}H\}$ NMR spectrum from the 1:1 reaction mixture of **1** and **H_2O** in presence of 10 mol% of **NHC^{Me_2}** in THF/C_6D_6 at RT.

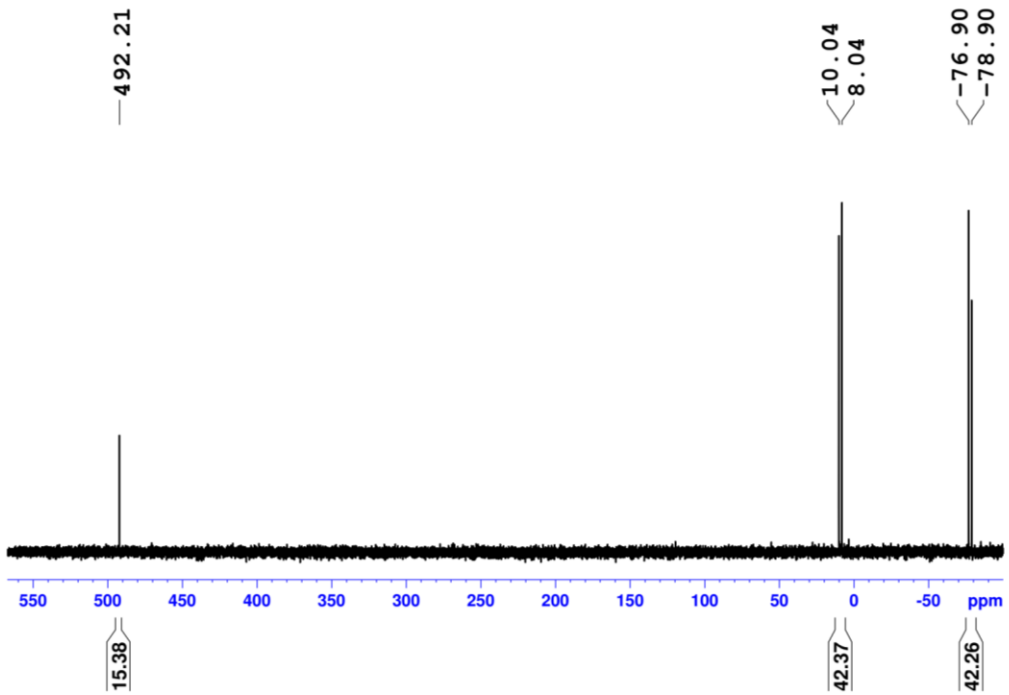


Figure S40. $^{31}P\{^{1}H\}$ NMR spectrum from the 1:1 reaction mixture of **1** and **H_2O** in presence of 10 mol% of **NHC^{iPrMe}** in THF/C_6D_6 at RT.

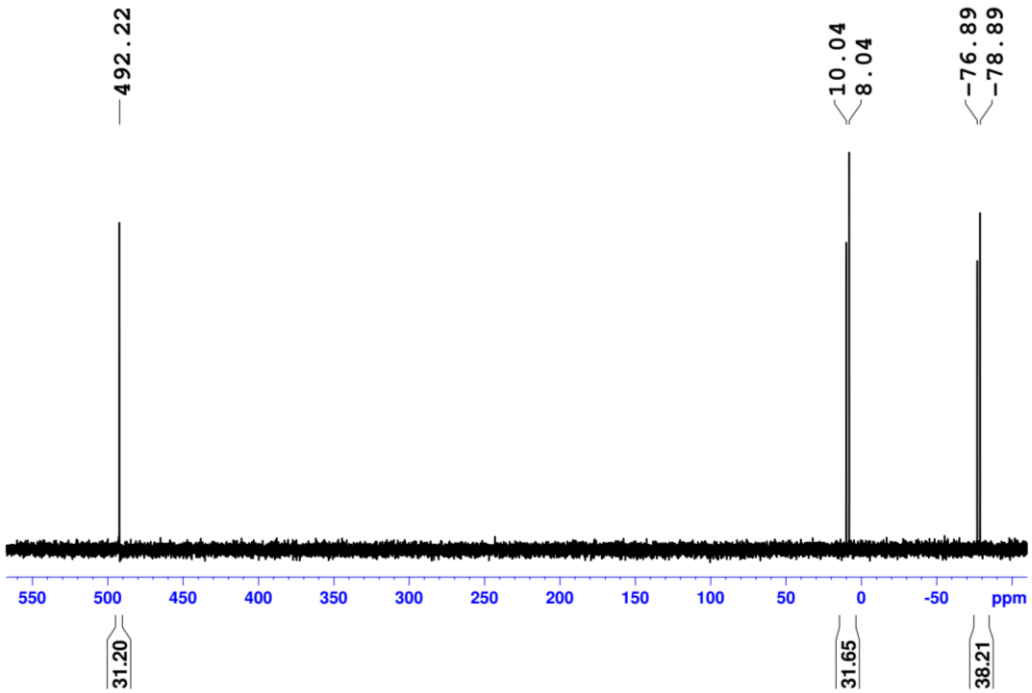


Figure 41. $^{31}P\{^{1}H\}$ NMR spectrum from the 1:1 reaction mixture of **1** and **H_2O** in presence of 10 mol% of **NHC^{iPr_2}** in THF/C_6D_6 at RT.

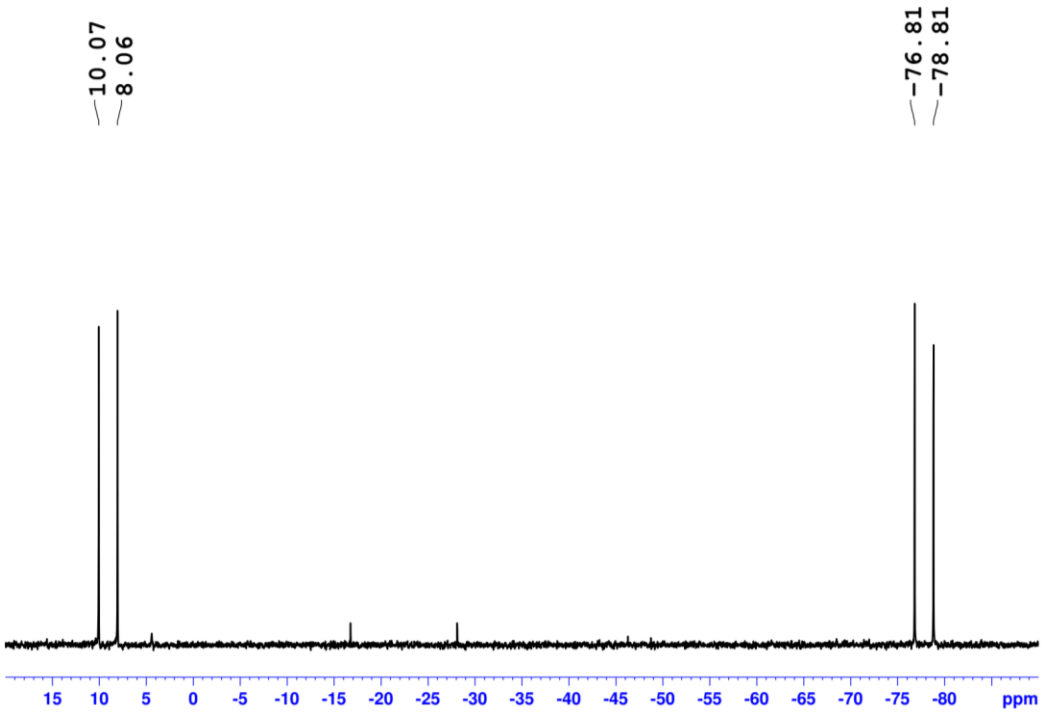


Figure S42. $^{31}P\{^{1}H\}$ NMR spectrum from the 1:1 reaction mixture of **1** and **H_2O** in presence of 10 mol% of **NHC^{tBu_2}** in THF/C_6D_6 at RT.

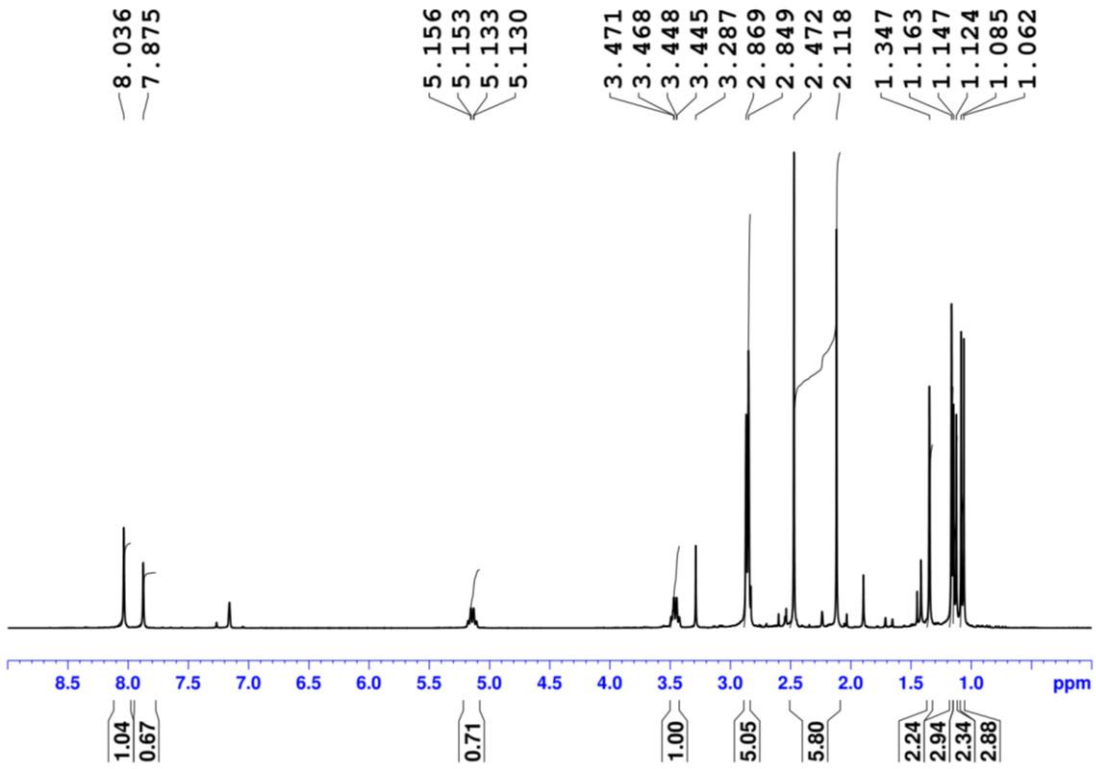


Figure S43. ^{1}H NMR spectrum of water hydrolysis of **NHC^{Me_4}** in C_6D_6 at RT.

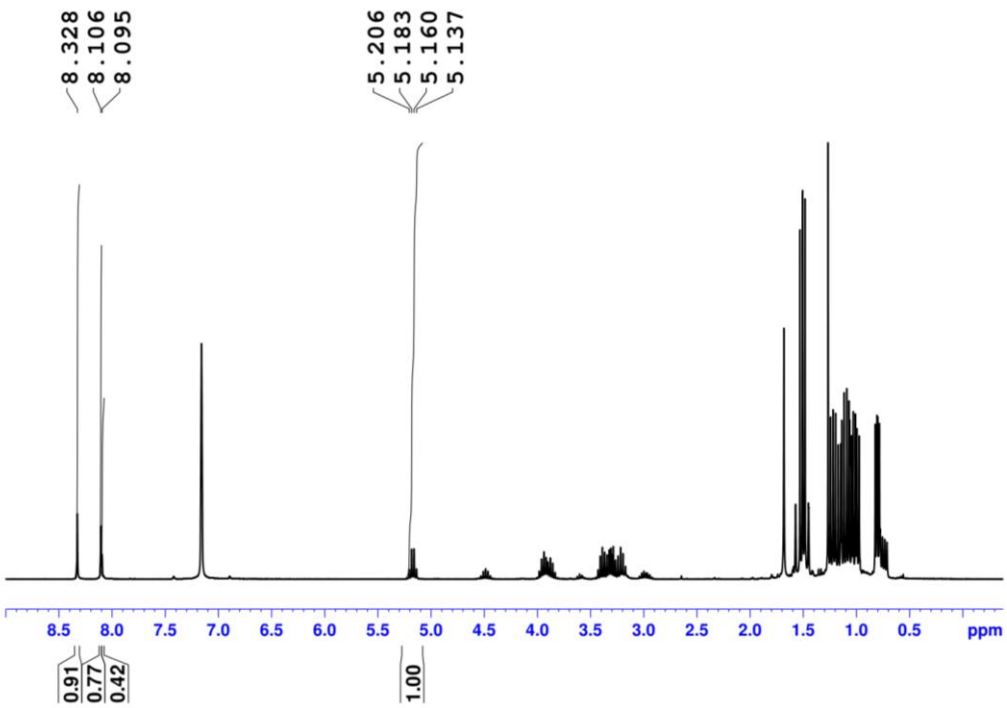


Figure S44. ^{1}H NMR spectrum of water hydrolysis of **NHC^{iPr_2Me_2}** in C_6D_6 at RT.

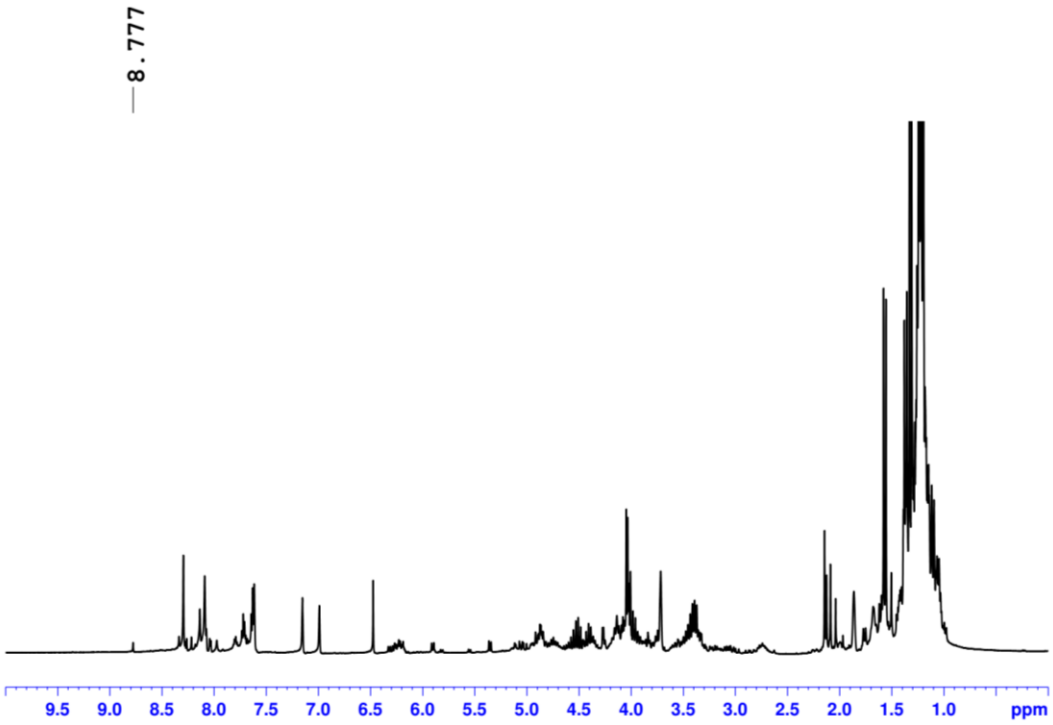


Figure S45. ^{1}H NMR spectrum of water hydrolysis of **NHC^{iPr_2}** in C_6D_6 at RT.

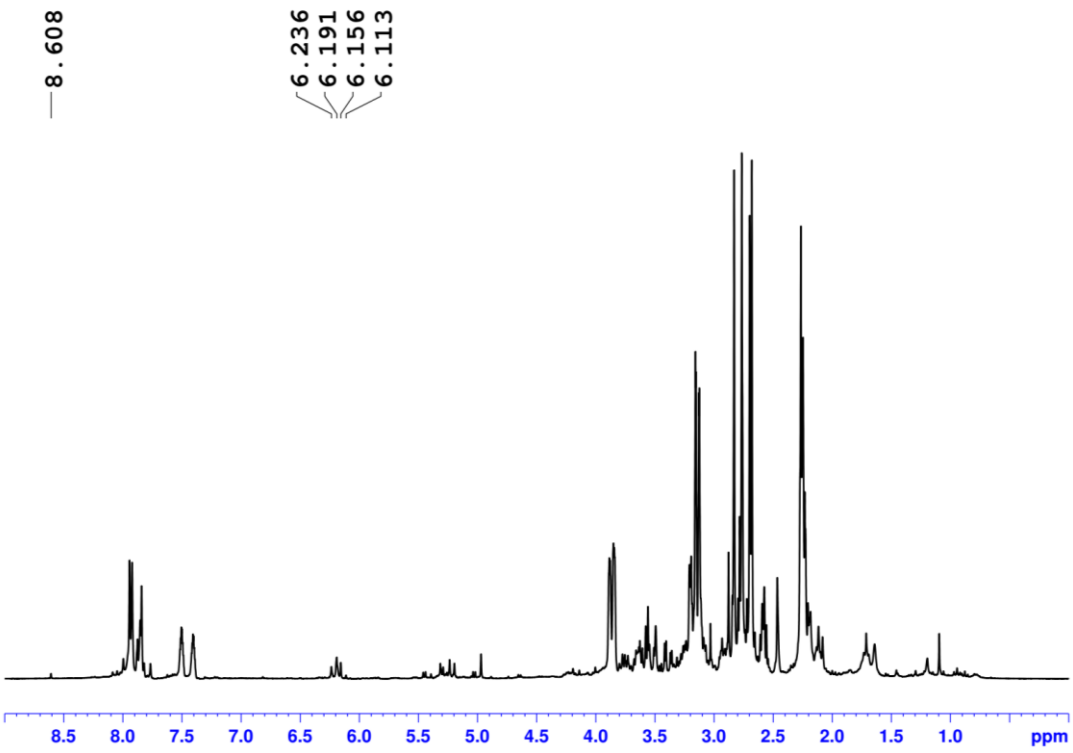


Figure S46. ^{1}H NMR spectrum of water hydrolysis of **NHC^{Me2}** in C_6D_6 at RT.

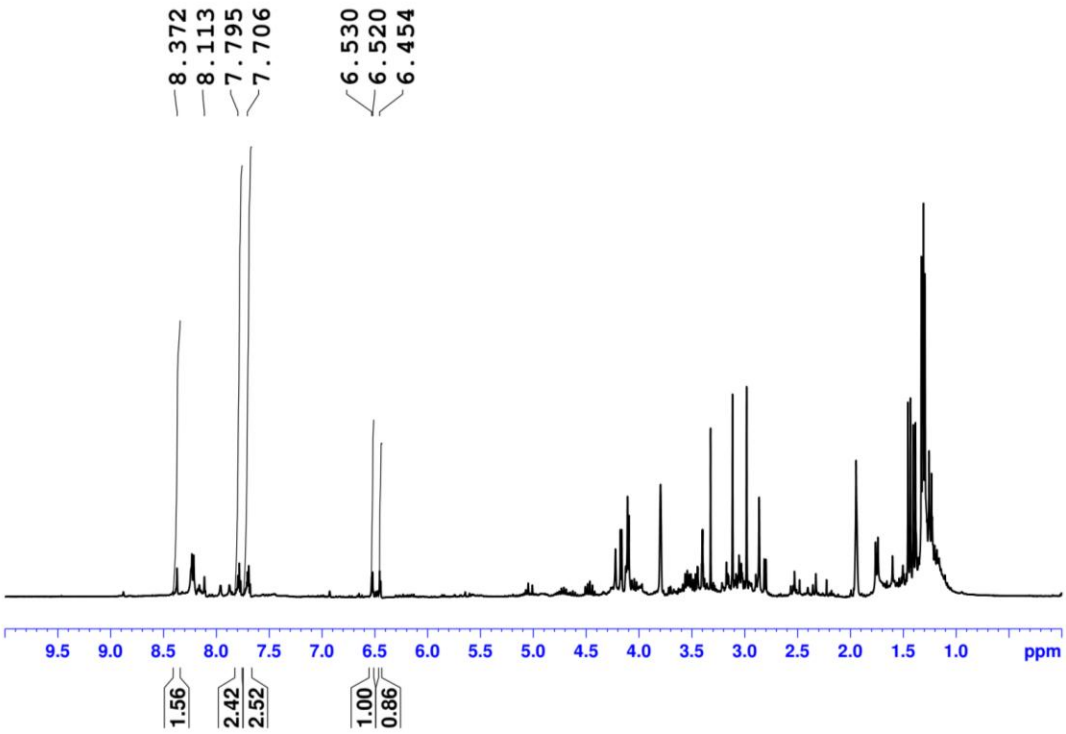


Figure S47. ^{1}H NMR spectrum of water hydrolysis of **NHC^{iPrMe}** in C_6D_6 at RT.

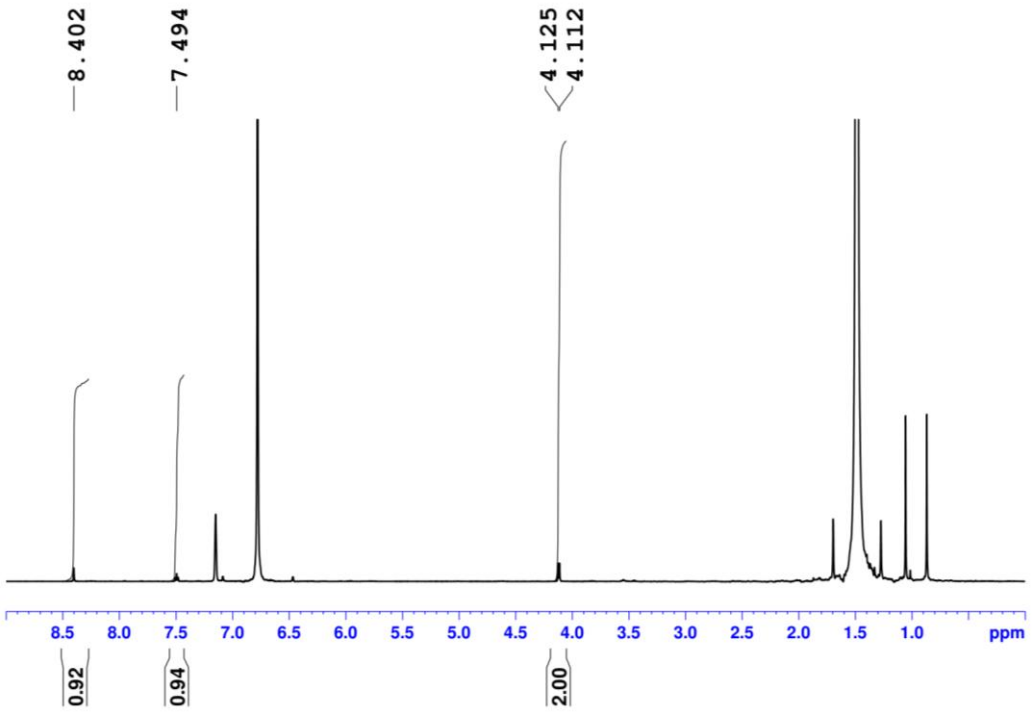


Figure S48. ^{1}H NMR spectrum of water hydrolysis of **NHC^{tBu_2}** in C_6D_6 at RT.

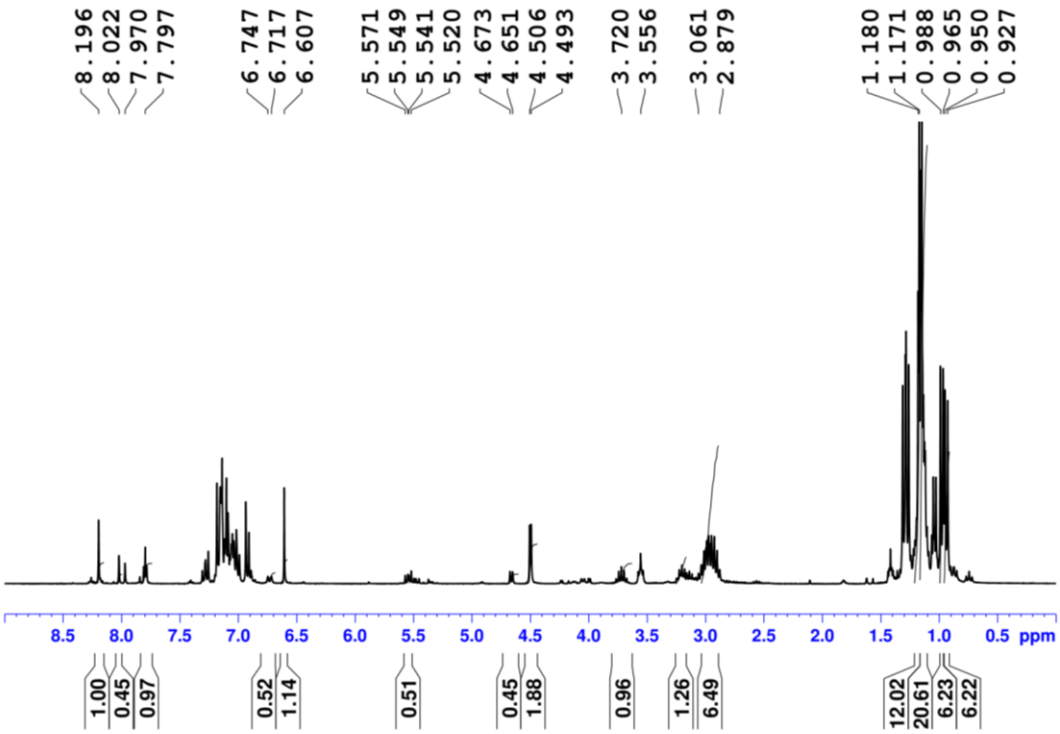


Figure S49. ^{1}H NMR spectrum of water hydrolysis of **NHC^{Dip_2}** in C_6D_6 at RT.

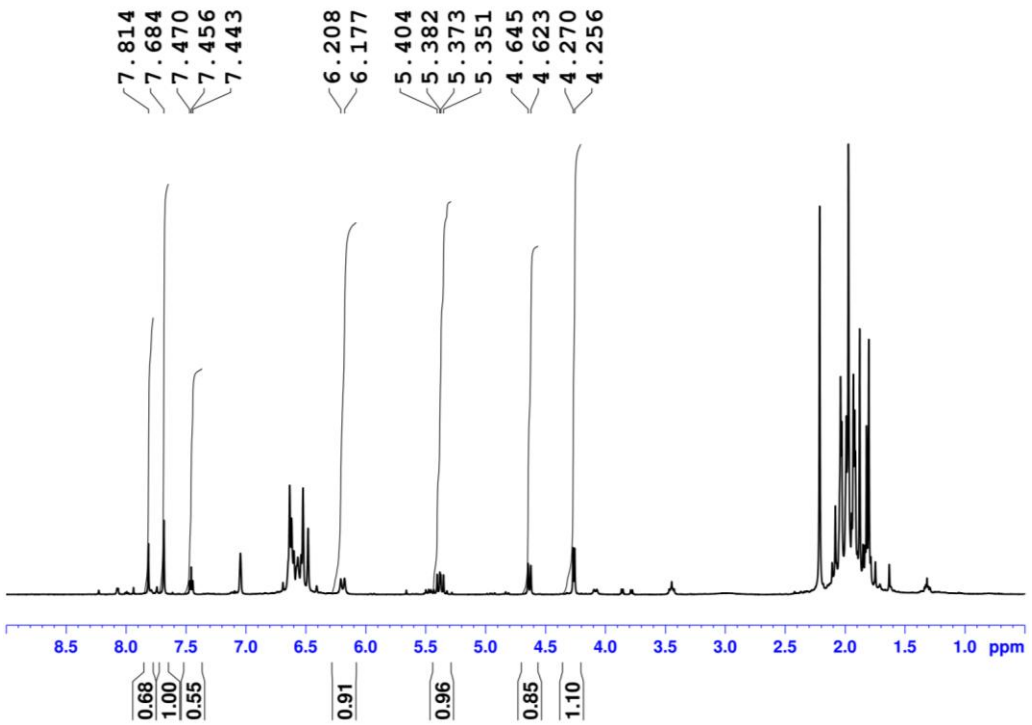


Figure S50. ^{1}H NMR spectrum of water hydrolysis of **NHC^{Mes_2}** in C_6D_6 at RT.

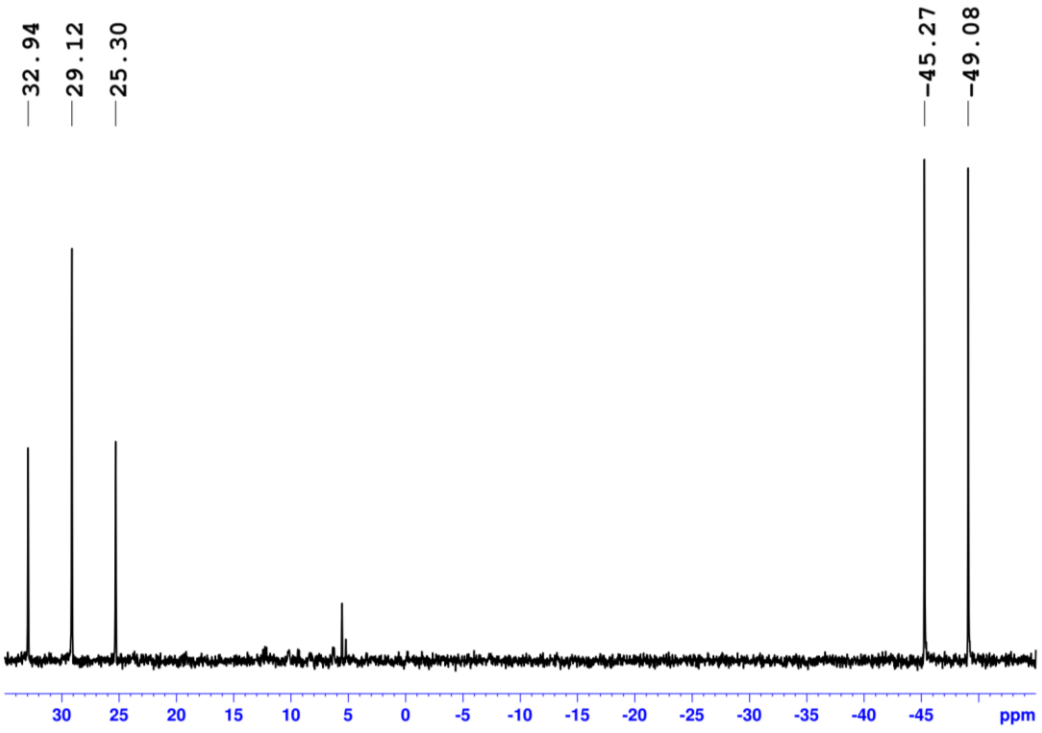


Figure S51. ^{31}P NMR spectrum from 1:2:2 reaction mixture of **1**, **NHC^{Me_4}**, and **H_2O** in C_6D_6 at RT.

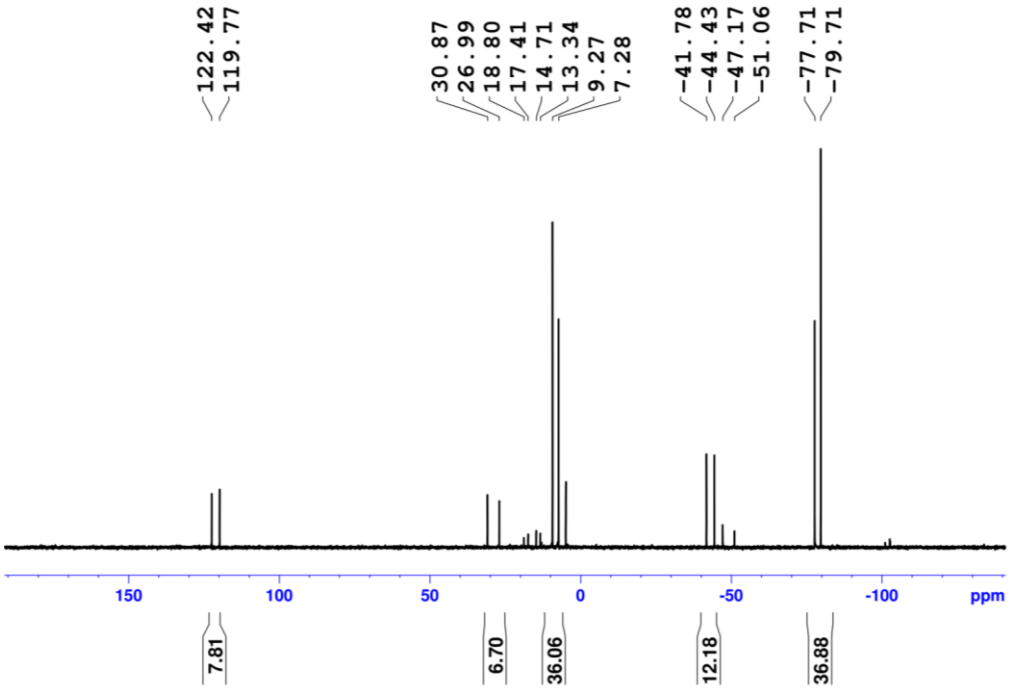


Figure S52. ^{31}P NMR spectrum from 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in C_6D_6 at RT with delay time d1 = 2 sec.

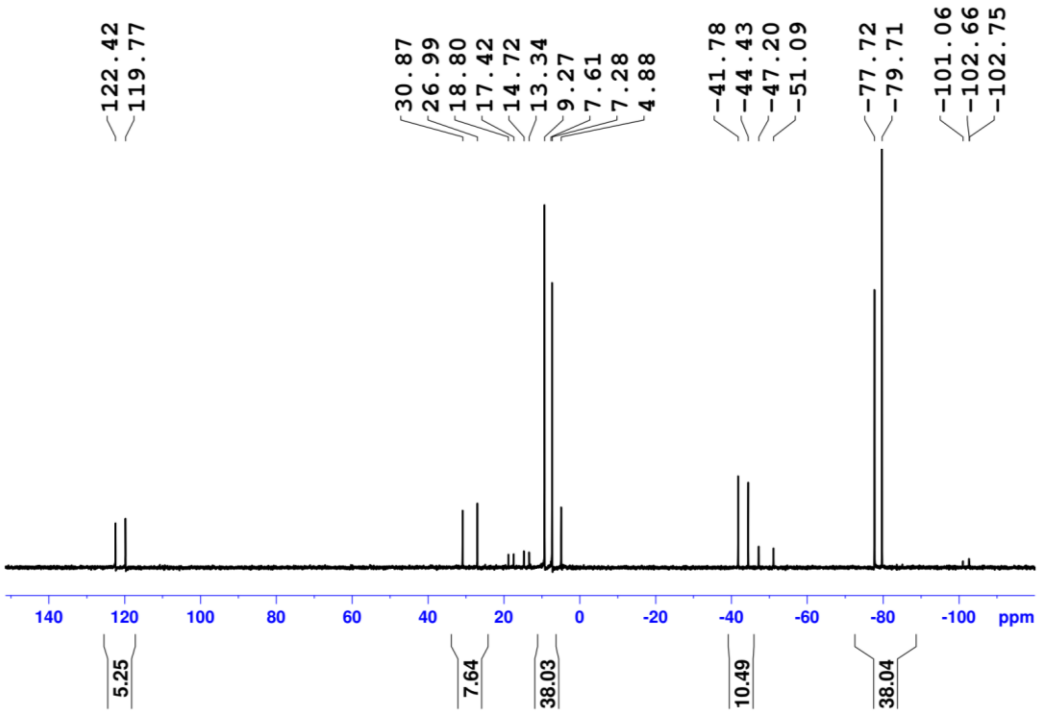


Figure S53. ^{31}P NMR spectrum from 1:1:1 reaction mixture of **1**, **NHC^{iPr_2Me_2}**, and **H_2O** in C_6D_6 at RT with delay time d1 = 40 sec.

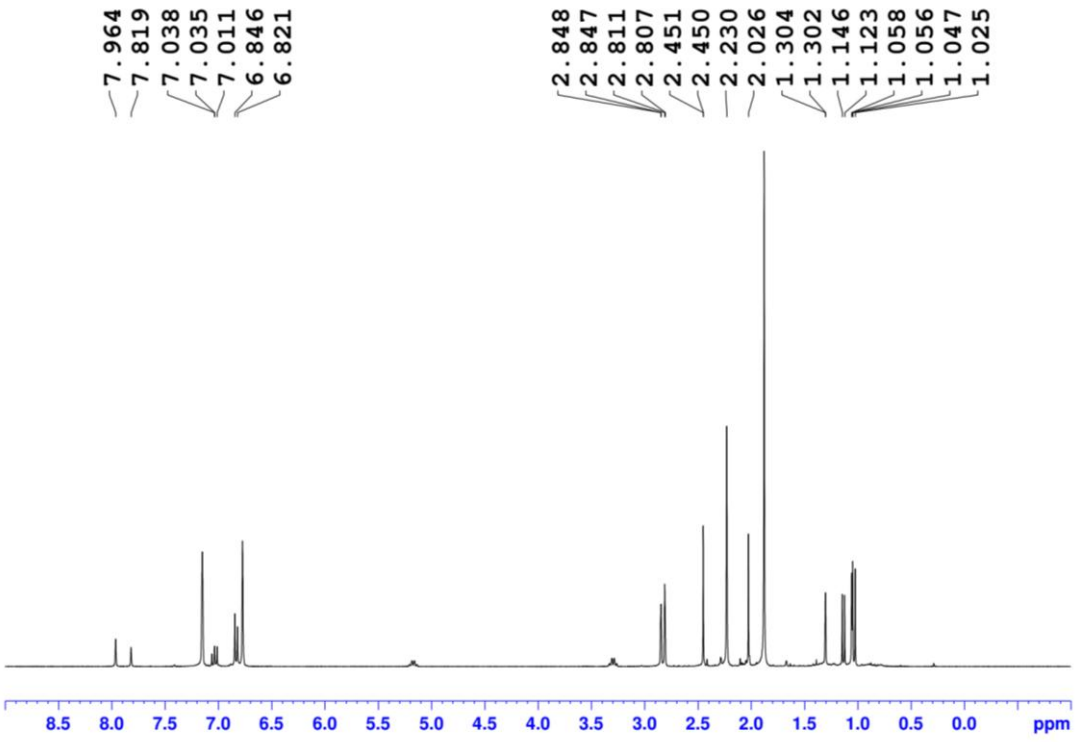


Figure S54. ^{1}H NMR spectrum from the reaction mixture of 1:1 hydrolyzed product of **NHC^{Me_4}** and **1** along with excess of H_2O in C_6D_6 at RT.

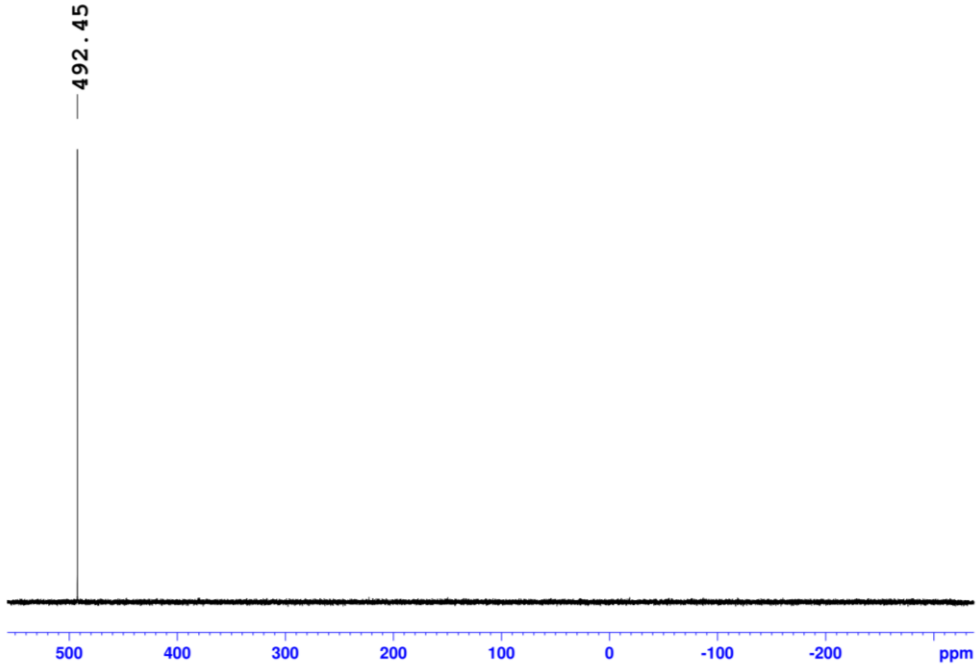


Figure S55. ^{31}P NMR spectrum from the reaction mixture of 1:1 hydrolyzed product of **NHC^{Me_4}** and **1** along with excess of H_2O in C_6D_6 at RT.

UV/vis Spectra

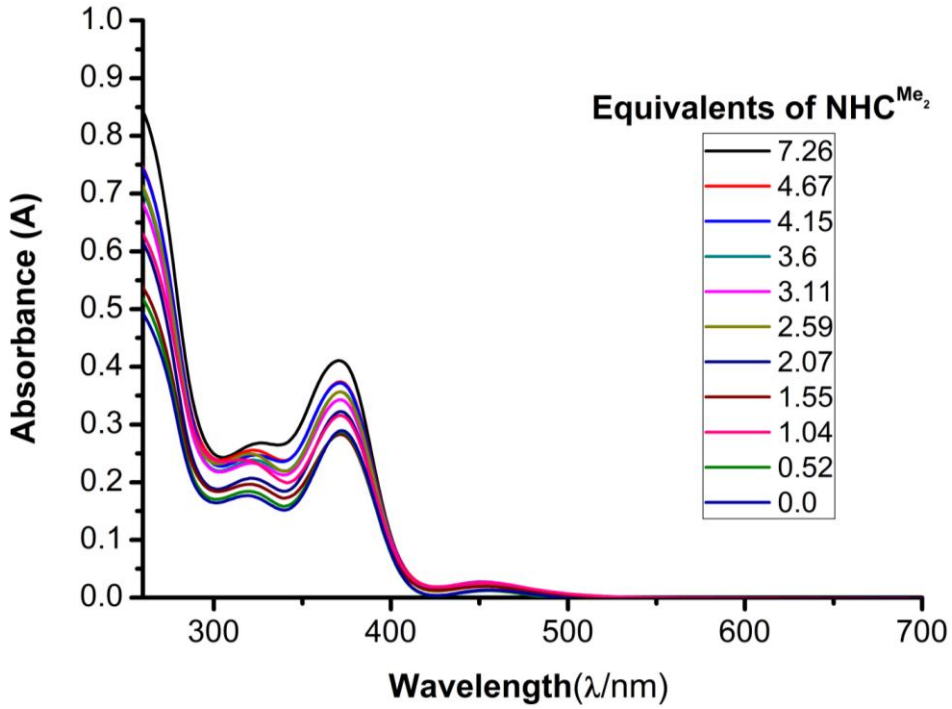


Figure S56. UV/vis spectra of **1** in THF with increasing concentrations of **NHC^{Me_2}**.

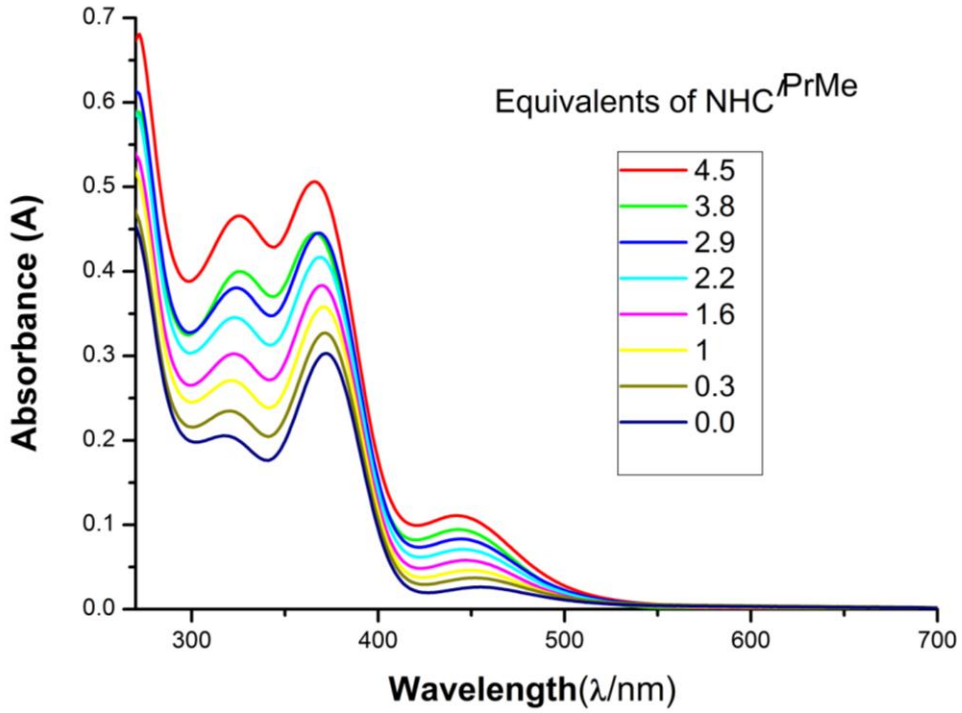


Figure S57. UV/vis spectra of **1** in THF with increasing concentrations of **NHC^{iPrMe}**.

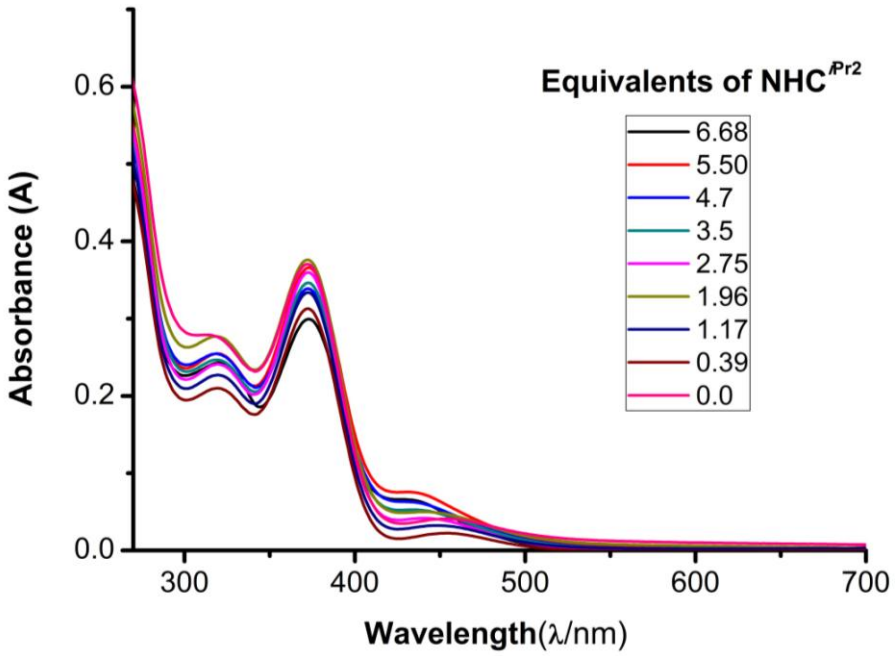


Figure S58. UV/vis spectra of **1** in THF with increasing concentrations of **NHC^{iPr_2}**.

HRMS (ESI-TOF) Spectrum

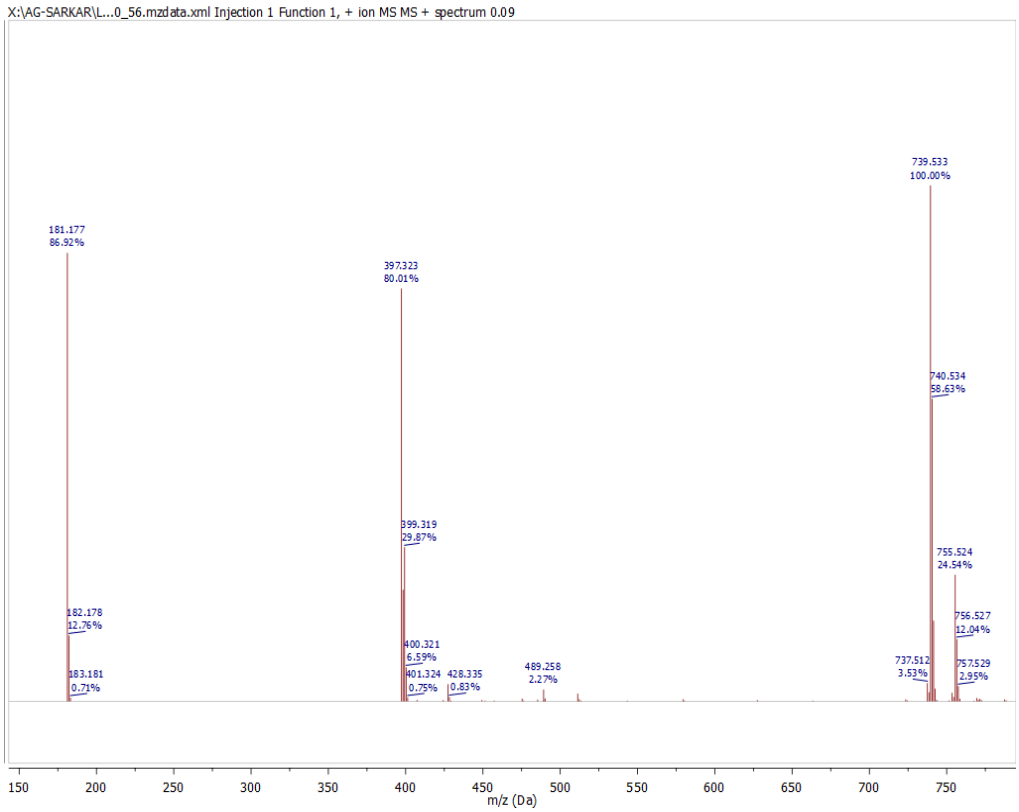


Figure S59. HRMS (ESI-TOF) spectrum of **4·NHC^{iPr_2Me_2}**.

Crystallographic Details

Single crystal X-ray data of **1·NHC^{Me_2}**, **4·NHC$^{Me\,iPr}$** and **4·NHC^{iPr_2Me_2}·toluene** were collected at 293 K and 120 K respectively using a Rigaku XtaLAB AFC12 (RINC): Kappa single diffractometer with graphite-monochromated Mo *K*α radiation, λ = 0.71073 Å. The unit cell parameters and the data reduction was obtained with the CrysAlisPro software from Rigaku Oxford Diffraction.[S7] A multi-scan absorption correction was applied to the collected reflections during data processing with SCALE3 ABSPACK also integrated in the CrysAlisPro software.[S7] The structure was solved by SHELXT[S8] structure solution program using Intrinsic phasing and refined by full matrix least-squares method based on F^2 using SHELXL[S9] refinement programme in the Olex-2 software.[S10] All non-hydrogen-atoms were refined with anisotropic displacement parameters. Hydrogens were placed in geometrically calculated positions or found in the Fourier difference map and include in the refinement process using riding model. The program Diamond (version 3.2k) is used for creating the crystallographic figures.[S11]

Table S10. Crystal data and structure refinement for **1·NHC^{Me_2}** (CCDC: 1870009)

Empirical formula	$C_{53}H_{58}N_2P_2$
Formula weight	784.95
Temperature/K	120.03(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	21.6214(12)
b/Å	10.9205(5)
c/Å	20.4742(10)
α/°	90
β/°	104.226(6)
γ/°	90
Volume/Å^3	4686.0(4)
Z	4
ρ_{calc}g/cm^3	1.113
μ/mm^{-1}	0.128
F(000)	1680.0
Crystal size/mm^3	0.407 × 0.131 × 0.119
Radiation	MoKα (λ = 0.71073)
2*Θ* range for data collection/°	5.388 to 52.996
Index ranges	-27 ≤ h ≤ 27, -13 ≤ k ≤ 13, -25 ≤ l ≤ 25
Reflections collected	64797
Independent reflections	9713 [R_{int} = 0.0680, R_{sigma} = 0.0536]
Data/restraints/parameters	9713/0/528
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0627, wR_2 = 0.1323
Final R indexes [all data]	R_1 = 0.0825, wR_2 = 0.1396
Largest diff. peak/hole / e Å^{-3}	0.33/-0.30

Table S11. Crystal data and structure refinement for for **4·NHC$^{Me\textit{i}Pr}$** (CCDC: 1870413)

Empirical formula	$C_{55}H_{64}N_2OP_2$
Formula weight	831.02
Temperature/K	120.01(10)
Crystal system	monoclinic
Space group	*C*c
a/Å	16.7505(7)
b/Å	16.1364(8)
c/Å	18.1430(8)
α/°	90
β/°	98.797(5)
γ/°	90
Volume/Å^3	4846.2(4)
Z	4
ρ_{calc}g/cm^3	1.139
μ/mm^{-1}	0.129
F(000)	1784.0
Crystal size/mm^3	0.23 × 0.176 × 0.128
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.446 to 50.994
Index ranges	-19 ≤ h ≤ 20, -17 ≤ k ≤ 19, -21 ≤ l ≤ 21
Reflections collected	24543
Independent reflections	8042 [R_{int} = 0.0511, R_{sigma} = 0.0624]
Data/restraints/parameters	8042/2/559
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0813
Final R indexes [all data]	R_1 = 0.0517, wR_2 = 0.0847
Largest diff. peak/hole / e Å^{-3}	0.20/-0.23

Table S12. Crystal data and structure refinement for **4·NHC^{iPr_2Me_2}.toluene** (CCDC: 1870412)

Empirical formula	$C_{66}H_{79.5}N_2OP_2$
Formula weight	978.75
Temperature/K	293(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	12.9095(6)
b/Å	21.2248(12)
c/Å	23.3462(11)
α/°	66.943(5)
β/°	81.227(4)
γ/°	81.959(4)
Volume/Å^3	5794.4(5)
Z	4
ρ_{calc}g/cm^3	1.122
μ/mm^{-1}	0.117
F(000)	2110.0
Crystal size/mm^3	0.602 × 0.097 × 0.078
Radiation	MoKα (λ = 0.71073)
2*Θ* range for data collection/°	5.044 to 53
Index ranges	-16 ≤ h ≤ 16, -25 ≤ k ≤ 26, -28 ≤ l ≤ 29
Reflections collected	120222
Independent reflections	23931 [R_{int} = 0.0829, R_{sigma} = 0.0680]
Data/restraints/parameters	23931/0/1325
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0575, wR_2 = 0.1325
Final R indexes [all data]	R_1 = 0.0945, wR_2 = 0.1484
Largest diff. peak/hole / e Å^{-3}	1.21/-0.73

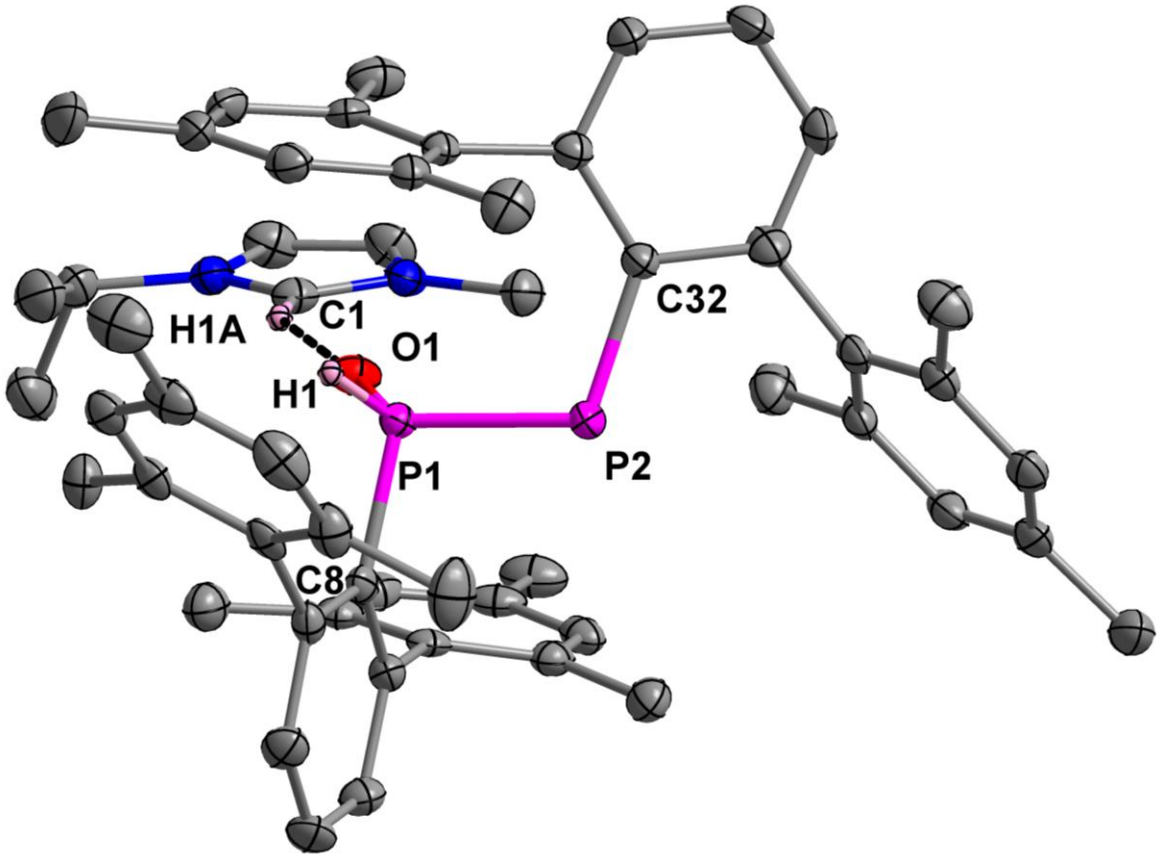


Figure S60. Molecular structure of **4·NHC**^{iPrMe} with thermal ellipsoids probability at 50%. All hydrogen atoms except P1-H and C1-H are omitted for clarity. It has been crystalized from saturated toluene solution at room temperature.

Computational details

All geometry optimization calculations are performed using B3LYP[S12-S14] exchange-correlation functional along with 6-31G(d) basis set for all atoms. Additionally, we employ Grimme's D3 dispersion model to account for the non-covalent interactions.[S15] Electronic energies are further refined with single point calculations at the M062X-D3/6-311++G(d,p) level of theory.[S16-S17] Solvent (THF) effects are taken into account using SMD solvation model by Truhlar and Cramer.[S18] All thermochemical data are estimated within ideal gas-rigid rotor-simple harmonic oscillator approximations at 298.15 K and 1 atm pressure. All calculations are performed using Gaussian16 package.[S19]

Table S13. Association Gibbs free energy of the adduct between **1** and various **NHC**s at 298.15 K

1·NHC$^{R'R''}$	**ΔG (kcal/mol)**
1·NHC^{Me_4}	−6.2
1·NHC^{Me_2}	−4.4
1·NHC^{iPrMe}	−3.4
1·NHC^{iPr_2}	1.9

Table S14. Relative stabilities (in terms of electronic energies at the B3LYP-D3/6-31G(d) level of theory) of the 1,1- and 1,2-water addition products during the hydrolysis of **1·NHC$^{R'R''}$**

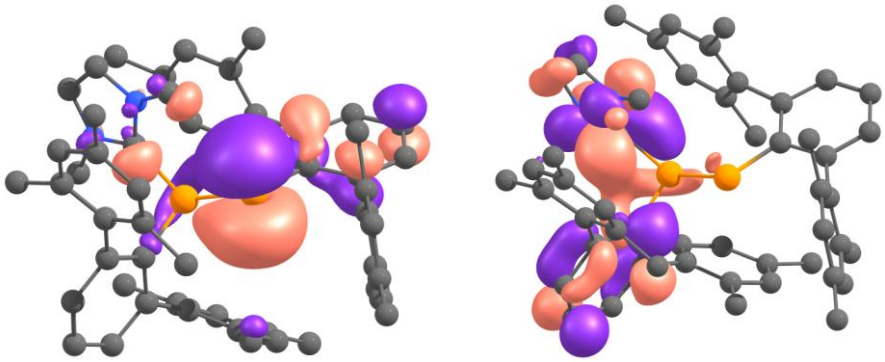
Addition product	**Relative electronic energy (kJ/mol)**	
	1,1-water addition product	1,2-water addition product
2·NHC^{Me_4}	102.9	0.0
2	38.9	0.0

Table S15. The calculated gas-phase proton detachment free energies (PDFEs) for various NHCs. The PDFE values are calculated following the equation $BH^+ \rightarrow B + H^+$

NHC(R'R")	[G(B)-G(BH^+)] (kcal/mol)	Hydrolysis
NHC^{tBu_2}	263.8	Very slow
NHC^{Mes_2}	265.2	Very slow
NHC^{iPrMe}	257.3	Fast
NHC^{Me_2}	255.9	Fast
NHC^{Me_4}	262.5	Very fast
NHC^{iPr_2}	258.4	Very fast
NHC^{iPr_2Me_2}	265.7	Very slow
NHC^{Dip_2}	264.5	Very slow

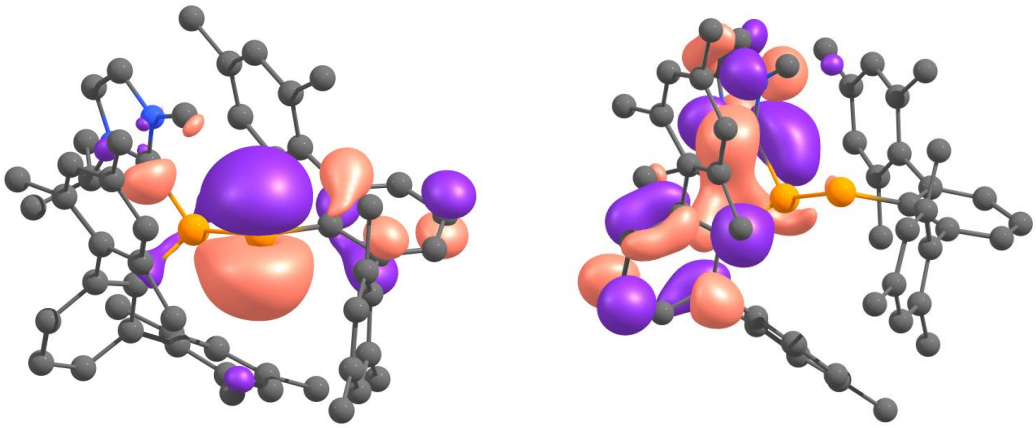
Table S16. The NPA atomic charges on the P1/P2 centre and Wiberg Bond Indices for the P1-P2 bonds in 1 and its NHC-adducts calculated at the B3LYP-D3/6-31G(d) level of theory

System	q_{P1} (e)	q_{P2} (e)	WBI
1	0.293	0.293	1.85
1·NHC^{Me_2}	0.512	-0.133	1.14
1·NHC^{iPrMe}	0.494	-0.144	1.15
1·NHC^{iPr_2}	0.513	-0.129	1.13



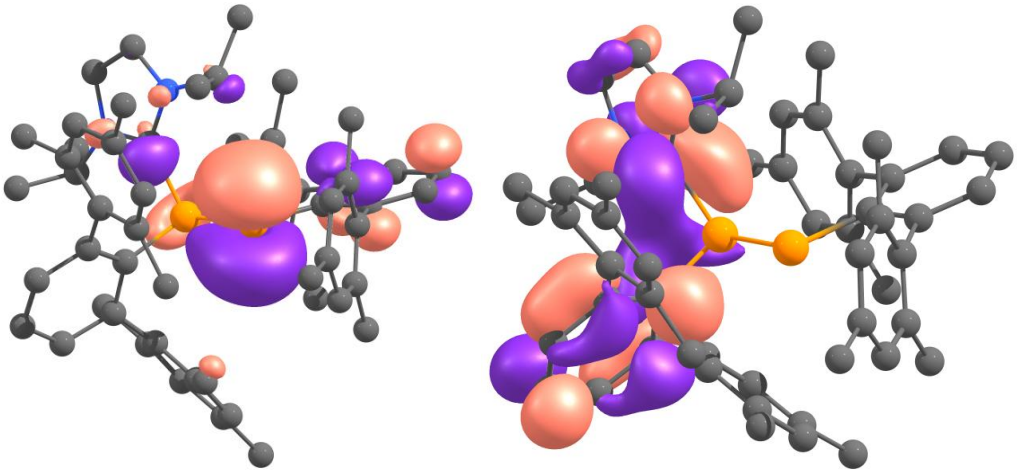
HOMO LUMO

Figure S61. Frontier molecular orbitals of 1·NHC^{Me_2}.



HOMO LUMO

Figure S62. Frontier molecular orbitals of the compound 1·NHC^{iPrMe}.



HOMO LUMO

Figure S63. Frontier molecular orbitals of the compound **1·NHC^{iPr_2}**.

Absolute energy data for the computed structures

E_{gas}= gas-phase absolute electronic energy (hartree) at B3LYP-D3/6-31G(d) level of theory
ΔH_{corr}= Enthalpy correction term at 298.15 K (hartree)
ΔG_{cor}r= Free energy correction term at 298.15 K (hartree)
$\mathbf{E^{sp}_{gas}}$ = gas-phase absolute single point energy (hartree) M062X-D3/6-311++G(d,p) level of theory
$\mathbf{E^{sp}_{sol}}$ = solvent-phase absolute single point energy (hartree)
NImag= Number of imaginary frequencies

Table S17. Absolute energy data for the computed structures.

Structures	$\mathbf{E_{gas}}$	$\mathbf{\Delta H_{corr}}$	$\mathbf{\Delta G_{corr}}$	$\mathbf{E^{sp}_{gas}}$	$\mathbf{E^{sp}_{sol}}$	**NImag**
1	−2542.139758	0.893863	0.75437	−2541.655118	−2542.169919	0
1·NHC^{Me_4}	−2925.630978	1.092143	0.933434	−2925.062805	−2925.673347	0
NHC^{Me_4}	−383.4475745	0.194446	0.148868	−383.363497	−383.4668809	0
1·NHC^{iPr_2}	−3004.248034	1.152269	0.987851	−3003.655984	-3004.290635	0
1·NHC^{Me_2}	−2846.978092	1.032279	0.878827	−2846.43799	−2847.02098	0
1·NHC^{iPrMe}	−2925.617454	1.092806	0.936791	−2925.054105	−2925.660554	0
NHC^{iPr_2}	−462.0790419	0.254209	0.202879	−461.9717002	−462.0961326	0
NHC^{Me_2}	−304.8000201	0.134921	0.095922	−304.7445778	−304.8184162	0
NHC^{iPrMe}	−383.439407	0.194549	0.149004	−383.3580932	−383.4571328	0
[NHC^{Me4}H]$^+$	−383.8970072	0.208641	0.162373	−383.7953859	−383.9773082	0
[NHC^{iPr_2}H]$^+$	−462.5261483	0.266436	0.22037	−462.4010571	−462.6054134	0
[NHC^{Me_2}H]$^+$	−305.2395945	0.149354	0.109452	−305.16598	−305.3244056	0
[NHC^{iPrMe}H]$^+$	−383.8829422	0.207878	0.164479	−383.7836064	−383.9647962	0
NHC^{Dip_2}	−1160.114944	0.60439	0.512062	−1159.829123	−1160.140295	0
[NHC^{Dip_2}H]$^+$	−1160.566478	0.618405	0.523828	−1160.262353	−1160.644117	0
NHC^{Mes_2}	−924.2180394	0.423119	0.342329	−924.0077322	−924.2450621	0
[NHC^{Mes_2}H]$^+$	−924.6724301	0.437129	0.355137	−924.4431127	−924.7491915	0
NHC^{tBu_2}	−540.7146642	0.312806	0.25676	−540.5846947	−540.7313537	0
[NHC^{tBu_2}H]$^+$	−541.1670585	0.327198	0.271175	−541.0194898	−541.2435357	0
NHC^{iPr_2Me_2}	−540.7248718	0.313771	0.25489	−540.5893201	−540.742194	0
[NHC^{iPr_2Me_2}H]$^+$	−541.1813637	0.327966	0.271092	−541.0289087	−541.2565153	0

Table S18. Relative absolute energies of the isomers for the water addition products

Structures	**Addition products**	**E_{gas} (hartree)**
2·NHC^{Me_4}	**1,1**	−3002.04509942
	1,2	−3002.08427086
2	**1,1**	−2618.56710866
	1.2	−2618.58196355

Cartesian coordinates of the optimized structures at the B3LYP-D3/6-31G(d) level of theory

1

100

C	0.01235600	2.27130800	-0.38818300
C	-1.02474200	2.68930400	-1.25388800
C	-0.91710800	3.93281500	-1.89546400
H	-1.72430200	4.24614400	-2.55236100
C	0.18722500	4.75803200	-1.70259100
H	0.24624600	5.71920700	-2.20629600
C	1.21624200	4.33909800	-0.86241200
H	2.09565800	4.96008300	-0.71215900
C	1.13938900	3.10658400	-0.20570800
C	2.28992800	2.67032800	0.64839600
C	2.32405600	2.99231000	2.02049000
C	3.42749100	2.59751300	2.78153400
H	3.44886600	2.83595000	3.84321900
C	4.50448600	1.91161100	2.21290000
C	4.46057200	1.62631300	0.84558700
H	5.29857400	1.10956100	0.38387500
C	3.36710700	1.98162800	0.05190000
C	3.33444700	1.61780700	-1.41342600
H	3.10391100	2.48493800	-2.04152900
H	2.56224200	0.86286700	-1.61003800
H	4.29004200	1.19612800	-1.73650200
C	5.67089500	1.45597500	3.05722600
H	5.79715100	2.08404700	3.94557100
H	6.60896200	1.47463800	2.49120900
H	5.52296100	0.42446600	3.40564900
C	1.17640100	3.73689700	2.66153500
H	0.25678300	3.13845100	2.63924500
H	0.95746800	4.67065900	2.13119900

H	1.39515300	3.97825000	3.70631000
C	-2.25808200	1.88776100	-1.53392600
C	-2.36236800	1.18080700	-2.75184600
C	-3.54693900	0.49989700	-3.04053700
H	-3.62229200	-0.05484600	-3.97408700
C	-4.64220100	0.52517700	-2.17048200
C	-4.52368400	1.25033100	-0.98535500
H	-5.36725500	1.29132600	-0.30068900
C	-3.34419300	1.91924300	-0.64096500
C	-3.25396000	2.63138700	0.68879900
H	-4.24880300	2.90582400	1.05520400
H	-2.64630300	3.53934900	0.63021700
H	-2.79939100	1.97674200	1.44416000
C	-5.90287300	-0.24127600	-2.49187400
H	-5.79743700	-1.30088500	-2.22184300
H	-6.13748200	-0.20401700	-3.56169000
H	-6.76443000	0.15194700	-1.94154200
C	-1.21775300	1.15894300	-3.73969000
H	-1.44252300	0.50035200	-4.58452500
H	-0.29264900	0.80531800	-3.27191200
H	-1.00973400	2.15963800	-4.13646700
C	0.01248600	-2.27143200	0.38801400
C	1.13954800	-3.10666000	0.20551200
C	1.21636300	-4.33924900	0.86207200
H	2.09579800	-4.96021000	0.71182800
C	0.18728700	-4.75829600	1.70212600
H	0.24629300	-5.71953600	2.20571200
C	-0.91704700	-3.93309800	1.89506900
H	-1.72425000	-4.24648800	2.55192500
C	-1.02463800	-2.68950300	1.25364500
C	-2.25788900	-1.88789000	1.53384000
C	-2.36200100	-1.18101800	2.75180300

C	-3.54650000	-0.50004300	3.04067600
H	-3.62170400	0.05464200	3.97426900
C	-4.64185700	-0.52520700	2.17075200
C	-4.52350200	-1.25027600	0.98554500
H	-5.36715800	-1.29122600	0.30097900
C	-3.34409700	-1.91922800	0.64097400
C	-3.25402100	-2.63127800	-0.68885200
H	-4.24893300	-2.90537400	-1.05532800
H	-2.64664500	-3.53943100	-0.63032100
H	-2.79921600	-1.97670500	-1.44412700
C	-5.90248300	0.24125000	2.49230600
H	-5.79758600	1.30059500	2.22099900
H	-6.13621800	0.20512200	3.56234600
H	-6.76437100	-0.15282500	1.94309800
C	-1.21731800	-1.15940600	3.73958000
H	-1.44180000	-0.50060300	4.58432700
H	-0.29209700	-0.80621700	3.27171900
H	-1.00967900	-2.16012700	4.13650600
C	2.29014600	-2.67024100	-0.64842500
C	3.36712800	-1.98133200	-0.05181900
C	4.46064700	-1.62587800	-0.84537200
H	5.29849500	-1.10896800	-0.38355500
C	4.50481200	-1.91126100	-2.21265800
C	3.42800500	-2.59736200	-2.78140700
H	3.44957100	-2.83584000	-3.84307800
C	2.32452200	-2.99229300	-2.02050200
C	1.17707300	-3.73707000	-2.66169400
H	0.25737000	-3.13874800	-2.63956300
H	0.95818000	-4.67084200	-2.13136300
H	1.39602200	-3.97842600	-3.70642700
C	5.67136100	-1.45558000	-3.05677100
H	6.60964400	-1.47614400	-2.49116000

H	5.52443400	-0.42337000	-3.40351700
H	5.79657800	-2.08242600	-3.94612300
C	3.33420500	-1.61737500	1.41347100
H	4.28993400	-1.19619300	1.73681500
H	3.10298800	-2.48431700	2.04158100
H	2.56237600	-0.86197100	1.60974800
P	-0.03012300	0.75330300	0.68857600
P	-0.03007400	-0.75336400	-0.68863800

1·NHC^{Me_2}

115

P	-0.69968900	-0.51049500	0.20583600
P	0.83695900	0.80146500	-0.56562500
N	-2.73583100	0.56531300	-1.68720200
N	-3.38247100	-1.10368600	-0.47052600
C	1.61407100	-1.40349100	-2.43268300
C	-2.47522300	2.20871600	1.35863000
C	0.28841700	-2.09915500	-2.42418400
C	-3.80650000	2.30113200	0.90917100
C	-1.57868700	3.27794200	1.11570200
C	0.42539500	-1.79516500	2.79864800

C	-2.03990000	1.10771700	2.28131200
C	3.21134900	0.32931100	-1.85915000
C	-0.66144000	-0.77538800	2.98579800
C	-1.16580100	0.04197700	1.93609500
C	-4.20326100	3.41341100	0.15526800
H	-5.23228700	3.47001700	-0.19673100
C	1.91244300	-0.23886600	-1.67520900
C	-2.01818400	4.37322400	0.36646300
H	-1.32597000	5.19255800	0.18375000
C	-0.72676200	-1.67391100	-3.30131000
C	0.09307700	-3.24385000	-1.62663500
C	-3.32248300	4.45825400	-0.13257900
C	0.15212600	-3.17550200	2.75738000
C	1.76919100	-1.34957600	2.83908600
C	2.54305400	-3.66438600	2.67414400
C	3.64244600	1.54812000	-1.09874100
C	2.79749100	-2.29232500	2.76380900
H	3.82789800	-1.94618800	2.79303300
C	1.21450800	-4.08424600	2.69530700
H	0.99123700	-5.14948300	2.65520500
C	-2.35917300	-0.21457300	-0.63842500
C	2.57322100	-1.96237600	-3.29163400
H	2.30315700	-2.85761400	-3.84816200
C	3.38969500	2.83921400	-1.59863100
C	4.13728600	-0.24264500	-2.73445400
H	5.11306400	0.22740100	-2.83570800
C	2.10677800	0.11527000	2.98545700
H	1.93548100	0.64682900	2.04080100
H	3.15750600	0.24799300	3.25821700
H	1.48892300	0.59723200	3.75027000
C	3.83261800	-1.39589700	-3.45459900
H	4.55864800	-1.83993800	-4.13027000

C	-1.12874800	-3.91943000	-1.69203900
H	-1.27968100	-4.79870700	-1.06663500
C	-3.97119900	0.16725800	-2.16076600
C	-2.47449200	1.25030500	3.61014700
H	-3.14992600	2.06853900	3.84640400
C	1.18124600	-3.70779500	-0.69244400
H	2.09931700	-3.95163500	-1.23911000
H	0.87172100	-4.58948800	-0.12421500
H	1.43666200	-2.92158800	0.02556700
C	-1.93945300	-2.37126000	-3.33612100
H	-2.72672200	-2.03103200	-4.00602700
C	3.79536800	3.94951300	-0.85099900
H	3.58773100	4.94756500	-1.23378400
C	-0.20172500	3.29813100	1.73594200
H	-0.26890600	3.19974200	2.82640500
H	0.31754800	4.23295500	1.50445000
H	0.42426700	2.47738400	1.37398400
C	-4.37786900	-0.87882100	-1.39723900
C	-1.10778800	-0.59114300	4.30068000
H	-0.70620100	-1.23550900	5.07819100
C	-0.49056800	-0.49870600	-4.22024100
H	-0.07929300	0.35688600	-3.67634800
H	-1.41610100	-0.19023700	-4.71907500
H	0.24246200	-0.75358000	-4.99555100
C	4.33125200	1.38792200	0.12001100
C	-4.84954300	1.26834300	1.27692700
H	-4.40232200	0.31883200	1.57349800
H	-5.53360300	1.08374900	0.44208700
H	-5.45334800	1.61546100	2.12570000
C	-1.25396600	-3.73131800	2.77270200
H	-1.99716200	-2.97116000	3.02093800
H	-1.34411400	-4.54168600	3.50578400

H	-1.51280000	-4.15673000	1.79474100
C	-2.03472800	0.39805500	4.61551800
H	-2.38388600	0.52347600	5.63702000
C	4.71628800	2.52012900	0.84089700
H	5.23293900	2.39207700	1.79092600
C	3.67434300	-4.65453700	2.53509100
H	3.95589300	-4.77725800	1.48064600
H	3.39537500	-5.64308500	2.91612900
H	4.56948700	-4.32198200	3.07234300
C	2.66293300	3.02465800	-2.91057900
H	3.14673600	2.46568800	-3.71955200
H	2.62390700	4.08096100	-3.19680600
H	1.63379900	2.65176200	-2.83610400
C	-2.16126500	-3.49349700	-2.53469500
C	-3.75399600	5.63706900	-0.97330400
H	-4.84193100	5.76366100	-0.96209100
H	-3.44924900	5.51061800	-2.02122000
H	-3.30012200	6.56896200	-0.61830500
C	4.45185500	3.81183200	0.37442900
C	4.63615900	0.00245800	0.63590400
H	3.72527400	-0.60063300	0.70419000
H	5.10010900	0.04105800	1.62702000
H	5.31625400	-0.53197200	-0.03835600
C	-3.47124800	-4.24489300	-2.59716100
H	-3.43254600	-5.06189400	-3.32992600
H	-4.29632400	-3.58606000	-2.89174400
H	-3.72388400	-4.69507100	-1.62968600
C	4.89708100	5.02324100	1.16084900
H	5.94916100	5.26729700	0.95911100
H	4.80665900	4.85523800	2.24024900
H	4.30332800	5.90805900	0.90613500
C	-2.06884100	1.76974700	-2.18113900

H	-2.51266800	2.64224000	-1.70350900
H	-1.00539800	1.71541900	-1.93158800
H	-2.20321800	1.81502200	-3.26396500
C	-3.38787800	-2.18125800	0.50819800
H	-2.50310800	-2.79912600	0.35192700
H	-3.37138100	-1.77470300	1.52131000
H	-4.29042200	-2.77686800	0.36281500
H	-4.44534200	0.67014400	-2.98855300
H	-5.27138000	-1.48117500	-1.43252700

1·NHC$^{i\text{PrMe}}$

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P	-0.73212800	-0.10504600	0.21662700
P	1.17103900	0.36320300	-0.68971600
N	-2.14190900	1.74131500	-1.63018200
N	-3.45546700	0.54422800	-0.38789200
C	0.89173400	-2.11064100	-2.30581200
C	-0.63725200	3.16923500	1.24408400
C	-0.58359500	-1.96121100	-2.51066000
C	-1.65699600	3.99603200	0.72538900
C	0.71705500	3.49363200	0.98738000
C	-0.45514800	-1.68897400	2.86017600
C	-0.92764700	2.06361300	2.21850100
C	3.10769800	-1.36062700	-1.66158900
C	-0.84616800	-0.24556600	3.00975700
C	-0.81468500	0.67668700	1.92529700
C	-1.31661900	5.05120000	-0.12848700
H	-2.11078900	5.67722000	-0.53203800
C	1.69099200	-1.18179700	-1.58737600

C	1.01007500	4.54843000	0.11517600
H	2.05311500	4.77588800	-0.09391800
C	-1.03994600	-1.10598900	-3.53624800
C	-1.49960700	-2.77179800	-1.81538700
C	0.00949900	5.32736800	-0.46980000
C	-1.38976800	-2.74126900	2.90682500
C	0.92779200	-1.99214800	2.80093000
C	0.40492400	-4.37622000	2.64069000
C	4.05202700	-0.42856000	-0.96198000
C	1.32649800	-3.32586000	2.68547100
H	2.38884800	-3.55324400	2.64417200
C	-0.94536100	-4.06252500	2.78084500
H	-1.68086000	-4.86562300	2.79676100
C	-2.14026700	0.86899200	-0.58654600
C	1.48047600	-3.19236400	-2.97831500
H	0.82998100	-3.88594600	-3.50732600
C	4.39501000	0.81868900	-1.51883300
C	3.66401600	-2.42911100	-2.37048400
H	4.74722900	-2.52466800	-2.39835000
C	1.97720800	-0.90909000	2.88608100
H	2.14372300	-0.45194000	1.90272200
H	2.93077100	-1.31987100	3.22878600
H	1.68197000	-0.10988700	3.57208200
C	2.86003100	-3.36543000	-3.01682300
H	3.30030800	-4.20038200	-3.55534200
C	-2.85769800	-2.70188500	-2.14702000
H	-3.55665900	-3.35539500	-1.62748100
C	-3.42970500	1.94304600	-2.08334100
C	-1.20879900	2.47269900	3.53294000
H	-1.29091600	3.53742200	3.73682000
C	-1.02121900	-3.70987400	-0.73404800
H	-0.38662800	-4.50445500	-1.14461700

H	-1.86163900	-4.18006800	-0.21324600
H	-0.42299900	-3.17581500	0.01011100
C	-2.40771500	-1.03773200	-3.81382400
H	-2.75513000	-0.37602400	-4.60616500
C	5.23963000	1.67462900	-0.80361600
H	5.49104500	2.64403700	-1.23137500
C	1.84225300	2.79097700	1.70866800
H	1.75074800	2.93715700	2.79259200
H	2.81496700	3.17328900	1.38572100
H	1.83931600	1.71675800	1.51515200
C	-4.25513900	1.20316300	-1.30032600
C	-1.13024000	0.20346400	4.30569600
H	-1.15843100	-0.52363600	5.11296600
C	-0.04921800	-0.33819900	-4.38072200
H	0.67166300	0.20696900	-3.76270000
H	-0.55630100	0.36965400	-5.04594500
H	0.53766000	-1.02545700	-5.00273600
C	4.61734300	-0.82407000	0.26792400
C	-3.11144800	3.78860700	1.08184000
H	-3.52202900	2.89157200	0.61384500
H	-3.71649900	4.63871100	0.75092600
H	-3.25342300	3.67242700	2.16060600
C	-2.87135500	-2.51747300	3.11164000
H	-3.10252900	-1.47699600	3.34112300
H	-3.24092200	-3.13144300	3.94186400
H	-3.44404700	-2.81248600	2.22308100
C	-1.34638300	1.55361900	4.56772400
H	-1.57222200	1.89036200	5.57605300
C	5.44889000	0.06146600	0.95670000
H	5.86201500	-0.23990300	1.91817700
C	0.86244300	-5.80038100	2.43687600
H	0.98102400	-6.02024100	1.36747500

H	0.14104200	-6.51897600	2.84103300
H	1.83151600	-5.98444100	2.91403700
C	3.84247300	1.25215200	-2.85734400
H	3.87671800	0.43696400	-3.58790500
H	4.40437000	2.10191400	-3.25966700
H	2.79156300	1.55360000	-2.76016600
C	-3.33433300	-1.83643400	-3.13560000
C	0.35141500	6.42848100	-1.44534300
H	-0.41536000	7.21095200	-1.45586200
H	0.43404700	6.03775900	-2.46897100
H	1.31158400	6.89655900	-1.20247500
C	5.76306200	1.32343000	0.44256200
C	4.33421700	-2.19867800	0.82686500
H	3.26418900	-2.42291300	0.80940800
H	4.69446000	-2.29014700	1.85671700
H	4.82530000	-2.97634800	0.22899400
C	-4.80425100	-1.76185300	-3.47879600
H	-5.36410700	-2.59685000	-3.04378500
H	-4.96304800	-1.78200100	-4.56350700
H	-5.25454200	-0.83142200	-3.10728400
C	6.67813700	2.25926200	1.19834900
H	7.73425100	1.99793800	1.04565200
H	6.48923800	2.21803100	2.27738700
H	6.54892300	3.29730700	0.87285800
C	-3.96630800	-0.31484900	0.70200400
C	-5.12885200	-1.18264900	0.21985300
C	-4.36128200	0.53531000	1.91423600
H	-3.12048300	-0.95848400	0.95355400
H	-4.87182900	-1.70922200	-0.69938400
H	-5.35910900	-1.92224100	0.99276500
H	-6.03864100	-0.59369900	0.05447200
H	-3.50410500	1.07037200	2.32607500

H	-5.13214400	1.26329200	1.63544700
H	-4.77534000	-0.10959700	2.69482200
C	-0.99405800	2.43642100	-2.21613500
H	-0.28740300	2.70429000	-1.43913100
H	-0.49884700	1.79343200	-2.94076900
H	-1.37167000	3.34315400	-2.69272100
H	-3.64120900	2.59889100	-2.91273000
H	-5.32678800	1.09862900	-1.31195100

1·NHC^{iPr_2}

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P	-0.71952200	-0.45532300	0.10586300
P	0.93342800	0.92710700	-0.00314900
N	0.48833900	-1.92749200	2.42404400
N	-1.30888100	-2.82866700	1.58766200
C	-0.48000600	2.66415800	2.00395900
C	1.73637000	-2.62230700	-1.27227300
C	-1.77403800	1.91052800	2.03257500
C	2.10697200	-3.75568800	-0.51359500
C	2.74928200	-1.76108500	-1.76192700
C	-2.55610700	-0.00409500	-2.42629700
C	0.34568600	-2.46293100	-1.82729700
C	1.68962200	3.29352700	1.10685700
C	-1.68185600	-1.23226500	-2.39812300
C	-0.60640000	-1.45708100	-1.48903500
C	3.45021400	-3.95614800	-0.18395000
H	3.72137700	-4.82952400	0.40681100
C	0.59961200	2.36206100	1.12817200

C	4.07744300	-1.98435800	-1.37930200
H	4.84168900	-1.29637300	-1.73505800
C	-2.09024900	1.01942500	3.07161500
C	-2.74459000	2.20181700	1.04763300
C	4.44974100	-3.06525400	-0.58070600
C	-3.91559300	-0.03559700	-2.06033600
C	-2.04518800	1.14192000	-3.08611400
C	-4.23968300	2.21251500	-2.96154700
C	2.85015500	3.06518700	0.18356600
C	-2.89358800	2.22293400	-3.33437300
H	-2.49088000	3.09708400	-3.84228200
C	-4.72962300	1.07078700	-2.32948300
H	-5.77896900	1.03088000	-2.04137200
C	-0.38422000	-1.84102600	1.37180000
C	-0.41756200	3.78785100	2.84438100
H	-1.26182600	3.97995500	3.50341100
C	4.00344400	2.41127600	0.65753500
C	1.70822900	4.41090900	1.94011800
H	2.55918300	5.08648800	1.88477900
C	-0.61073400	1.21060900	-3.54950900
H	0.06808300	1.24580300	-2.68956000
H	-0.43860700	2.10538000	-4.15587200
H	-0.33490100	0.33365300	-4.14524700
C	0.66390600	4.66196800	2.83075000
H	0.68584800	5.52874500	3.48564200
C	-3.98981400	1.57790800	1.10623700
H	-4.72696300	1.80570000	0.34044700
C	0.12550700	-2.98261500	3.24567500
C	0.08410400	-3.32464700	-2.90927500
H	0.81999200	-4.08924100	-3.14393300
C	-2.43617900	3.19344600	-0.04597100
H	-2.08290200	4.14310300	0.37095000

H	-3.31517700	3.38359100	-0.66515700
H	-1.64295100	2.81443700	-0.69877200
C	-3.34923800	0.40222000	3.09297100
H	-3.58631900	-0.27990900	3.90915000
C	5.03793500	2.11319500	-0.23397300
H	5.91622600	1.58364800	0.13199500
C	2.46105100	-0.64962200	-2.74322200
H	1.75002200	-0.96940300	-3.51170400
H	3.38328000	-0.32736200	-3.23691800
H	2.03550500	0.22221600	-2.23847100
C	-0.99331300	-3.54275500	2.72599000
C	-1.89787000	-2.11204900	-3.46777200
H	-2.73535400	-1.91948300	-4.13286300
C	-1.12489800	0.74806400	4.20098900
H	-0.09780100	0.98240700	3.91669100
H	-1.17762800	-0.29989400	4.51869000
H	-1.35998300	1.36588600	5.07810500
C	2.77335300	3.46094700	-1.16804600
C	1.09305500	-4.78712600	-0.07637500
H	0.32651600	-4.35365900	0.56715700
H	1.57618600	-5.59783800	0.47810200
H	0.57118000	-5.23139500	-0.93122000
C	-4.53170400	-1.21903100	-1.35579600
H	-4.06087700	-2.16308800	-1.64378000
H	-5.60317100	-1.29383800	-1.57081700
H	-4.42197900	-1.09977600	-0.27179100
C	-1.04904600	-3.18895900	-3.70034400
H	-1.23471200	-3.87396400	-4.52336200
C	3.83037200	3.15213500	-2.02745400
H	3.76007100	3.44096900	-3.07496200
C	-5.12231400	3.41262200	-3.20708800
H	-5.00151200	4.15845900	-2.40942200

H	-6.18162900	3.13547000	-3.23727700
H	-4.87263200	3.90882100	-4.15160600
C	4.11009300	2.01650400	2.11179500
H	4.20898200	2.89637100	2.75949000
H	4.97682000	1.36974400	2.28555100
H	3.20879100	1.48862000	2.43985400
C	-4.31446800	0.67132500	2.12317200
C	5.88228500	-3.25529100	-0.14372500
H	6.12231400	-4.31392000	0.00605200
H	6.07202200	-2.73998900	0.80778000
H	6.58491800	-2.84711400	-0.87836300
C	4.96469700	2.46447900	-1.58395100
C	1.54461200	4.16863600	-1.68949300
H	0.66916500	3.51073200	-1.63473900
H	1.67674600	4.47526000	-2.73234700
H	1.31192600	5.05855700	-1.09393500
C	-5.69516000	0.05902500	2.19368300
H	-6.43853600	0.79987700	2.51615800
H	-5.73403500	-0.77368900	2.90422800
H	-6.02270400	-0.31608300	1.21694500
C	6.08995200	2.13462200	-2.53747300
H	6.76662900	2.98941400	-2.67304700
H	5.70758200	1.86629600	-3.52918100
H	6.69366100	1.29686800	-2.17065700
C	-2.54827700	-3.03553000	0.80635500
C	-3.75325200	-3.11219400	1.74619800
C	-2.44148000	-4.24714800	-0.11945700
H	-2.63895600	-2.13129600	0.20763800
H	-3.76607500	-2.25362500	2.42180000
H	-4.67085000	-3.09594700	1.15065300
H	-3.75921600	-4.03634700	2.33544600
H	-1.64690500	-4.11449800	-0.85482300

H	-2.25004600	-5.16413600	0.45081000
H	-3.38721000	-4.37385200	-0.65616000
H	0.68798100	-3.24436500	4.12476900
H	-1.57944000	-4.38186400	3.06213100
C	1.65847300	-1.04757200	2.72732200
C	2.88936400	-1.48913100	1.94830400
C	1.94650900	-1.00519000	4.23095000
H	1.36623000	-0.05639400	2.37600300
H	2.72884900	-1.36819100	0.87975600
H	3.73893800	-0.86166600	2.23377500
H	3.13619400	-2.53286900	2.16439400
H	1.05136500	-0.83120300	4.83169700
H	2.43705900	-1.92204900	4.57953200
H	2.64111400	-0.17965700	4.41373500

NHC^{Dip_2}

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N	-1.08656000	0.02873500	0.56709500
N	1.03556600	0.11481400	0.55709300
C	-0.03032400	0.10299300	-0.30690300
C	0.65997400	0.04994400	1.90051800
C	-0.69338700	-0.00576700	1.90707800
C	-2.45925600	-0.06995500	0.15046000
C	-2.97948900	-1.34311900	-0.14745300
C	-4.31892400	-1.41690700	-0.54784800
C	-5.10332300	-0.26950100	-0.63771800
C	-4.56341800	0.97836100	-0.33452600
C	-3.22850500	1.10489200	0.06672300
C	-2.09588600	-2.58448000	-0.09811600
C	-1.42765800	-2.80798600	-1.47021200
C	-2.83822700	-3.84667200	0.36768600

C	-2.59906500	2.46841000	0.32598500
C	-1.97620800	3.00332700	-0.97932900
C	-3.56883100	3.49117800	0.93657300
C	2.40718000	0.10603800	0.13036200
C	3.06168500	-1.13147200	0.00273800
C	4.40872100	-1.11878600	-0.38041700
C	5.06862100	0.07963600	-0.63625600
C	4.39061800	1.29193300	-0.52076100
C	3.04700200	1.33163900	-0.13232400
C	2.34586500	-2.45427700	0.24751200
C	2.95797500	-3.21347300	1.43830000
C	2.33122300	-3.32139800	-1.02426500
C	2.27815600	2.64509900	-0.07902000
C	3.08913600	3.80586500	0.51765200
C	1.75994900	2.98947000	-1.48958400
H	1.38122400	0.04822700	2.70339800
H	-1.40435800	-0.06507700	2.71702500
H	-4.75491600	-2.38035400	-0.79199300
H	-6.14211300	-0.34788700	-0.94827500
H	-5.18764500	1.86246800	-0.41476200
H	-1.29565100	-2.39460800	0.62649700
H	-0.76001300	-3.67760200	-1.43505100
H	-0.84217900	-1.92862400	-1.75592000
H	-2.18664700	-2.99001100	-2.24109100
H	-2.12455300	-4.66633700	0.50885200
H	-3.57452000	-4.18480800	-0.37069900
H	-3.36192300	-3.68064700	1.31590600
H	-1.78162400	2.32837000	1.04230300
H	-1.45930000	3.95418800	-0.79991000
H	-2.75461500	3.17380600	-1.73322200
H	-1.25645200	2.28552900	-1.38275900
H	-3.02389200	4.40029900	1.21490700

H	-4.05927200	3.09713900	1.83388800
H	-4.34987400	3.78867600	0.22719400
H	4.94256400	-2.05940100	-0.48492100
H	6.11376300	0.07032800	-0.93480700
H	4.91344400	2.21792300	-0.73926000
H	1.30359800	-2.23679000	0.49626000
H	2.40716300	-4.14300500	1.62497800
H	2.92570400	-2.60810900	2.35132600
H	4.00531300	-3.47709900	1.24897700
H	1.76566100	-4.24436400	-0.84865000
H	3.34502600	-3.60388500	-1.33165200
H	1.86049500	-2.78445000	-1.85376000
H	1.40259300	2.49445000	0.56151200
H	3.92766300	4.09445400	-0.12671100
H	3.49386700	3.54867700	1.50303900
H	2.44951900	4.68883100	0.62960600
H	1.14990200	3.90042300	-1.46680400
H	1.14865800	2.16978000	-1.87871300
H	2.59871400	3.15469500	-2.17715500

[NHC^{Dip_2}]H$^+$

66

N	-1.11207100	-0.00021100	0.61977500
N	1.06291400	-0.00004000	0.60083300
C	-0.03110500	0.00010600	-0.16786700
C	0.66967700	-0.00046200	1.92943100
C	-0.69452500	-0.00057600	1.94169400
C	-2.48427800	-0.00009100	0.14433700
C	-3.10032000	-1.24407800	-0.07766700
C	-4.41076900	-1.21128500	-0.56734100

C	-5.05538200	0.00014200	-0.80959600
C	-4.41061300	1.21144200	-0.56717500
C	-3.10016300	1.24399300	-0.07746800
C	-2.36801000	-2.56353300	0.14300700
C	-1.77956400	-3.07549100	-1.18777200
C	-3.25187700	-3.63673200	0.80065100
C	-2.36775200	2.56335300	0.14343200
C	-1.77992200	3.07588000	-1.18739100
C	-3.25137200	3.63622300	0.80195500
C	2.42662900	0.00006100	0.10422800
C	3.04219900	-1.24284500	-0.12425300
C	4.35299300	-1.20991700	-0.61352500
C	4.99984500	0.00026100	-0.85440600
C	4.35267900	1.21034000	-0.61387200
C	3.04190800	1.24305900	-0.12453400
C	2.33851300	-2.57365300	0.11550100
C	3.11055400	-3.45046800	1.11870300
C	2.10505300	-3.31736700	-1.21367700
C	2.33798400	2.57374700	0.11517000
C	3.10999900	3.45078200	1.11823000
C	2.10423400	3.31732100	-1.21401900
H	1.39580200	-0.00061400	2.72674000
H	-1.40621700	-0.00085600	2.75200600
H	-4.93254000	-2.14187400	-0.76265500
H	-6.07240200	0.00023400	-1.19046800
H	-4.93224800	2.14213700	-0.76236600
H	-1.52869400	-2.38178000	0.82567500
H	-1.22099000	-4.00429900	-1.02911900
H	-1.09805900	-2.34470400	-1.63911700
H	-2.57667400	-3.27586500	-1.91197800
H	-2.64820500	-4.51752200	1.04288100
H	-4.05483000	-3.96789900	0.13390500

H	-3.70872700	-3.26866100	1.72502400
H	-1.52812100	2.38132300	0.82564000
H	-1.22136800	4.00467900	-1.02861000
H	-2.57734900	3.27647600	-1.91118600
H	-1.09854100	2.34532600	-1.63930400
H	-2.64766200	4.51698100	1.04421200
H	-3.70770600	3.26774700	1.72642300
H	-4.05471100	3.96755600	0.13575900
H	4.87079600	-2.14326200	-0.81043100
H	6.01701900	0.00033700	-1.23476400
H	4.87022200	2.14377000	-0.81106500
H	1.35336800	-2.37618500	0.55455300
H	2.55577300	-4.37352000	1.31794000
H	3.26320300	-2.92927600	2.06993000
H	4.09467900	-3.73281700	0.73014500
H	1.55806600	-4.24977400	-1.03692400
H	3.05458200	-3.57143300	-1.69682400
H	1.52520400	-2.70976100	-1.91765100
H	1.35295000	2.37612100	0.55439400
H	4.09401800	3.73329200	0.72952500
H	3.26285800	2.92966800	2.06946300
H	2.55506000	4.37373700	1.31747700
H	1.55720600	4.24970400	-1.03727500
H	1.52431400	2.70961300	-1.91785700
H	3.05366100	3.57139900	-1.69736600
H	-0.03934800	0.00047700	-1.24563400

NHC^{iPr_2Me_2}

33

C	0.00000000	0.00000000	0.91539400
N	-0.04944300	1.06064300	0.05629600
C	-0.02399600	0.68128900	-1.29297400
C	0.00000000	2.45222200	0.53447500
H	-0.35154300	3.08149800	-0.29067100
C	-0.04833300	1.64941500	-2.43056600
H	0.00429300	1.11792600	-3.38510400
H	-0.96601000	2.25235700	-2.44051600
H	0.79877100	2.34693600	-2.39521900
C	-0.93953600	2.64712200	1.72661900
H	-0.91176900	3.69143400	2.05800800
H	-0.63933500	1.99632800	2.55115100
H	-1.96884000	2.39243100	1.45334600
C	1.44675100	2.83569100	0.86954800
H	1.81862000	2.18496300	1.66781400
H	1.50800900	3.87830800	1.20209200
H	2.09715700	2.71104700	-0.00376700
N	0.04944300	-1.06064300	0.05629600
C	0.02399600	-0.68128900	-1.29297400
C	0.00000000	-2.45222200	0.53447500
H	0.35154300	-3.08149800	-0.29067100
C	0.04833300	-1.64941500	-2.43056600
H	-0.00429300	-1.11792600	-3.38510400
H	0.96601000	-2.25235700	-2.44051600
H	-0.79877100	-2.34693600	-2.39521900
C	0.93953600	-2.64712200	1.72661900
H	0.91176900	-3.69143400	2.05800800
H	0.63933500	-1.99632800	2.55115100
H	1.96884000	-2.39243100	1.45334600
C	-1.44675100	-2.83569100	0.86954800
H	-1.81862000	-2.18496300	1.66781400
H	-1.50800900	-3.87830800	1.20209200

H	-2.09715700	-2.71104700	-0.00376700

[NHC^{iPr_2Me_2}]H$^+$

34

C	0.00000000	0.00000000	0.83150000
N	0.00000000	1.08900400	0.05553500
C	0.00354400	0.68693700	-1.27944800
C	0.09609300	2.49702800	0.53897800
H	-0.40809900	3.08976500	-0.22876800
C	0.00179200	1.65570400	-2.41529700
H	0.04460400	1.12055600	-3.36568800
H	-0.90737800	2.26808800	-2.42101500
H	0.86337900	2.33064000	-2.37561400
C	-0.64998700	2.67549700	1.86145100
H	-0.67793400	3.74034500	2.10812000
H	-0.14203700	2.16810100	2.68924200
H	-1.68062600	2.31345200	1.79614600
C	1.56846300	2.91147500	0.62674100
H	2.09008200	2.31981900	1.38693800
H	1.63636400	3.96654600	0.90772000
H	2.08458700	2.77827200	-0.32868800
N	0.00000000	-1.08900400	0.05553500
C	-0.00354400	-0.68693700	-1.27944800
C	-0.09609300	-2.49702800	0.53897800
H	0.40809900	-3.08976500	-0.22876800
C	-0.00179200	-1.65570400	-2.41529700
H	-0.04460400	-1.12055600	-3.36568800
H	0.90737800	-2.26808800	-2.42101500
H	-0.86337900	-2.33064000	-2.37561400
C	0.64998700	-2.67549700	1.86145100

H	0.67793400	-3.74034500	2.10812000
H	0.14203700	-2.16810100	2.68924200
H	1.68062600	-2.31345200	1.79614600
C	-1.56846300	-2.91147500	0.62674100
H	-2.09008200	-2.31981900	1.38693800
H	-1.63636400	-3.96654600	0.90772000
H	-2.08458700	-2.77827200	-0.32868800
H	0.00000000	0.00000000	1.90762200

NHC^{iPr_2}

27

C	0.00000000	0.00000000	0.41291700
N	0.00000000	1.06172200	-0.44934800
C	0.00000400	0.67878200	-1.78675500
C	0.00002900	2.45828400	0.01809200
H	0.00008900	3.07949600	-0.88606000
C	-1.27163300	2.74564000	0.82230700
H	-1.28494100	3.78783900	1.16080600
H	-1.30988400	2.08529900	1.69360600
H	-2.16488000	2.56388300	0.21495200
C	1.27165800	2.74558900	0.82237500
H	1.30980500	2.08529400	1.69370400
H	1.28502100	3.78782500	1.16081300
H	2.16492800	2.56374100	0.21507800
N	0.00000000	-1.06172200	-0.44934800
C	-0.00000400	-0.67878200	-1.78675500
C	-0.00002900	-2.45828400	0.01809200
H	-0.00008900	-3.07949600	-0.88606000
C	1.27163300	-2.74564000	0.82230700
H	1.28494100	-3.78783900	1.16080600

H	1.30988400	-2.08529900	1.69360600
H	2.16488000	-2.56388300	0.21495200
C	-1.27165800	-2.74558900	0.82237500
H	-1.30980500	-2.08529400	1.69370400
H	-1.28502100	-3.78782500	1.16081300
H	-2.16492800	-2.56374100	0.21507800
H	0.00000000	1.38712100	-2.60232200
H	0.00000000	-1.38712100	-2.60232200

[NHC^{iPr_2}]H$^+$

28

C	0.00000000	0.00000000	0.31161200
N	0.00000400	1.09052900	-0.46634500
C	0.00000400	0.68276200	-1.78534800
C	0.00000000	2.50584700	0.01701600
H	0.00003500	3.10148400	-0.90028500
C	-1.27945400	2.78870300	0.80691900
H	-1.30890700	3.84792900	1.07784900
H	-1.31024500	2.20771900	1.73556800
H	-2.17211700	2.55879400	0.21771000
C	1.27940700	2.78868300	0.80700300
H	1.31012600	2.20770400	1.73565800
H	1.30885900	3.84791000	1.07793000
H	2.17210400	2.55875600	0.21785500
N	-0.00000400	-1.09052900	-0.46634500
C	-0.00000400	-0.68276200	-1.78534800
C	0.00000000	-2.50584700	0.01701600
H	-0.00003500	-3.10148400	-0.90028500
C	1.27945400	-2.78870300	0.80691900
H	1.30890700	-3.84792900	1.07784900

H	1.31024500	-2.20771900	1.73556800
H	2.17211700	-2.55879400	0.21771000
C	-1.27940700	-2.78868300	0.80700300
H	-1.31012600	-2.20770400	1.73565800
H	-1.30885900	-3.84791000	1.07793000
H	-2.17210400	-2.55875600	0.21785500
H	0.00000700	1.38916000	-2.60086100
H	-0.00000700	-1.38916000	-2.60086100
H	0.00000000	0.00000000	1.38923200

NHC^{iPrMe}

21

C	0.46575300	-0.78701600	0.00007800
N	-0.32945700	0.32927200	-0.00019800
C	0.39498600	1.51625800	-0.00037500
C	-1.80001400	0.25022700	-0.00013100
H	-2.15788700	1.28727600	-0.00056900
C	-2.29211200	-0.44855100	-1.27142700
H	-3.38693500	-0.49489600	-1.28486900
H	-1.89005300	-1.46520600	-1.30904000
H	-1.95391800	0.08710900	-2.16500800
C	-2.29206600	-0.44732000	1.27182800
H	-1.88881800	-1.46342800	1.31093700
H	-3.38689800	-0.49498300	1.28470200
H	-1.95513500	0.08996900	2.16489100
N	1.71825600	-0.23306400	-0.00004300
C	1.70417400	1.15906500	-0.00029700
C	2.93056100	-1.03215600	0.00039300
H	3.53418800	-0.82600100	0.89190100
H	-0.07213700	2.49054700	-0.00073100

H	2.60204700	1.75962900	-0.00054900
H	2.63129900	-2.08075500	0.00014000
H	3.53496000	-0.82576800	-0.89053400

[NHC$^{i\text{PrMe}}$]H^{+}

22

C	0.50257200	-0.67567100	0.00024700
N	-0.35099700	0.35521600	-0.00029800
C	0.38287000	1.52559800	-0.00076500
C	-1.84493500	0.25268600	-0.00028000
H	-2.18229700	1.29304600	-0.00121300
C	-2.32130100	-0.43817600	-1.27943100
H	-3.41454300	-0.42546400	-1.30876000
H	-2.00116200	-1.48578300	-1.30919300
H	-1.94702100	0.07071100	-2.17261500
C	-2.32138800	-0.43593400	1.28004900
H	-2.00118200	-1.48346500	1.31167800
H	-3.41463300	-0.42321900	1.30927200
H	-1.94719800	0.07454300	2.17236300
N	1.75553500	-0.20229300	0.00008700
C	1.70256700	1.17884900	-0.00053000
C	2.98250900	-1.01049100	0.00057400
H	3.56518400	-0.78274600	0.89548500
H	-0.09099100	2.49501600	-0.00123900
H	2.59525000	1.78518900	-0.00076100
H	2.71283800	-2.06708600	0.00056300
H	3.56577100	-0.78289700	-0.89398900
H	0.23085900	-1.71946900	0.00071000

NHC^{Me_2}

15

C	0.00000000	0.99067200	-0.00000200
N	1.06172900	0.12146100	-0.00010600
C	0.67822000	-1.21650600	-0.00001500
C	2.44230500	0.57069800	-0.00001500
H	2.97048600	0.21206500	-0.89098400
N	-1.06172900	0.12146100	0.00010500
C	-0.67822000	-1.21650600	0.00001500
C	-2.44230500	0.57069800	0.00001800
H	-2.97048800	0.21205100	0.89097900
H	1.38543400	-2.03327900	0.00078900
H	-1.38543400	-2.03327900	-0.00079100
H	-2.43120300	1.66104300	0.00047100
H	-2.97010900	0.21279400	-0.89147200
H	2.43120300	1.66104400	-0.00045200
H	2.97011100	0.21278000	0.89146700

$[NHC^{Me_2}]H^+$

16

C	0.00000000	0.86391500	-0.00012500
N	1.08840500	0.08535700	0.00007400
C	0.68173500	-1.23658700	0.00001300
C	2.48279800	0.55112900	0.00002800
H	2.98661800	0.18107500	-0.89514500
N	-1.08840500	0.08535700	-0.00007500
C	-0.68173500	-1.23658700	-0.00005600
C	-2.48279800	0.55112900	0.00009700
H	-2.98655000	0.18108900	0.89531400
H	1.38947600	-2.05139500	0.00011600

H	-1.38947600	-2.05139500	-0.00011600
H	-2.49377900	1.64149700	-0.00022000
H	-2.98690900	0.18059000	-0.89471000
H	2.49377900	1.64149700	0.00032800
H	2.98684100	0.18060400	0.89488000
H	0.00000000	1.94345100	-0.00017900

NHC^{Me_4}

21

C	0.00000000	1.57942200	0.00000200
N	-1.05961600	0.71019700	0.00001300
C	-0.68121500	-0.63793800	-0.00000200
C	-2.43637200	1.16552500	-0.00002100
H	-2.97115200	0.81157300	0.88964000
N	1.05961600	0.71019700	-0.00001200
C	0.68121500	-0.63793800	0.00000100
C	2.43637200	1.16552500	0.00002200
H	2.97115000	0.81157900	-0.88964300
H	2.41733800	2.25581800	-0.00011100
H	2.97103800	0.81179900	0.88984300
H	-2.41733800	2.25581800	0.00011800
H	-2.97103700	0.81180500	-0.88984600
C	1.66482200	-1.76043300	0.00002100
H	2.31684300	-1.73321900	-0.88317800
H	2.31679500	-1.73323000	0.88325600
H	1.14918200	-2.72530700	0.00000000
C	-1.66482200	-1.76043300	-0.00002300
H	-2.31682800	-1.73323300	0.88318800
H	-2.31681000	-1.73321700	-0.88324600
H	-1.14918300	-2.72530700	-0.00002500

[NHC^{Me4}]H^{+}

22

C	0.00000000	0.86391500	-0.00012500
N	1.08840500	0.08535700	0.00007400
C	0.68173500	-1.23658700	0.00001300
C	2.48279800	0.55112900	0.00002800
H	2.98661800	0.18107500	-0.89514500
N	-1.08840500	0.08535700	-0.00007500
C	-0.68173500	-1.23658700	-0.00005600
C	-2.48279800	0.55112900	0.00009700
H	-2.98655000	0.18108900	0.89531400
H	1.38947600	-2.05139500	0.00011600
H	-1.38947600	-2.05139500	-0.00011600
H	-2.49377900	1.64149700	-0.00022000
H	-2.98690900	0.18059000	-0.89471000
H	2.49377900	1.64149700	0.00032800
H	2.98684100	0.18060400	0.89488000
H	0.00000000	1.94345100	-0.00017900

NHC^{Mes2}

47

C	-0.00003000	0.00049200	-0.28688800
N	1.06093900	0.00432500	0.58503500
C	0.67737000	0.00098000	1.92835500
N	-1.06095800	-0.00586200	0.58504600
C	-0.67736300	-0.00636100	1.92836400
H	1.39305300	0.00459800	2.73661100

H	-1.39302900	-0.01219000	2.73662200
C	2.42925200	0.01118400	0.15453800
C	3.11761200	-1.20588900	0.05773500
C	3.03670900	1.23439300	-0.16187300
C	4.45521100	-1.17457400	-0.34748000
C	4.37481800	1.21832200	-0.56480300
C	5.10180600	0.02653600	-0.65595900
H	5.00184800	-2.11165300	-0.43186700
H	4.85945600	2.15909000	-0.81810100
C	-2.42928200	-0.01162600	0.15455900
C	-3.11697400	1.20595600	0.05874000
C	-3.03737300	-1.23418900	-0.16286200
C	-4.45451900	1.17571600	-0.34653900
C	-4.37552800	-1.21706400	-0.56578900
C	-5.10181500	-0.02483800	-0.65597000
H	-5.00065900	2.11315500	-0.43021600
H	-4.86064800	-2.15736400	-0.81987400
C	2.24627400	2.51768000	-0.09214500
H	1.38139700	2.46865700	-0.76332000
H	1.85198700	2.69049200	0.91662000
H	2.86184200	3.37763900	-0.37232500
C	2.41212100	-2.50660600	0.35452000
H	2.07787800	-2.55620800	1.39787100
H	1.51483900	-2.60630700	-0.26697000
H	3.06597600	-3.36300000	0.16496100
C	6.55804900	0.03984300	-1.05928000
H	7.20934300	0.17255600	-0.18491500
H	6.84959100	-0.89883800	-1.54252400
H	6.77487200	0.85970400	-1.75264900
C	-2.24759900	-2.51795000	-0.09431000
H	-1.38233500	-2.46851500	-0.76496400
H	-1.85394600	-2.69227100	0.91444200

H	-2.86341600	-3.37725800	-0.37592800
C	-6.55809700	-0.03666500	-1.05919800
H	-6.77764500	-0.86129200	-1.74598300
H	-7.20980200	-0.16007400	-0.18377300
H	-6.84656400	0.89911700	-1.54990400
C	-2.41067500	2.50596000	0.35668200
H	-2.07546700	2.55390600	1.39980000
H	-1.51390400	2.60610200	-0.26547100
H	-3.06432200	3.36290600	0.16890300

[NHC^{Mes2}]H^{+}

48

C	0.00000000	0.00010900	-0.12909500
N	-1.08902300	0.00051100	0.64917400
C	-0.68183700	0.00060700	1.97463100
N	1.08902300	-0.00008400	0.64917200
C	0.68183900	0.00029900	1.97462900
H	-1.39986800	0.00085400	2.77954200
H	1.39987100	0.00032400	2.77954000
C	-2.45884000	0.00035300	0.17365100
C	-3.08554200	1.23566000	-0.04248400
C	-3.08552800	-1.23526100	-0.04170200
C	-4.40584300	1.20473200	-0.49723300
C	-4.40568900	-1.20468200	-0.49642800
C	-5.08215300	-0.00000500	-0.72608000
H	-4.91913100	2.14565700	-0.67726800
H	-4.91899200	-2.14572400	-0.67593300
C	2.45883900	-0.00019600	0.17364700
C	3.08537400	-1.23564900	-0.04227100
C	3.08569300	1.23527200	-0.04192400

C	4.40565900	-1.20498800	-0.49702300
C	4.40587000	1.20442500	-0.49664900
C	5.08215200	-0.00037000	-0.72608400
H	4.91882100	-2.14601500	-0.67690300
H	4.91929600	2.14536700	-0.67631300
C	-2.36257600	-2.53916000	0.19938000
H	-1.49024300	-2.64641500	-0.45793800
H	-1.99968200	-2.61799600	1.23112300
H	-3.02201500	-3.38976400	0.01257400
C	-2.36273200	2.53981600	0.19765300
H	-1.99901800	2.61904600	1.22907100
H	-1.49096900	2.64709100	-0.46042000
H	-3.02253000	3.39020100	0.01111800
C	-6.51955000	-0.00083300	-1.18449500
H	-7.19786400	-0.01610200	-0.32185500
H	-6.75521500	0.89277000	-1.77032700
H	-6.74617700	-0.88098300	-1.79395900
C	2.36293700	2.53932300	0.19891900
H	1.49053400	2.64651900	-0.45831300
H	2.00018600	2.61846500	1.23068900
H	3.02246100	3.38979700	0.01181700
C	6.51955500	-0.00001700	-1.18448400
H	6.74766000	0.88213200	-1.79047100
H	7.19787800	0.01062400	-0.32178100
H	6.75373900	-0.89171500	-1.77382900
C	2.36236900	-2.53965300	0.19810800
H	1.99856100	-2.61859500	1.22951500
H	1.49064500	-2.64696700	-0.46001100
H	3.02206900	-3.39016900	0.01182200
H	-0.00000200	-0.00006400	-1.20791400

NHC^{tBu_2}

33

N	-1.07566700	0.28082600	-0.00002800
N	1.05907100	0.24066700	-0.00001000
C	-0.02128800	-0.59526300	-0.00001400
C	0.69247300	1.58674200	-0.00002300
C	-0.66296500	1.61090200	0.00000700
C	-2.47927600	-0.21637600	-0.00000200
C	-3.46369400	0.95995700	-0.00003600
C	-2.68518500	-1.07013600	-1.26301800
C	-2.68515200	-1.07003500	1.26308700
C	2.46964900	-0.22116400	0.00000000
C	3.16479400	0.31436400	1.26540000
C	3.16490500	0.31463700	-1.26522500
C	2.50783000	-1.75442100	-0.00016600
H	1.40019400	2.40129600	0.00007300
H	-1.33497400	2.45360200	-0.00006800
H	-4.48594600	0.56896600	-0.00002400
H	-3.34668000	1.58693500	-0.89105600
H	-3.34668100	1.58698800	0.89094900
H	-3.69697100	-1.49148100	-1.27813800
H	-1.95500100	-1.88282000	-1.28294800
H	-2.54810200	-0.46155900	-2.16416700
H	-3.69696400	-1.49131100	1.27832000
H	-2.54795500	-0.46140000	2.16418100
H	-1.95502500	-1.88276500	1.28302700
H	2.65121600	-0.04668600	2.16250800
H	3.17041300	1.40946800	1.29179000
H	4.20509800	-0.02739600	1.29832700
H	4.20523400	-0.02705300	-1.29810100
H	3.17045700	1.40974800	-1.29140700

H	2.65145200	-0.04627700	-2.16246600
H	3.55417900	-2.08134500	-0.00023500
H	2.00480500	-2.16121000	-0.88038300
H	2.00488000	-2.16139600	0.88001200

[NHC^{tBu_2}]H$^+$

34

N	-1.10107100	0.29701900	0.00000100
N	1.08900400	0.26227800	0.00000500
C	-0.01643700	-0.49278800	-0.00002700
C	0.69539900	1.58863300	0.00005100
C	-0.66772200	1.61017300	0.00004700
C	-2.52803900	-0.21608500	-0.00001000
C	-3.48515500	0.97994100	-0.00000800
C	-2.72344500	-1.05740700	-1.27088700
C	-2.72345600	-1.05742400	1.27085500
C	2.52406600	-0.21628900	-0.00000200
C	3.19423600	0.32870800	1.27069600
C	3.19426300	0.32882500	-1.27063600
C	2.54417200	-1.74841100	-0.00007400
H	1.40360300	2.40061700	0.00008200
H	-1.34509900	2.44668600	0.00007200
H	-4.50994900	0.59971600	-0.00002600
H	-3.36496700	1.60056300	-0.89392300
H	-3.36499200	1.60054100	0.89392600
H	-3.75438200	-1.42081300	-1.30751400
H	-2.06540400	-1.93256800	-1.28721000
H	-2.53663600	-0.46175800	-2.16983100
H	-3.75439200	-1.42083400	1.30746700
H	-2.53665800	-0.46178500	2.16980800

H	-2.06540900	-1.93258100	1.28717300
H	2.68636200	-0.03297200	2.17024700
H	3.20298400	1.42280000	1.29018400
H	4.23333900	-0.01120600	1.30182800
H	4.23336700	-0.01108700	-1.30177700
H	3.20301500	1.42291900	-1.29002200
H	2.68640700	-0.03277000	-2.17023000
H	3.58569900	-2.07953900	-0.00008200
H	2.06950300	-2.16510900	-0.89507200
H	2.06949200	-2.16519300	0.89488000
H	-0.03870700	-1.56796200	-0.00006600

2·NHC^{Me_4} (1,1-water addition product)

124

P	-0.46301600	-0.62267500	0.36212500
P	1.32609300	0.12781100	-0.43847000
N	-3.13931800	2.99240800	0.15679800
N	-4.99564100	2.25641200	0.87423800
C	0.72096200	-0.47700000	-3.16892800
C	1.49366500	0.87440400	2.74279500
C	-0.73905300	-0.38453100	-2.86664100
C	0.78001500	2.09131000	2.69533200
C	2.88810300	0.86579000	2.53262400
C	-1.66350500	-2.98055800	1.65716500
C	0.77251600	-0.39274800	3.07124400
C	3.08516400	-0.40641400	-2.53733800
C	-0.73660100	-2.23007200	2.56819300
C	-0.02227200	-1.08423000	2.12029800
C	1.46197300	3.25735300	2.31466600
H	0.91094900	4.19456500	2.26190800

C	1.71749400	-0.29267500	-2.18201500
C	3.53144600	2.04840200	2.15601400
H	4.59635800	2.02297300	1.93812600
C	-1.38063300	0.86785600	-2.85259800
C	-1.46715700	-1.56466100	-2.60967500
C	2.83137800	3.24982700	2.01395100
C	-3.02632400	-2.62610200	1.58943600
C	-1.17724000	-4.06456300	0.89960000
C	-3.41354200	-4.44153900	-0.00184200
C	4.21719800	-0.24045500	-1.56778200
C	-2.06015900	-4.78105300	0.08864400
H	-1.68058300	-5.61827700	-0.49467200
C	-3.87572400	-3.36487700	0.75842400
H	-4.92722500	-3.08761100	0.70251100
C	-3.64869600	2.07003500	1.02846600
C	1.10518900	-0.77410300	-4.48245700
H	0.32674100	-0.91381700	-5.22742800
C	4.84832300	1.00997200	-1.42064900
C	3.42634000	-0.71018000	-3.86167600
H	4.47846500	-0.80043700	-4.11792600
C	-1.70952900	3.19213700	-0.01656800
H	-1.32303300	3.92658100	0.69967400
H	-1.49648300	3.54327800	-1.02659600
H	-1.20643500	2.23719300	0.13166900
C	0.29060400	-4.41501500	0.93268400
H	0.88656000	-3.57365900	0.55410800
H	0.50587200	-5.29260400	0.31468800
H	0.63892800	-4.61552700	1.95229500
C	2.44665200	-0.89061200	-4.83364800
H	2.72759700	-1.12184000	-5.85766900
C	-2.81174300	-1.46076000	-2.25562900
H	-3.35837500	-2.36385200	-1.99717100

C	-4.12475400	3.72445700	-0.51556200
C	0.88109600	-0.87147900	4.38425500
H	1.50164500	-0.32034700	5.08715200
C	-0.78830500	-2.91221600	-2.64942300
H	-0.31068200	-3.10102200	-3.61786900
H	-1.50071900	-3.71549300	-2.44780800
H	-0.00674800	-2.96602600	-1.88210400
C	-2.73059700	0.92693100	-2.49249900
H	-3.22904500	1.89192700	-2.45438600
C	5.94266700	1.11429100	-0.55471000
H	6.42902800	2.08104100	-0.43839300
C	3.68391300	-0.40740900	2.70482300
H	3.73745300	-0.69421700	3.76191900
H	4.70084500	-0.29090200	2.32537700
H	3.22101500	-1.25130300	2.18200800
C	-5.31768000	3.24613300	-0.06054600
C	-0.61543500	-2.67727500	3.88805100
H	-1.17412300	-3.55940100	4.19132600
C	-0.62657000	2.12236200	-3.23433700
H	0.14085200	2.37181900	-2.49333100
H	-1.30728800	2.97541300	-3.32500000
H	-0.11340800	2.00015000	-4.19540600
C	4.69448900	-1.36545000	-0.86315300
C	-0.67914600	2.14057800	3.07532600
H	-1.32280100	1.59264000	2.37850300
H	-1.04224900	3.17238400	3.11242800
H	-0.83048100	1.68900600	4.06257600
C	-3.56649300	-1.44461100	2.36094700
H	-3.18258900	-1.41850200	3.38602300
H	-4.66075400	-1.48423700	2.40823400
H	-3.28780700	-0.49113800	1.88958200
C	0.19987200	-2.01139300	4.80017500

H	0.29119300	-2.36638400	5.82315600
C	5.79769900	-1.21938400	-0.01915000
H	6.16406100	-2.08754700	0.52531200
C	-4.33940800	-5.19100100	-0.93160900
H	-4.32777300	-4.75269500	-1.93961000
H	-5.37606200	-5.16165700	-0.57840500
H	-4.04499700	-6.24149400	-1.03375400
C	4.36100400	2.22067200	-2.18152900
H	4.35575900	2.03784000	-3.26237500
H	4.99914300	3.08876600	-1.98691500
H	3.33579400	2.46991000	-1.89028900
C	-3.44954800	-0.22110800	-2.15445800
C	-3.82184900	4.78997100	-1.51662300
H	-3.19754500	5.58553100	-1.09028000
H	-4.74630800	5.25078700	-1.87661100
H	-3.28883100	4.39434500	-2.39174600
C	3.52971200	4.49011400	1.51030200
H	2.97266000	5.39916700	1.76025500
H	3.63599700	4.45553400	0.41774000
H	4.53764400	4.58133400	1.93037300
C	-5.98296700	1.47984500	1.59876000
H	-6.57696500	0.86096400	0.91542400
H	-6.66231000	2.13287400	2.15859800
H	-5.44783000	0.83377500	2.29388600
C	6.43186700	0.01498800	0.15481800
C	4.00647100	-2.70439900	-0.99865400
H	2.96899100	-2.65797400	-0.64197000
H	4.52381200	-3.47591300	-0.42065300
H	3.95892800	-3.03022500	-2.04390700
C	-6.72263000	3.60456900	-0.41414400
H	-7.26983400	2.74598100	-0.82570400
H	-6.74065900	4.39842600	-1.16645200

H	-7.28767500	3.96056700	0.45746600
C	-4.86589000	-0.13364400	-1.64131300
H	-5.50796000	-0.90207300	-2.08790200
H	-5.30684400	0.84916700	-1.83764800
H	-4.87306000	-0.28419800	-0.55503000
C	7.58700100	0.16052700	1.11748700
H	8.21143000	-0.73947000	1.13560800
H	7.22686000	0.32428300	2.14260400
H	8.22447500	1.01188600	0.85646200
H	2.46958000	-0.32925000	0.22438200
O	1.54411600	1.77298500	-0.55418400
H	1.36630500	2.20028400	0.30910700

2·NHC^{Me_4} (1,2-water addition product)

124

P	-0.23847900	0.43116400	0.49791300
P	-1.57174200	-1.36610000	-0.05366000
O	1.12063200	0.06476000	-0.21219400
C	-4.59619400	1.96093900	-1.63336500
H	-5.65479800	1.95295400	-1.38158500
C	-3.98611200	0.76454900	-2.02614500
C	-1.13441900	0.37621300	3.20485200
C	-1.91619400	-0.47905200	-2.79414100
C	2.79951700	-1.53142600	1.78997500
C	-3.32325500	-0.76130500	2.77223100
C	1.26297500	0.07743200	2.95809000
C	-3.88215900	3.15654200	-1.54198000
C	-2.61498000	0.76610800	-2.33943000
C	-0.01548300	0.17572800	2.35481300
C	-2.53714800	0.41178000	2.67536300

C	-2.52953800	3.14456300	-1.89662200
H	-1.96333200	4.07488800	-1.86170600
C	2.52680400	-0.21321000	2.20697400
C	1.50926300	-5.58304400	-0.28307200
C	-1.88552400	1.97344100	-2.30206000
C	-0.96969600	0.49581600	4.58892600
H	-1.85123100	0.64270000	5.20879400
C	1.52414500	-3.45695400	-1.48845600
C	-1.81161000	-0.66681500	-4.17886500
H	-2.28239500	0.05755300	-4.83941400
C	4.01626600	-1.80504400	1.16401100
H	4.22251500	-2.82357800	0.84176700
C	0.29497900	0.42293500	5.16925400
H	0.41651300	0.52165900	6.24488400
C	-1.32823200	-1.41070900	-1.89978900
C	-3.09717300	1.58449800	2.13677600
C	0.12194900	-5.63368800	-0.43460600
H	-0.42726200	-6.48176600	-0.02938900
C	0.12030300	-3.52341600	-1.62304700
C	-0.49262400	-2.64008300	-3.83873700
H	0.07286700	-3.48227100	-4.22964400
C	1.39764300	0.20650100	4.34986700
H	2.39090500	0.11572200	4.78425500
C	-0.58306000	-4.63175000	-1.10904900
C	-4.42174100	1.56085800	1.68374600
H	-4.84795900	2.47084900	1.26826200
C	-0.58945700	-2.48865800	-2.44710800
C	4.68369800	0.48966300	1.36192700
H	5.41655700	1.28062100	1.20186000
C	-4.63545700	-0.74393100	2.29756700
H	-5.23230800	-1.65190900	2.36314000
C	3.47758200	0.79998000	2.00274500

C	-5.20249800	0.40819000	1.74084500
C	2.19129200	-4.49463500	-0.83177400
H	3.27459100	-4.44421900	-0.73680200
C	4.97050700	-0.80779800	0.93359000
C	-0.43513400	2.00708700	-2.72886800
H	0.15363700	1.24733800	-2.20574900
H	0.00783200	2.98996200	-2.53150900
H	-0.33554900	1.80491800	-3.80257100
C	-1.11014500	-1.74671600	-4.70741800
H	-1.04117200	-1.88618100	-5.78337200
C	1.78216800	-2.62525900	1.99726800
H	1.34564400	-2.58225600	3.00058100
H	2.22274900	-3.61388700	1.84588300
H	0.96099800	-2.52171500	1.27960300
C	-2.75450900	-2.02764800	3.37324700
H	-1.82545200	-2.32084100	2.87364500
H	-3.46415600	-2.85596000	3.28114300
H	-2.51793700	-1.89630700	4.43574000
C	3.20616200	2.21810300	2.45572100
H	2.17589600	2.51480800	2.23210400
H	3.88745500	2.92645200	1.96952600
H	3.32780800	2.32865800	3.54037900
C	-4.79822100	-0.50883600	-2.07961100
H	-5.86518400	-0.28984000	-2.19402600
H	-4.67600500	-1.08840600	-1.15548700
H	-4.48772800	-1.15421200	-2.90668900
C	-4.53880200	4.42151800	-1.04270500
H	-5.62617100	4.38986900	-1.17086400
H	-4.16178100	5.30778200	-1.56645600
H	-4.33994400	4.56984700	0.02784200
C	-2.32238000	2.87807100	2.01777600
H	-1.37130800	2.83472100	2.55384400

H	-2.90586100	3.71711800	2.41836900
H	-2.11064000	3.08901400	0.96311600
C	2.25102900	-6.65307500	0.48295300
H	2.38123900	-6.36505400	1.53542600
H	3.25148900	-6.82457600	0.06918900
H	1.71112700	-7.60630500	0.47182400
C	2.29861300	-2.26987700	-2.01043700
H	2.13782100	-2.11703400	-3.08410800
H	3.37253800	-2.40224000	-1.83690300
H	1.96322500	-1.36602700	-1.48598000
C	-2.07797200	-4.74925400	-1.28471800
H	-2.43588700	-5.73790200	-0.97942500
H	-2.37346300	-4.58179300	-2.32676800
H	-2.59754400	-3.99572600	-0.67943100
C	6.26383700	-1.13596800	0.22355300
H	6.77863700	-1.98224100	0.69426900
H	6.95488300	-0.28492000	0.22712200
H	6.08696200	-1.41836300	-0.82387700
C	-6.61154300	0.39358500	1.19709600
H	-7.27404200	-0.22851900	1.80977600
H	-6.63490900	-0.01357700	0.17804300
H	-7.03629500	1.40256300	1.15540800
N	2.19691600	3.58367900	-0.57320100
N	3.68930400	2.29623300	-1.44713000
C	4.17366700	3.59876900	-1.57273000
C	3.22643800	4.41658600	-1.01659400
C	2.50002300	2.30660600	-0.83695700
H	1.89224100	1.38132200	-0.56977900
C	0.96357400	4.01499600	0.08320100
H	1.19943000	4.50498600	1.03159200
H	0.33874100	3.13461500	0.26658300
H	0.42410400	4.71011300	-0.56559300

C	3.17518100	5.89727600	-0.84970700
H	2.31082900	6.33155800	-1.36672600
H	4.07664200	6.35918100	-1.25937200
H	3.10349600	6.17984300	0.20756900
C	5.48864500	3.89816000	-2.20853400
H	6.31427600	3.41894500	-1.66829600
H	5.67366700	4.97492800	-2.21488500
H	5.52400100	3.54504300	-3.24629800
C	4.34392700	1.07580900	-1.91221800
H	4.37725300	1.06581300	-3.00544700
H	3.77449800	0.22205600	-1.54519700
H	5.35636600	1.02299900	-1.50844200
H	-2.76795700	-0.61212900	-0.06540100

2 (1,1-water addition product)

103

P	0.64899300	-0.41577900	-0.19944500
P	-1.03466500	0.45412800	0.66078600
O	0.69248800	-0.28078400	-1.86449200
C	-0.88436600	2.16665800	-0.09471600
C	0.18464800	3.07741700	0.09095500
C	0.11119300	4.36645600	-0.45760600
H	0.94848800	5.04364900	-0.30718800
C	-1.01010900	4.78707500	-1.16607900
H	-1.05586400	5.79239800	-1.57670100
C	-2.07553500	3.90676200	-1.33393700
H	-2.96324000	4.21654200	-1.87983900
C	-2.02607200	2.60688000	-0.81361900
C	1.42553000	2.74814500	0.86202600
C	1.40732400	2.72884600	2.27465900

C	2.59452800	2.47869400	2.96563300
H	2.57507300	2.45816100	4.05403400
C	3.80932500	2.27126800	2.30150600
C	3.81072700	2.31595000	0.90812600
H	4.74210200	2.16078900	0.37007300
C	2.63915400	2.54578400	0.17576300
C	0.13052200	2.98559500	3.03854400
H	-0.39550700	3.86496400	2.65112500
H	0.33298000	3.14468000	4.10255500
H	-0.55422500	2.13447500	2.94309900
C	5.07727500	2.01366900	3.08150100
H	4.96906900	1.14503500	3.74288900
H	5.33768000	2.86971000	3.71679200
H	5.92653600	1.82359000	2.41643200
C	2.70502300	2.56564400	-1.33744500
H	2.79701400	3.58906800	-1.72273900
H	1.80123700	2.14491800	-1.78773300
H	3.56979800	1.99477100	-1.69347800
C	-3.22413600	1.73192500	-1.04245700
C	-4.28036900	1.72765500	-0.11059100
C	-5.42721200	0.97759600	-0.38413600
H	-6.24585600	0.98589600	0.33252200
C	-5.54807300	0.21536000	-1.54867800
C	-4.48632100	0.22823400	-2.45690900
H	-4.56296300	-0.35385100	-3.37381300
C	-3.33008500	0.98118300	-2.22949600
C	-4.16892400	2.49756400	1.18502400
H	-3.40828700	2.05001100	1.83788300
H	-5.11899000	2.49608200	1.72937300
H	-3.86953800	3.53795500	1.01736600
C	-6.77923400	-0.62374400	-1.80005300
H	-6.68558900	-1.61834400	-1.34128600

H	-6.95098300	-0.77759900	-2.87103000
H	-7.67622800	-0.15859400	-1.37601300
C	-2.21015900	0.98636300	-3.24172200
H	-2.01396400	1.99967800	-3.61306200
H	-2.45191300	0.35096500	-4.10021200
H	-1.27602200	0.62525600	-2.79890700
C	0.92782700	-2.18994900	0.19159700
C	2.20882600	-2.71780800	-0.12382600
C	2.48556300	-4.06664200	0.12273000
H	3.47367400	-4.44783700	-0.12054400
C	1.51482200	-4.90865800	0.65753600
H	1.73854300	-5.95574500	0.84298100
C	0.25150500	-4.40006800	0.93810800
H	-0.52323700	-5.04650700	1.34051200
C	-0.06572300	-3.05268900	0.71119500
C	3.29513100	-1.90218300	-0.75781600
C	4.22213600	-1.20328300	0.03977200
C	5.22785700	-0.46236100	-0.58776200
H	5.94787900	0.07062700	0.02900000
C	5.32536300	-0.37635900	-1.97924700
C	4.41124200	-1.10102900	-2.75120600
H	4.49082200	-1.07297000	-3.83606000
C	3.40975000	-1.88421800	-2.16517900
C	4.11283000	-1.21997500	1.54565400
H	5.01398700	-0.80951400	2.00958300
H	3.95383900	-2.23325600	1.92833100
H	3.26760700	-0.60760100	1.88417800
C	6.37499000	0.49543200	-2.62705700
H	7.30170700	0.50851600	-2.04306700
H	6.02654200	1.53412100	-2.70568700
H	6.61500500	0.15427500	-3.63943800
C	2.48509200	-2.71604300	-3.02865900

H	2.64158600	-3.78605200	-2.84830000
H	2.66086500	-2.52318300	-4.09138700
H	1.43212900	-2.50947900	-2.81196400
C	-1.46245300	-2.63341300	1.04183800
C	-2.43858500	-2.57627900	0.02993700
C	-3.74542500	-2.22533000	0.37567100
H	-4.49313500	-2.15391300	-0.40851700
C	-4.10289100	-1.92779800	1.69149200
C	-3.11778400	-2.00262300	2.68121700
H	-3.38032500	-1.77131600	3.71205300
C	-1.80090500	-2.35107400	2.38057300
C	-2.07907500	-2.83189100	-1.41455400
H	-1.44501200	-2.02642800	-1.80585500
H	-2.97617100	-2.87377200	-2.03925100
H	-1.52565000	-3.77026500	-1.53853300
C	-5.51088400	-1.51491700	2.04817500
H	-6.20093800	-1.67374400	1.21391900
H	-5.54980900	-0.44950600	2.30616900
H	-5.88537400	-2.07472800	2.91382900
C	-0.74780000	-2.36856400	3.46463900
H	-1.18296600	-2.12653800	4.43904100
H	0.03500900	-1.62961400	3.25330400
H	-0.25483200	-3.34439000	3.54489100
H	1.91972300	0.12314200	0.06881100
H	1.61651400	-0.24900000	-2.18103300

2 (1,2-water addition product)

103

P	0.92732700	-0.37298400	-0.15576800
P	-1.01587900	0.49580400	0.60360900
C	-0.93814000	2.15478100	-0.25494500

C	0.06465200	3.14176700	-0.08412600
C	-0.04602400	4.36665800	-0.75460100
H	0.73239300	5.11145300	-0.61008800
C	-1.12410000	4.63236600	-1.59552900
H	-1.19548100	5.58762300	-2.10922300
C	-2.11230800	3.66824400	-1.76535800
H	-2.96601500	3.86357400	-2.40893400
C	-2.03775400	2.43412700	-1.10294900
C	1.26495300	2.93852100	0.78679000
C	1.16508300	3.12831900	2.18049200
C	2.29187200	2.91169900	2.97774200
H	2.21109200	3.04872200	4.05459400
C	3.52133500	2.53419900	2.42675300
C	3.60906100	2.40126100	1.04023300
H	4.55756300	2.11666300	0.59040500
C	2.50165100	2.59580400	0.20834200
C	-0.13100000	3.59575500	2.80479400
H	-0.44490300	4.55812700	2.38296800
H	-0.02595400	3.71673000	3.88743200
H	-0.95385700	2.89575200	2.62233700
C	4.71288300	2.24931700	3.31038600
H	4.71942100	1.19967900	3.63392000
H	4.70292900	2.86812700	4.21446500
H	5.65629000	2.43218400	2.78421500
C	2.66489500	2.44590200	-1.28857700
H	2.91081200	3.40848200	-1.75697700
H	1.74764000	2.08881000	-1.76460400
H	3.46970200	1.74116300	-1.52047700
C	-3.17637700	1.47640300	-1.31133700
C	-4.24651600	1.44751900	-0.39344800
C	-5.33601100	0.61001000	-0.64376800
H	-6.16170900	0.59456000	0.06461200

C	-5.38834900	-0.21457200	-1.77040600
C	-4.32221900	-0.16559100	-2.67106700
H	-4.34906700	-0.79041800	-3.56191600
C	-3.22203800	0.67488800	-2.46958600
C	-4.21255100	2.27571500	0.86882200
H	-3.53816300	1.81862800	1.60610000
H	-5.20586600	2.34295700	1.32455400
H	-3.84749500	3.29152400	0.68569500
C	-6.55018300	-1.15580200	-1.98641900
H	-6.38931600	-2.11035100	-1.46577200
H	-6.69092600	-1.38643400	-3.04792800
H	-7.48610200	-0.73416700	-1.60302800
C	-2.10214100	0.71216200	-3.48269200
H	-1.95356100	1.72393800	-3.87829200
H	-2.31458600	0.04651800	-4.32554800
H	-1.15664800	0.39994400	-3.02777300
C	1.00574700	-2.17739300	0.32145700
C	2.25775600	-2.74975400	-0.02773400
C	2.54144300	-4.08118600	0.29009500
H	3.50563500	-4.49599400	0.00743600
C	1.60313700	-4.86272400	0.96095000
H	1.82864100	-5.89569100	1.21276500
C	0.37164500	-4.31150800	1.29986700
H	-0.37547100	-4.91408700	1.80995100
C	0.05301000	-2.98056900	0.98529400
C	3.29160700	-1.95596700	-0.77274200
C	4.23955500	-1.18086100	-0.07221900
C	5.18686500	-0.45278300	-0.79597200
H	5.91758300	0.14420800	-0.25339700
C	5.21549600	-0.46126700	-2.19430200
C	4.28561700	-1.25845900	-2.86819200
H	4.31019300	-1.30028800	-3.95553100

C	3.33345500	-2.02177500	-2.18207200
C	4.19741700	-1.08875000	1.43274200
H	5.11260100	-0.63678200	1.82752100
H	4.06457600	-2.07097000	1.89773500
H	3.35469900	-0.45901200	1.74634900
C	6.20861800	0.38947100	-2.95060200
H	7.17258100	0.43798000	-2.43189000
H	5.84437100	1.42068200	-3.05327200
H	6.38503600	0.00325100	-3.95999800
C	2.37314500	-2.90963700	-2.94314000
H	2.52236000	-3.96450100	-2.68474500
H	2.51203700	-2.80391400	-4.02384200
H	1.33219500	-2.66945300	-2.70270300
C	-1.31217400	-2.50603700	1.36684700
C	-2.35309600	-2.54009500	0.41916200
C	-3.62906900	-2.12626300	0.80536700
H	-4.42715700	-2.12954300	0.06877800
C	-3.89466400	-1.66609300	2.09698300
C	-2.84760500	-1.64562900	3.02281100
H	-3.03762700	-1.29203900	4.03486200
C	-1.55876400	-2.06389100	2.68102800
C	-2.08352500	-2.94752000	-1.01010800
H	-1.41359500	-2.22893300	-1.49787200
H	-3.01094500	-2.98181300	-1.58937300
H	-1.59692000	-3.92836400	-1.06851200
C	-5.26779300	-1.16493000	2.47689100
H	-6.03964500	-1.56455900	1.81104100
H	-5.31469900	-0.07053000	2.40898600
H	-5.52744100	-1.44020800	3.50556700
C	-0.43954700	-2.00412300	3.69662700
H	-0.79504600	-1.60901800	4.65327200
H	0.37955000	-1.36141900	3.34983000

H	-0.00172600	-2.99281500	3.87715200
H	-0.36270000	0.86986700	1.81245500
O	0.48776300	-0.49957300	-1.79840600
H	1.28518500	-0.29582400	-2.31518000

2·NHC^{iPr_2Me_2} (1,2-water addition product)

136

P	-0.02672000	-0.55774600	-0.41706800
P	-1.87025100	-0.02152600	0.44560100
N	3.98637300	2.72543300	0.29689300
N	5.70423400	1.56113500	-0.22000900
C	-1.40823200	-1.29499000	2.96791100
C	-2.00985200	1.37246500	-2.48359000
C	0.06563600	-1.26807300	2.72932500
C	-1.39547600	2.57889600	-2.08669700
C	-3.41215600	1.24212700	-2.40396900
C	1.33073800	-2.49635900	-2.18725100
C	-1.18230900	0.26354100	-3.05191400
C	-3.73572900	-0.90496900	2.32032300
C	0.40642700	-1.57202200	-2.92662100
C	-0.38292800	-0.59714300	-2.25363200
C	-2.18302900	3.59048000	-1.51702300
H	-1.70390900	4.51416300	-1.19724900
C	-2.35027200	-0.81552600	2.03021200
C	-4.16353200	2.27120100	-1.82956700
H	-5.23649500	2.14160700	-1.72059600
C	0.81443500	-0.10911000	3.01341100
C	0.69758300	-2.42675800	2.23811300
C	-3.56695800	3.44178200	-1.35437200
C	2.69305300	-2.16582700	-2.03503400

C	0.84693500	-3.73263600	-1.71136900
C	3.08499300	-4.31206800	-0.92861700
C	-4.81948400	-0.44244500	1.39269000
C	1.73039700	-4.61944800	-1.09199100
H	1.35343000	-5.57536100	-0.73218300
C	3.54372100	-3.08384100	-1.40784700
H	4.59718000	-2.83150700	-1.29903000
C	4.54755700	2.06083400	-0.75745400
C	-1.86158700	-1.85086100	4.17169400
H	-1.12283600	-2.21513200	4.88012200
C	-5.39404000	0.83378100	1.55582100
C	-4.14674300	-1.47463000	3.53200100
H	-5.21161700	-1.54284300	3.73729800
C	2.73452400	3.46935200	0.07656600
H	2.48778200	3.19397900	-0.95012900
C	-0.61424500	-4.08310700	-1.85701300
H	-1.23546000	-3.35120600	-1.32459700
H	-0.82857600	-5.07600100	-1.44894900
H	-0.93150800	-4.06489800	-2.90618700
C	-3.21939500	-1.94164300	4.45905100
H	-3.55412200	-2.37611100	5.39723500
C	2.06912200	-2.38997300	1.98398100
H	2.54717400	-3.26494000	1.55498300
C	4.77117200	2.66126800	1.45672600
C	-1.20809000	0.11367000	-4.44612000
H	-1.83083200	0.78973900	-5.02746000
C	-0.10189600	-3.66690300	1.92035600
H	-0.64044900	-4.04505400	2.79712000
H	0.54435900	-4.46095100	1.53806400
H	-0.85044600	-3.44818800	1.14930800
C	2.18540100	-0.11762300	2.74767800
H	2.77009300	0.77709700	2.94546300

C	-6.45266300	1.20753200	0.72170700
H	-6.89300900	2.19540600	0.84333200
C	-4.10060400	-0.00293500	-2.91439700
H	-4.03792400	-0.06811600	-4.00681700
H	-5.15354300	-0.01626900	-2.62534100
H	-3.62891100	-0.91287400	-2.52639500
C	5.87148000	1.91950100	1.12621300
C	0.36154200	-1.69118800	-4.31981800
H	0.97712900	-2.45077600	-4.79532800
C	0.14830900	1.12285100	3.58382300
H	-0.51192000	1.59727300	2.84888800
H	0.89344500	1.86210100	3.89335000
H	-0.46940700	0.87606300	4.45515700
C	-5.32247100	-1.32888700	0.41830200
C	0.08810900	2.77066300	-2.26998900
H	0.65138200	2.04621400	-1.67159700
H	0.39639400	3.77906700	-1.97733000
H	0.37792400	2.61020200	-3.31431600
C	3.24540000	-0.84031900	-2.50453800
H	2.79699900	-0.51940400	-3.44930800
H	4.33001900	-0.89823700	-2.64467300
H	3.06796000	-0.03806300	-1.77709700
C	-0.44744600	-0.85791200	-5.08801800
H	-0.47571000	-0.95621800	-6.16978200
C	-6.38798800	-0.91798900	-0.38709000
H	-6.77556100	-1.60335500	-1.13836700
C	4.01790600	-5.26615100	-0.21950000
H	4.03001400	-5.08007100	0.86382400
H	5.04844600	-5.16020400	-0.57610900
H	3.71434700	-6.30906400	-0.36345000
C	-4.88831700	1.78359100	2.61586300
H	-4.97000400	1.34489700	3.61728600

H	-5.45872900	2.71819500	2.60871000
H	-3.83273100	2.01777000	2.44883800
C	2.82322000	-1.23796700	2.20804400
C	4.42390000	3.28282700	2.77243800
H	4.22941800	4.35708500	2.68439100
H	5.24919000	3.15774200	3.47892000
H	3.53584500	2.82920100	3.22753000
C	-4.39022700	4.48806400	-0.64347300
H	-3.89653500	5.46550100	-0.64674600
H	-4.55142700	4.20038700	0.40406800
H	-5.37815200	4.60213800	-1.10330100
C	6.65360700	0.86571200	-1.10512900
H	6.08194900	0.76929600	-2.03206300
C	-6.96076700	0.35054800	-0.25781000
C	-4.71215600	-2.69974000	0.23523100
H	-3.66459100	-2.63458800	-0.08713800
H	-5.25635500	-3.27747700	-0.51776800
H	-4.71157500	-3.26846000	1.17197400
C	7.00687400	1.49123800	2.00031100
H	6.96856500	0.41836600	2.22579800
H	6.97201600	2.02483000	2.95433300
H	7.98288900	1.69617300	1.54826500
C	4.28314300	-1.17662600	1.83753500
H	4.66168000	-2.15584200	1.52772500
H	4.89872200	-0.81743700	2.67139700
H	4.42992800	-0.47938500	1.00607400
C	-8.06918000	0.79690200	-1.18186500
H	-8.70212400	-0.04326100	-1.48753800
H	-7.66056600	1.24406400	-2.09900400
H	-8.70826800	1.55107800	-0.71036500
H	-2.96235800	-0.33306800	-0.37071500
O	-2.13104000	1.54823700	0.91696400

H	-1.93903500	2.16265400	0.17833300
C	7.02163700	-0.54249200	-0.62540000
H	7.59555000	-1.05271000	-1.40729100
H	7.63795300	-0.52843900	0.27841900
H	6.12255800	-1.13050100	-0.42186700
C	7.88538400	1.73126700	-1.40013100
H	7.57501300	2.71895800	-1.75522800
H	8.51599600	1.86537700	-0.51492200
H	8.49831900	1.25888500	-2.17630200
C	1.58952000	3.01102300	0.98243500
H	1.73485700	3.31989200	2.02197500
H	0.64961900	3.45747200	0.63814700
H	1.47615300	1.92441200	0.94765300
C	2.95430300	4.98668700	0.11295100
H	3.78289300	5.26885300	-0.54450400
H	2.04821300	5.49864900	-0.23212900
H	3.17237100	5.35059700	1.12244700

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