Supporting Information

for

Uncovering diverse reactivity of NHCs with diazoalkane: C-H activation, C=C bond formation, and access to N-heterocyclic methylenehydrazine

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Contents

1. General procedures and instrumentation

All manipulations and experiments were performed in an inert atmosphere of argon using standard Schlenk techniques (unless otherwise mentioned) and in an argon-filled MBRAUN glove box. The solvents, toluene, THF, and hexane were purified by MBRAUN solvent purification system MB SPS-800 and stored over activated 4 Å molecular sieves before use. All chemicals were purchased from Sigma Aldrich and TCI chemicals (0.6 M Me_3SiCHN_2 solution in hexane) and used without further purification. The starting materials 6-SIPr, 5-IPr, 5-SIPr, 5-I^{t}Bu, and DAC carbenes were synthesized using a literature procedure.[1] Deuterated NMR solvents, benzene-d_6, $CDCl_3$ and THF-d_8 were stored over 4 Å molecular sieves at least 48 h before use. The ^{1}H, ^{13}C, and ^{29}Si NMR spectra were recorded in a Bruker Avance DPX 400 and Bruker Avance DPX 500 spectrometer. High-resolution mass spectra (HRMS) were obtained using a Q Exactive Thermo Scientific. The IR Spectra were acquired by using Bruker Alpha-II ECO-ATR spectrophotometer using solid samples in the 500-4000 cm^{-1} range. Melting points were measured in a sealed glass tube on a Stuart SMP-30 melting point apparatus.

2. Experimental section with spectroscopic details

Synthesis of 1: 5-SIPr (0.200 g, 0.51 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C for 10 min. After that, Me_3SiCHN_2 (0.938 mL, 0.56 mmol) was added to the solution resulting in a yellow-colored solution. The reaction was run for 18 hours while slowly warming to room temperature. All the volatiles were removed and the residue was dissolved in 6-8 mL of hexane. The solution was filtered using a cannula, concentrated to 2 mL, and stored at room temperature to get block-shaped yellow crystals of **1** and **2** after one day with a total yield of 56% of **1** and 9% of **2** calculated from NMR. **2** resulted from the hydrolysis of 5-SIPr due to the adventitious amount of water.

1 and **2** could not be separated as both crystallized simultaneously.

^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = -0.38 (singlet, 9 H, Si(C***H***$_3$)$_3$), δ = 1.21 (d, *J* = 6.75 Hz, 6 H, CH(C***H***$_3$)$_2$), δ = 1.27 (d, *J* = 6.88 Hz, 6 H, CH(C***H***$_3$)$_2$), δ = 1.34 (d, *J* = 6.88 Hz, 6 H, CH(C***H***$_3$)$_2$), δ = 1.49 (d, *J* = 6.88 Hz, 6 H, CH(C***H***$_3$)$_2$), 3.47 (multiplet, merging sept with NC*H*$_2$C***H***$_2$N, *J* = 6.88 Hz, 2 H, C***H***(CH$_3$)$_2$), 3.48

(multiplet, merging quart with C***H***$(CH_3)_2$), *J* = 2.63 Hz, 2 H, NCH_2C***H***$_2$N), 3.77 (quart, *J* = 2.63 Hz, 2 H, NC***H***$_2$CH_2N), 4.19 (sept, *J* = 6.88 Hz, 2 H, C***H***$(CH_3)_2$), 5.14 (singlet, C-***H***), 7.09 (multiplet, 4 H, Ar-***H***), 7.19 (t, 2 H, Ar-***H***) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, C_6D_6): δ = -1.62 (Si(***C***$H_3)_3$), δ = 23.89, 24.26, 26.11, 26.26 (CH(***C***$H_3)_2$), 27.65 (***C***H$(CH_3)_2$), 28.80 (N***C***H_2***C***H_2N), 53.06 (SiMe_3***C***NN), 83.92 (N***C***N), 124.44, (Ar-C), 124.77 (Ar-C), 127.76 (Ar-C), 139.75 (Ar-C), 149.20 (Ar-C), 151.75 (Ar-C).

^{29}Si (79.49 MHz, 298 K, C_6D_6): -2.10 ppm

HRMS: m/z calcd for $[M+H]^+$ $C_{31}H_{49}N_4Si$, 505.84; found **505.37**.

IR (cm^{-1}): 2960.88, 2037.15, 1653.64, 1453.63, 1255.69, 1096.93, 1045.38, 802.07.

Melting point range: 77-85 ˚C.

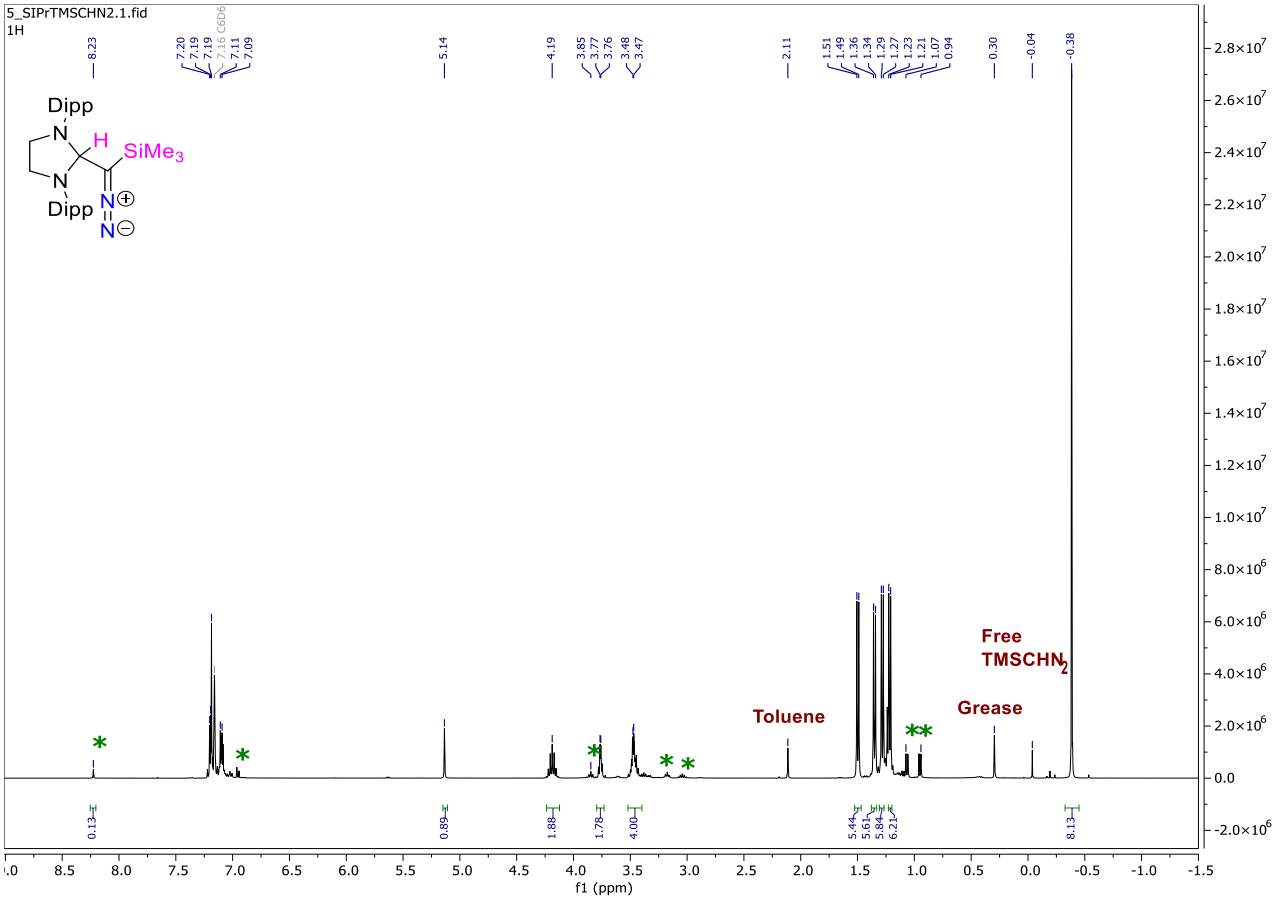


Figure S1: ^{1}H NMR spectrum of **1** (Peak at -0.04 belongs to free Me_3SiCHN_2, Peaks with green asterisks belong to **2**)

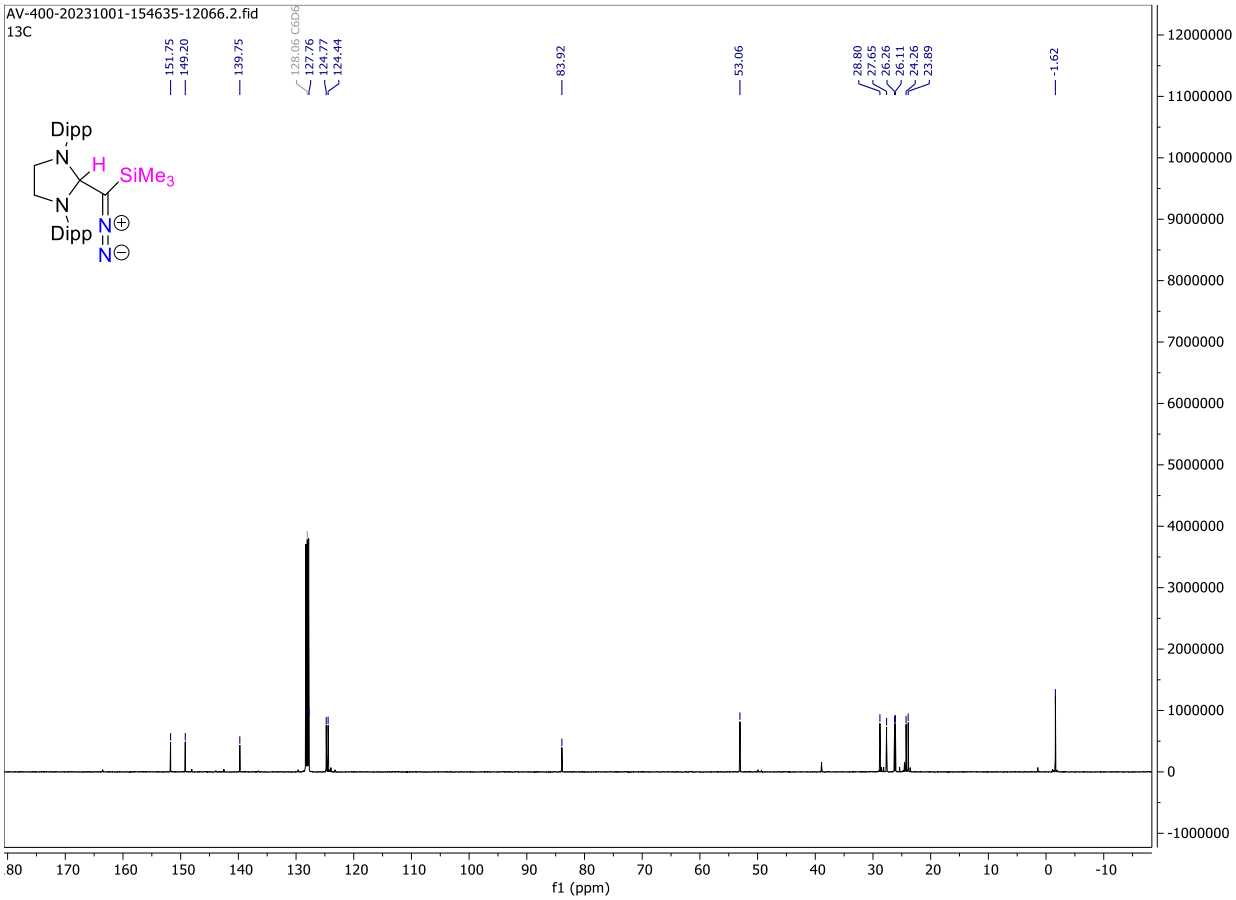


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **1**

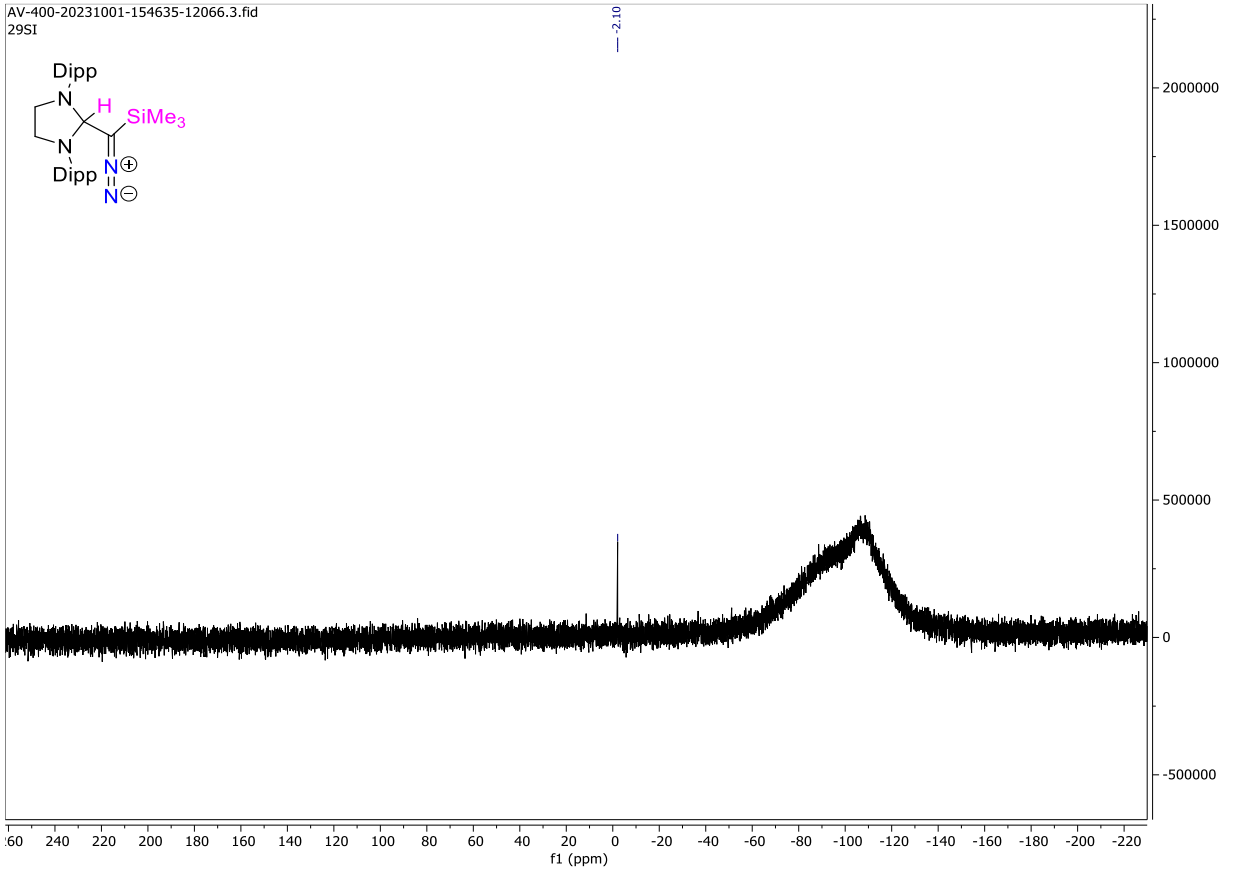


Figure S3: $^{29}Si\{^{1}H\}$ NMR spectrum of **1**

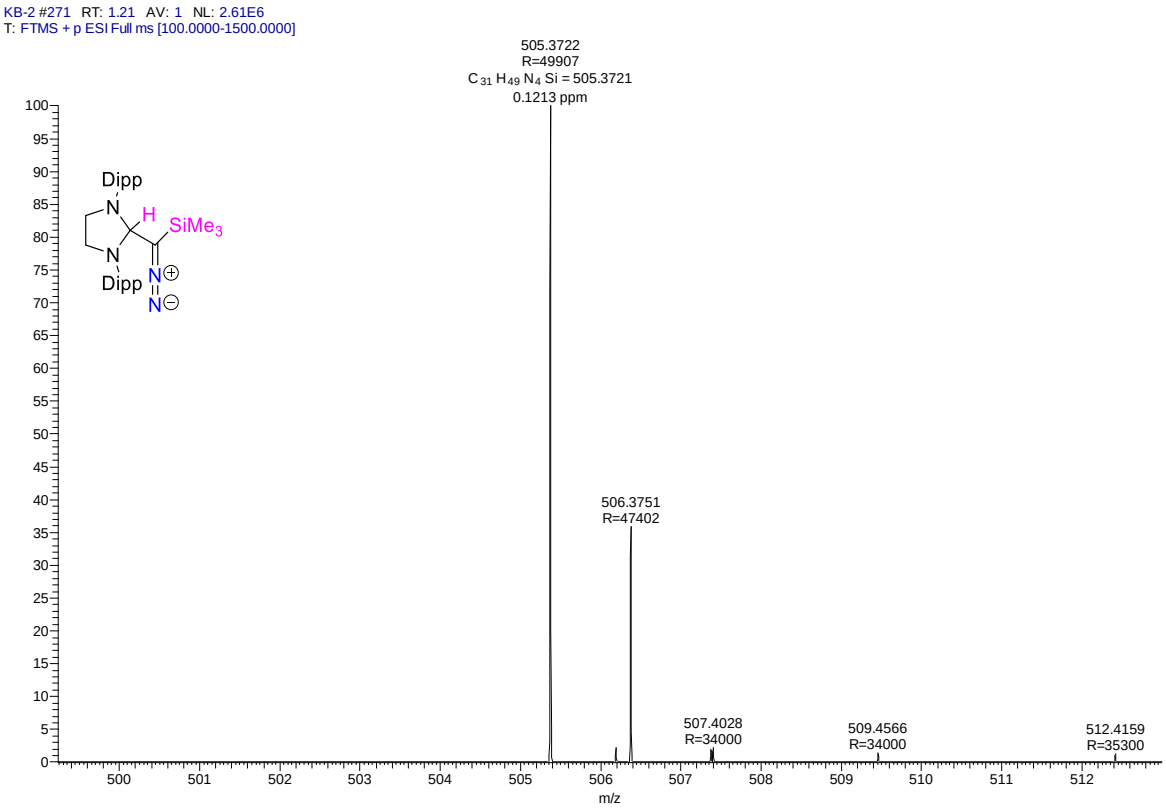


Figure S4: HRMS spectrum of **1**

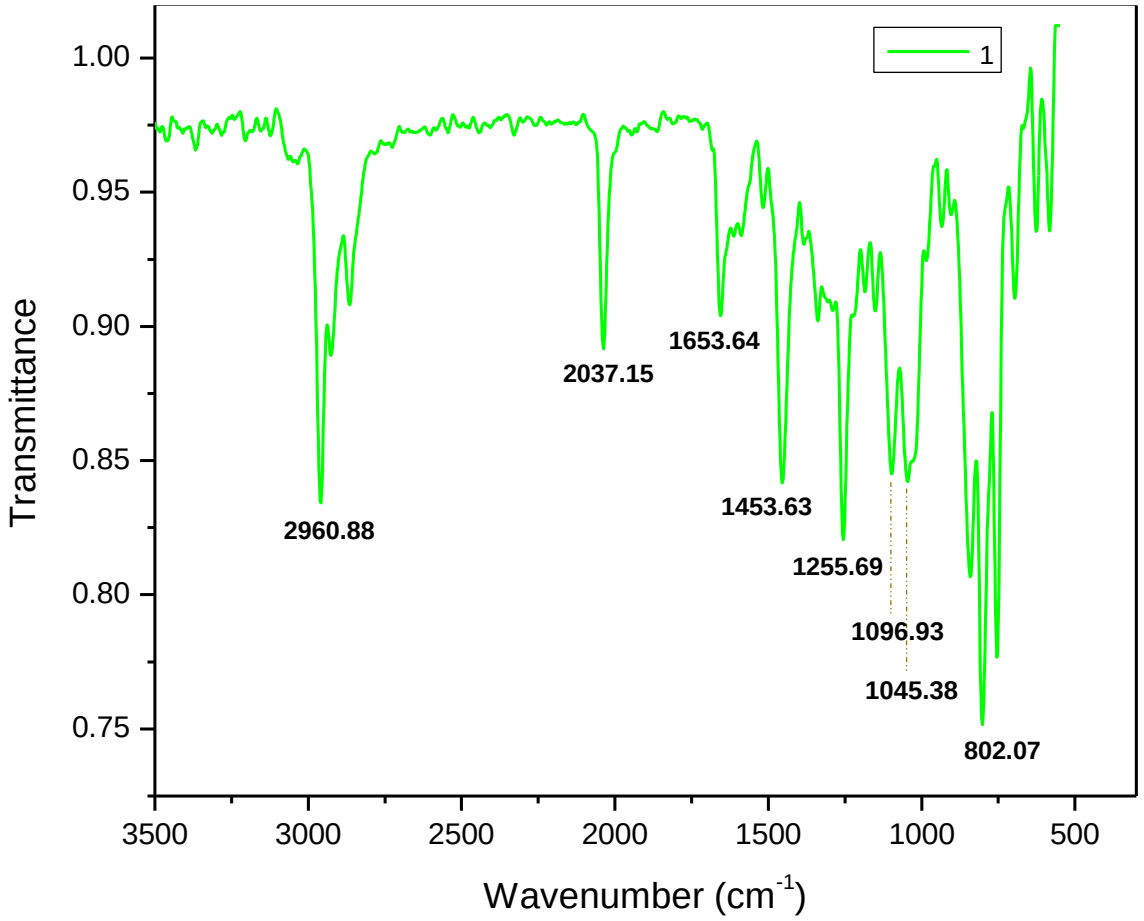


Figure S5: IR (ATR) spectrum of **1**

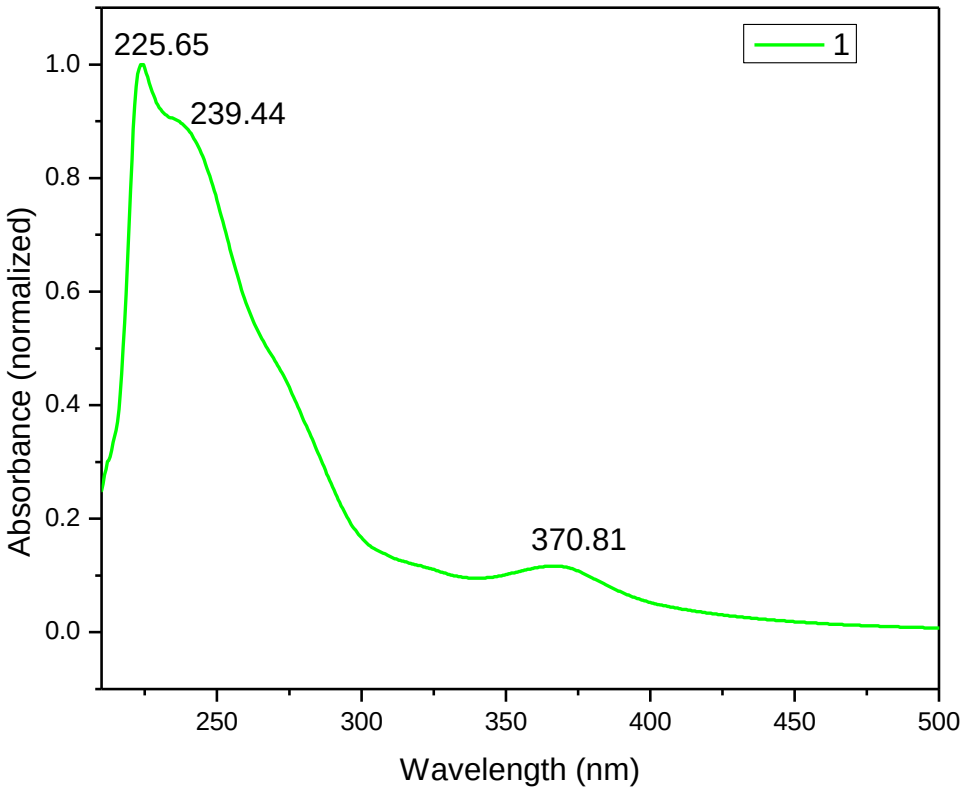


Figure S6: UV-VIS spectrum of **1** in THF

Synthesis of 3: 6-SIPr (0.200 g, 0.49 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C for 10 min. After that, Me_3SiCHN_2 (0.90 mL, 0.54 mmol) was added to it resulting in a yellow-colored solution. The reaction was run for 20 hours while slowly warming to room temperature. All the volatiles were removed and the residue was dissolved in 6-8 mL of hexane. The solution was filtered using a cannula, concentrated to 3 mL, and stored at room temperature to get plate-shaped yellow crystals of **3** after a day with a yield of 68%.

^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = -0.21 (singlet, 9 H, Si(C***H***$_3$)$_3$), 1.31 (broad d, *J*= 4.77 Hz, 12 H, CH(***C***H$_3$)$_2$), 1.42 (broad d, *J*= 13.20 Hz, 12 H, CH(***C***H$_3$)$_2$), 1.62 (quint, *J* = 5.99 Hz, 2 H, NCH$_2$***C***H$_2$CH$_2$N), 3.14 (t, *J* = 5.99 Hz, 4 H, NC***H***$_2$CH$_2$C***H***$_2$N), 3.33 (sept, *J* = 6.72, 4 H, C***H***(CH$_3$)$_2$), 7.08 (broad, 4 H, Ar-H), 7.40 (singlet, 1 H, NNC***H***SiMe$_3$) ppm.

^{13}C{^{1}H} NMR (125.7 MHz, 298 K, $CDCl_3$): δ = -1.70 (Si(***C***H$_3$)$_3$), 23.46 (NCH$_2$***C***H$_2$CH$_2$N), 24.18(CH(***C***H$_3$)$_3$), 24.93 (CH(***C***H$_3$)$_3$), 28.92 (***C***H(CH$_3$)$_3$), 49.28 (N***C***H$_2$CH$_2$CH$_2$N), 52.91(NCH$_2$CH$_2$***C***H$_2$N), 123.74 (Ar-C), 126.70 (Ar-C), 127.40 (Ar-C), 141.02 (Ar-C), 144.24 (Ar-C), 146.23 (Ar-C), 151.37 (***C***NNCHSiMe$_3$), 156.01 (NN***C***HSiMe$_3$) ppm.

^{29}Si (79.49 MHz, 298 K, $CDCl_3$): -11.16 ppm.

HRMS: m/z calcd for [M+H]$^+$ $C_{34}H_{51}N_4Si$, 519.87; found **519.38**.

IR (cm^{-1}): 2956.76, 1550.54, 1494.87, 1455.70, 1290.74, 1249.51, 1210.33, 1045.38, 833.00.

Melting point range: 125-130 ˚C.

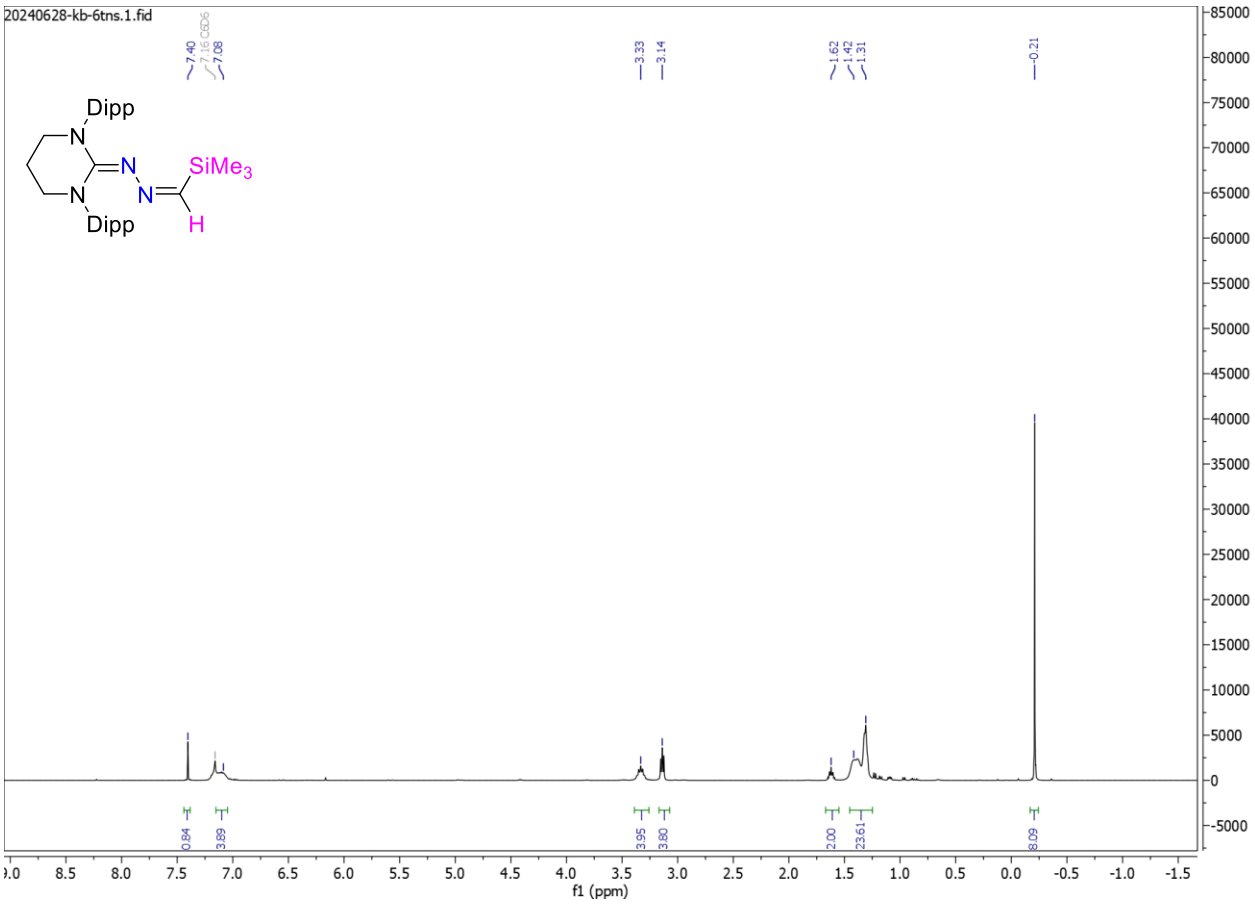


Figure S7: ^{1}H NMR spectrum of **3** (Smaller peaks in the region 1.4-0.75 ppm belong to minor impurities)

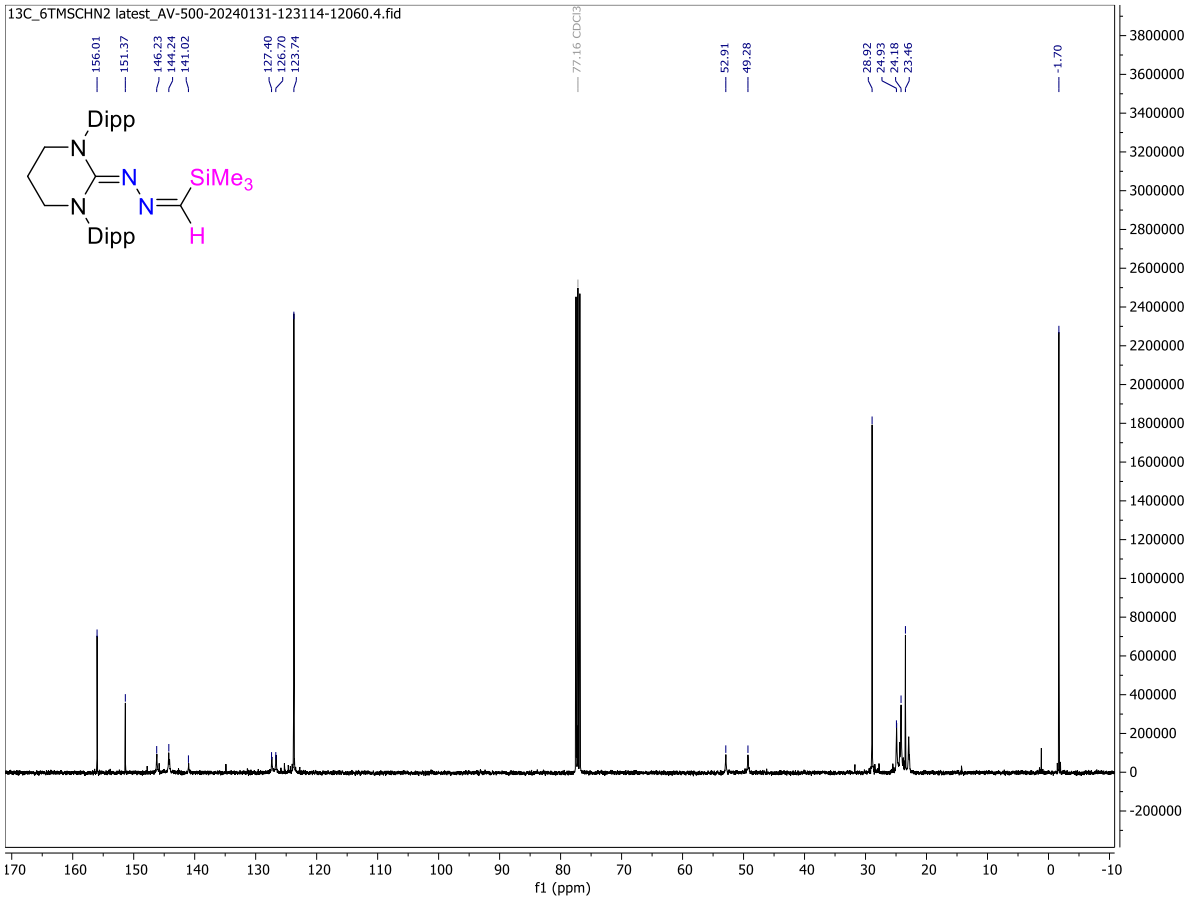


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of **3**

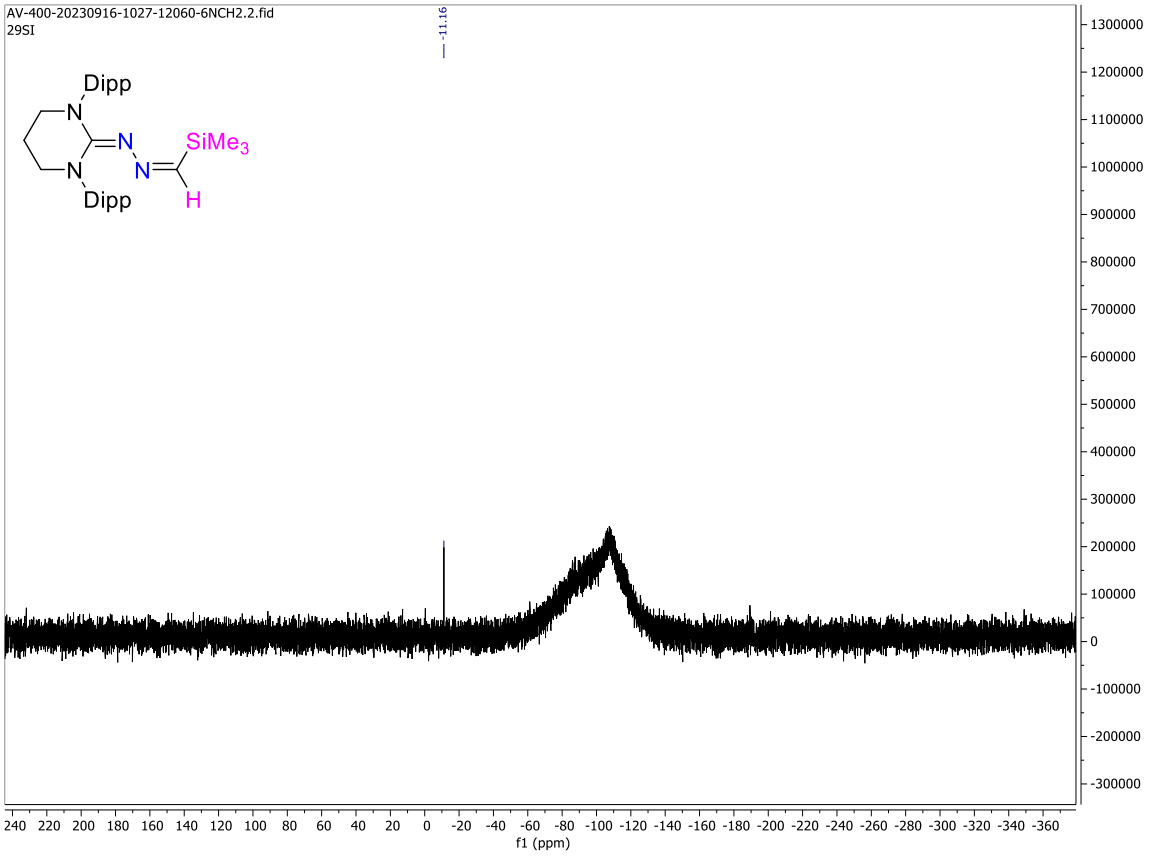


Figure S9: ^{29}Si NMR spectrum of **3**

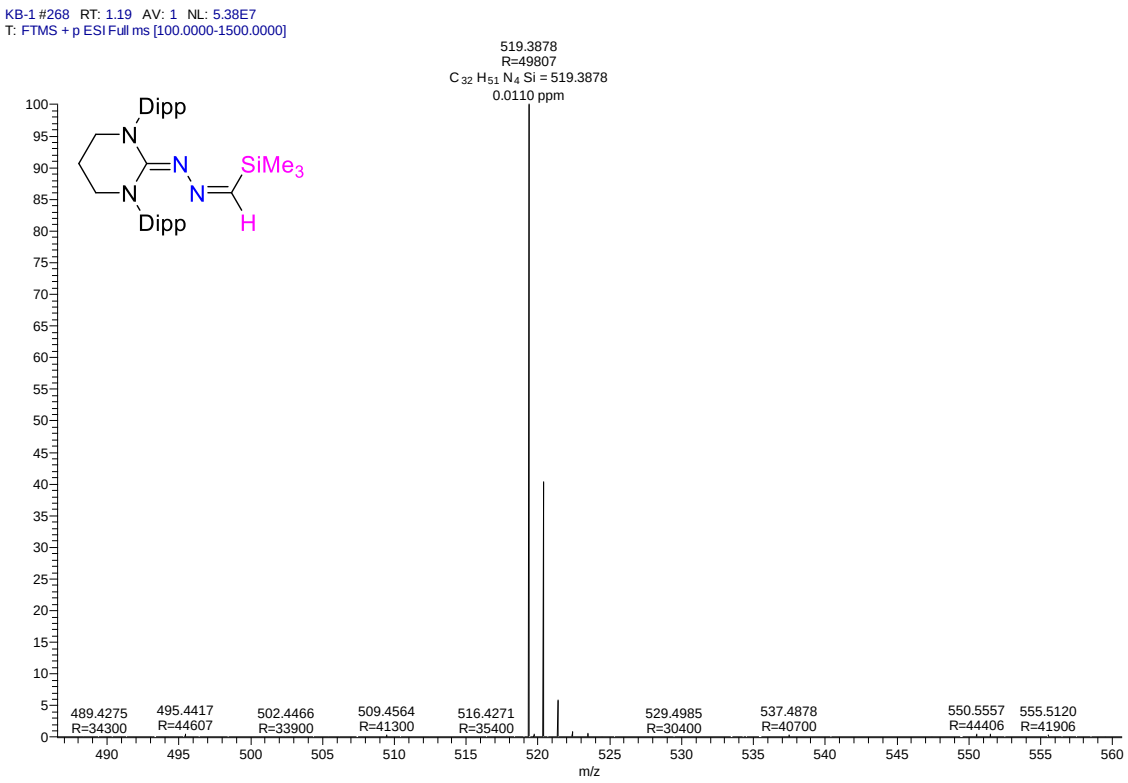


Figure S10: HRMS spectrum of **3**

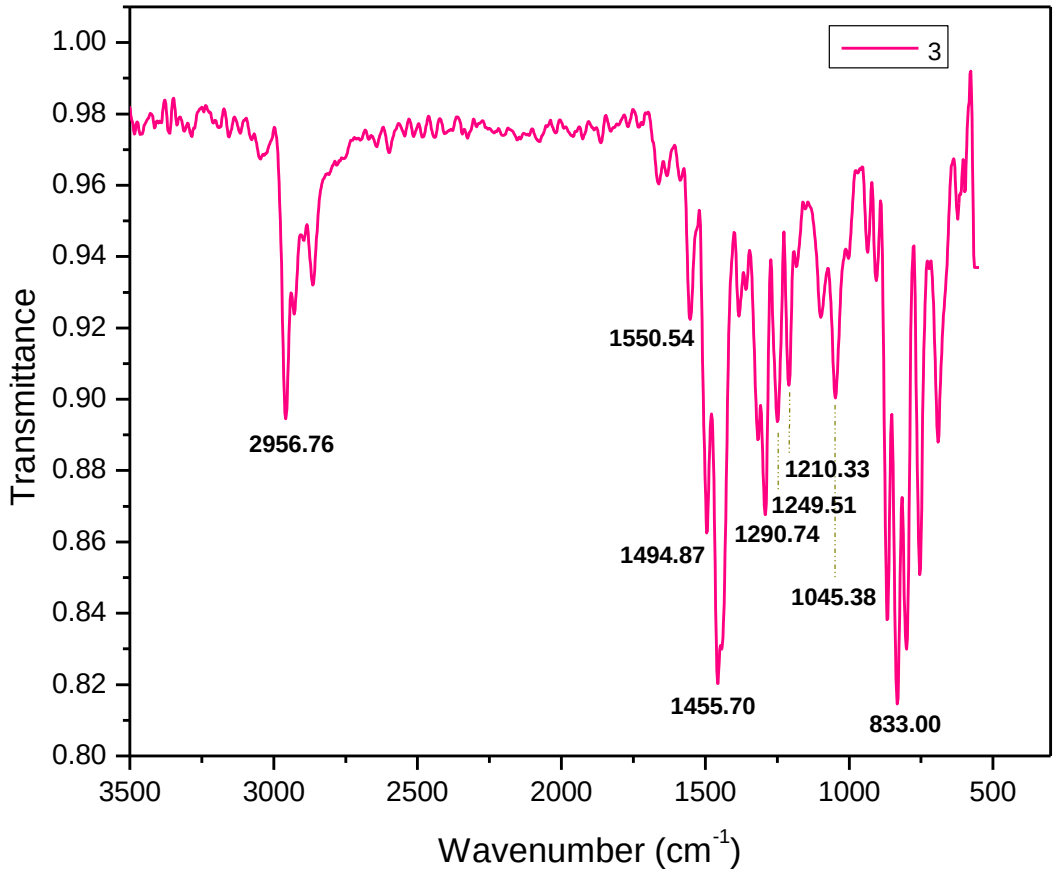


Figure S11: IR (ATR) spectrum of **3**

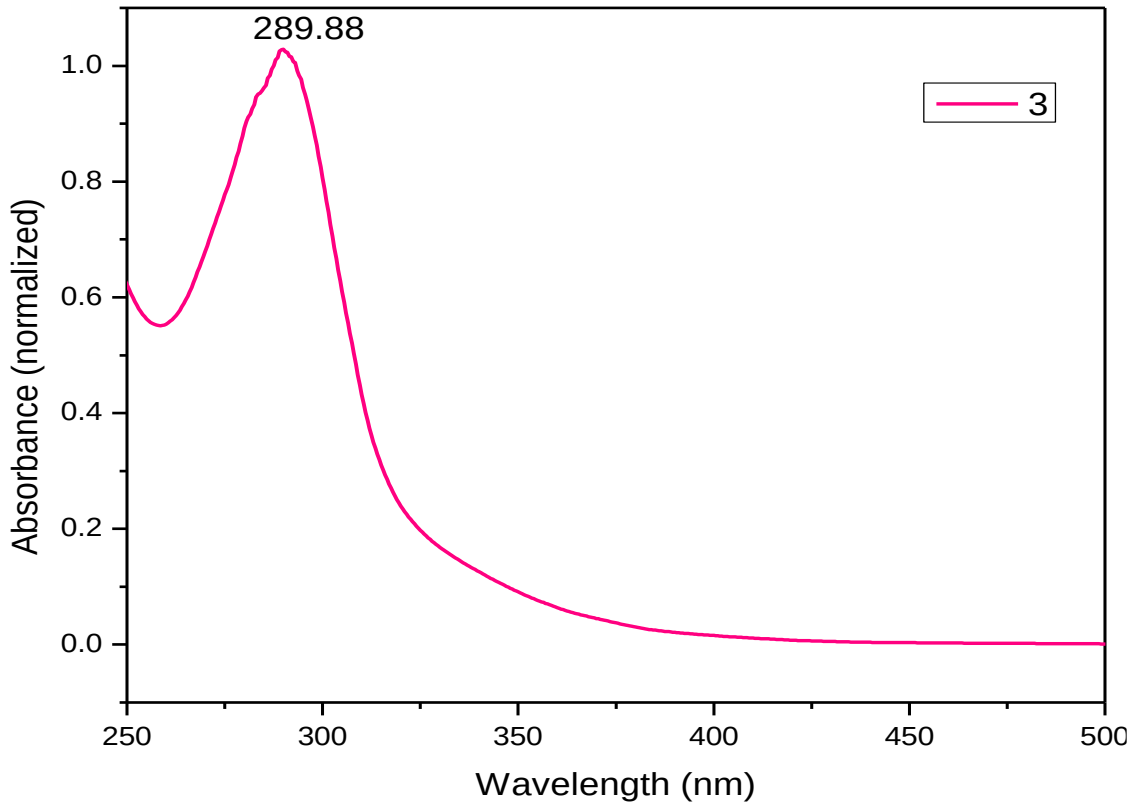


Figure S12: UV-VIS spectra of **3** in THF

Synthesis of 4: 5-IPr (0.200 g, 0.51 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C for 10 min. After that, $SiMe_3CHN_2$ (0.943 mL, 0.56 mmol) was added to it at low temperature. The reaction was run for 24 hours while slowly warming to room temperature, resulting in a deep red solution. The solution was filtered using a cannula. All the volatiles were removed, resulting in a red-colored sticky compound, which gets solidified after keeping the flask in a glove box to afford pure red-colored solid, **4** within 24 h with a yield of 85%.

After several attempts, crystals of **4** were obtained by slow evaporation of $CDCl_3$ in a *vial* at room temperature.

^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = -0.18 (singlet, 9 H, Si(C***H***$_3$)$_3$), 1.23 (d, *J* = 6.88 Hz, 12 H, CH(C***H***$_3$)$_2$), 1.38 (d, *J* = 6.88 Hz, 12 H, CH(C***H***$_3$)$_2$), 3.18 (broad sept, 4 H, C***H***(CH$_3$)$_2$), 5.83 (broad singlet, 2 H, NC***H***C***H***N), 7.12 (d, *J* = 7.75 Hz, 4 H, Ar-H), 7.23 (t, 2 H, *J* = 7.50 Hz, Ar-H), 7.68 (singlet, 1 H, NNC***H***SiMe$_3$) ppm.

^{13}C{^{1}H} NMR (125.7 MHz, 298 K, $CDCl_3$): δ= -1.95 (Si(***C***H$_3$)$_3$), 22.69, 23.97 (CH(***C***H$_3$)$_2$, 28.95 (***C***H(CH$_3$)$_2$, 114.74 (N***C***HCHN), 117.10 (NCH***C***HN), 123.35 (Ar-C), 124.04 (Ar-C), 128.36 (Ar-C), 129.17 (Ar-C), 145.50 (Ar-C), 147.27 (Ar-C), 150.60 (***C***NNCHSiMe$_3$), 155.22 (NN***C***HSiMe$_3$).

^{29}Si (79.49 MHz, 298 K, C_6D_6): -10.88 ppm.

IR (cm^{-1}): 2958.82, 1591.78, 1503.12, 1463.94, 1356.73, 1249.51, 1055.69, 938.16, 837.13.

HRMS: m/z calcd for $[M+H]^+$ $C_{31}H_{47}N_4Si$, 503.35; found **503.35.**

Melting point range: 90-95 ˚C.

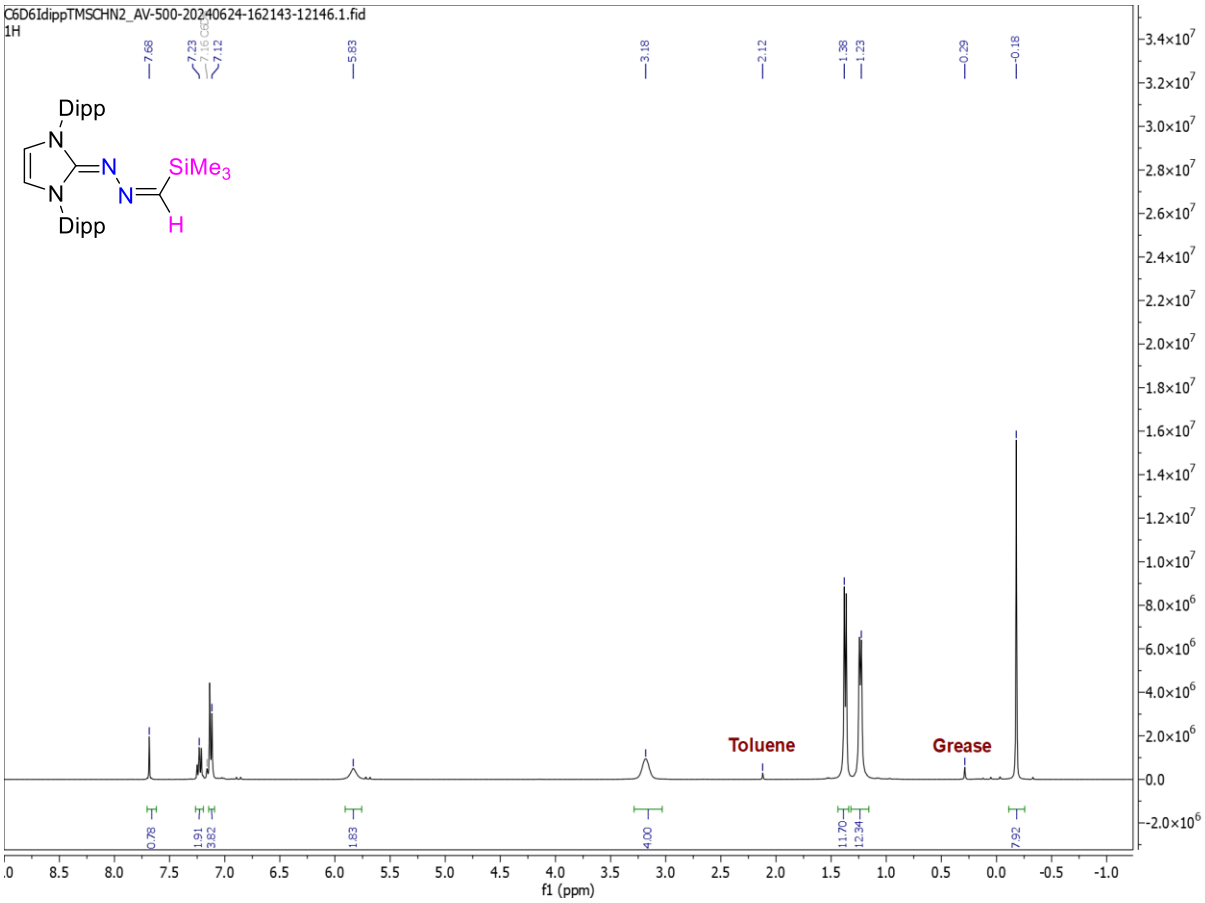


Figure S13: ^{1}H NMR spectrum of **4**

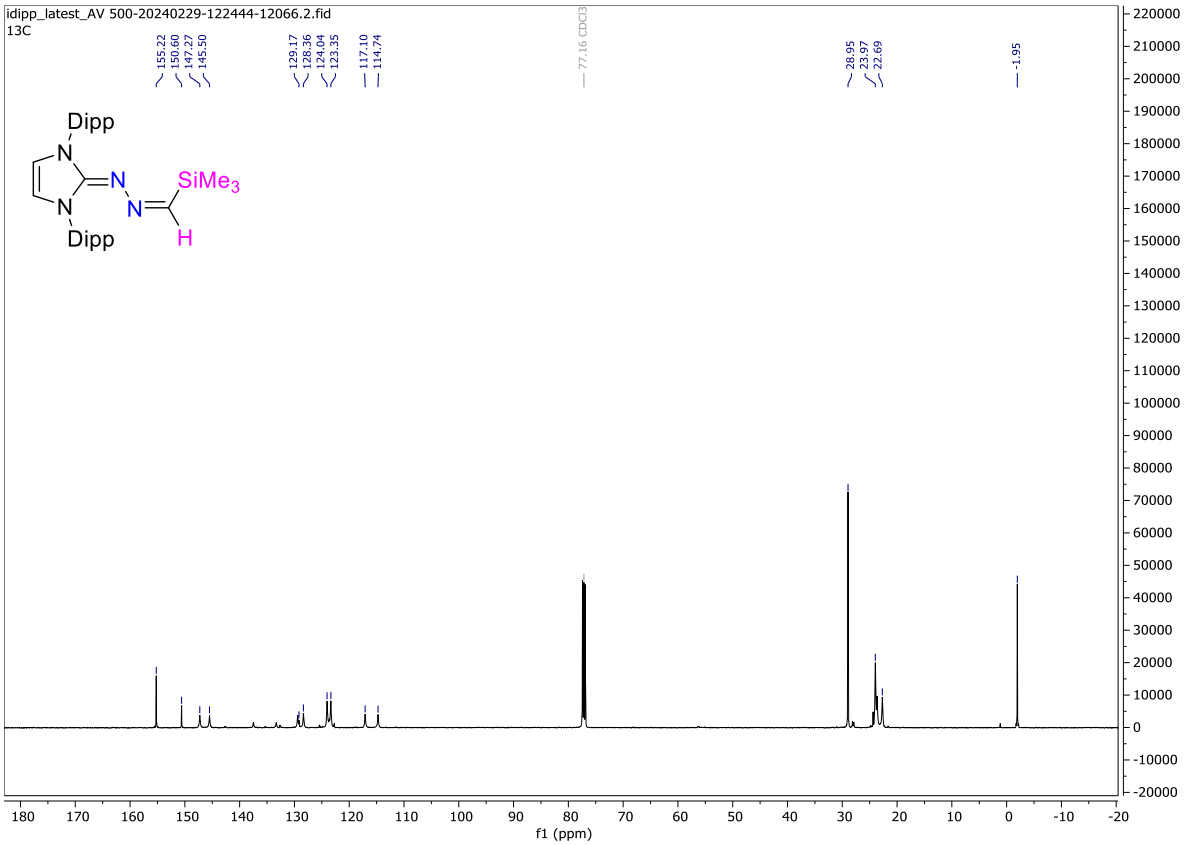


Figure S14: $^{13}C\{^{1}H\}$ NMR spectrum of **4**

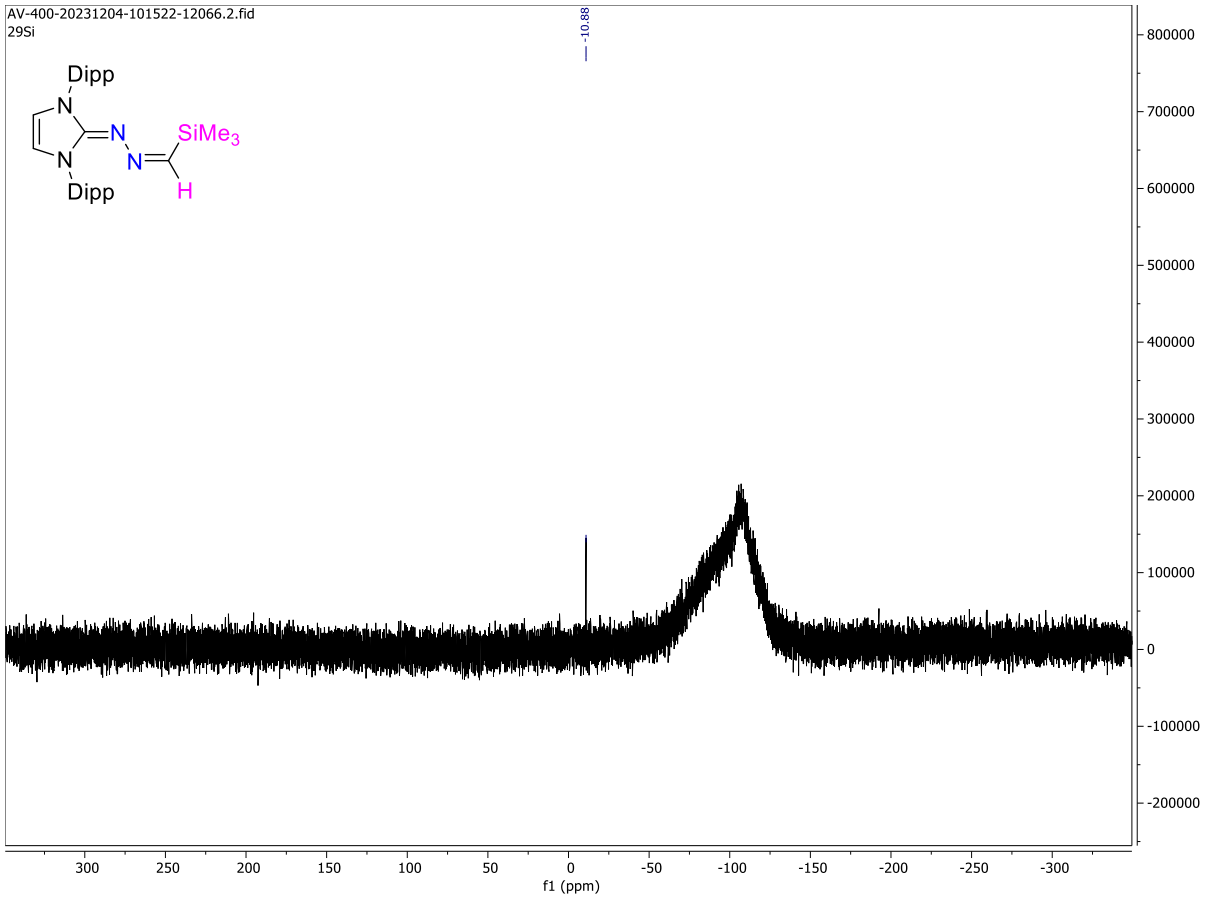


Figure S15: $^{29}Si\{^{1}H\}$ NMR spectrum of **4**

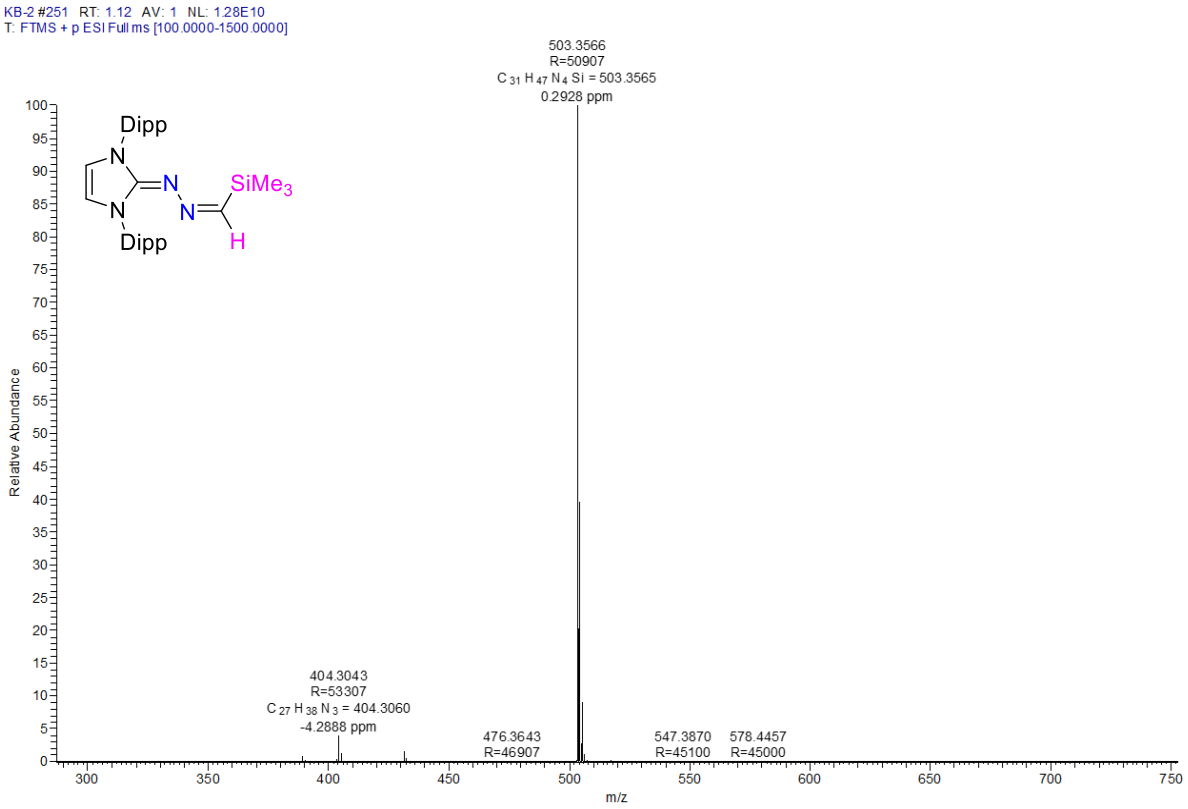


Figure S16: HRMS spectrum of **4**

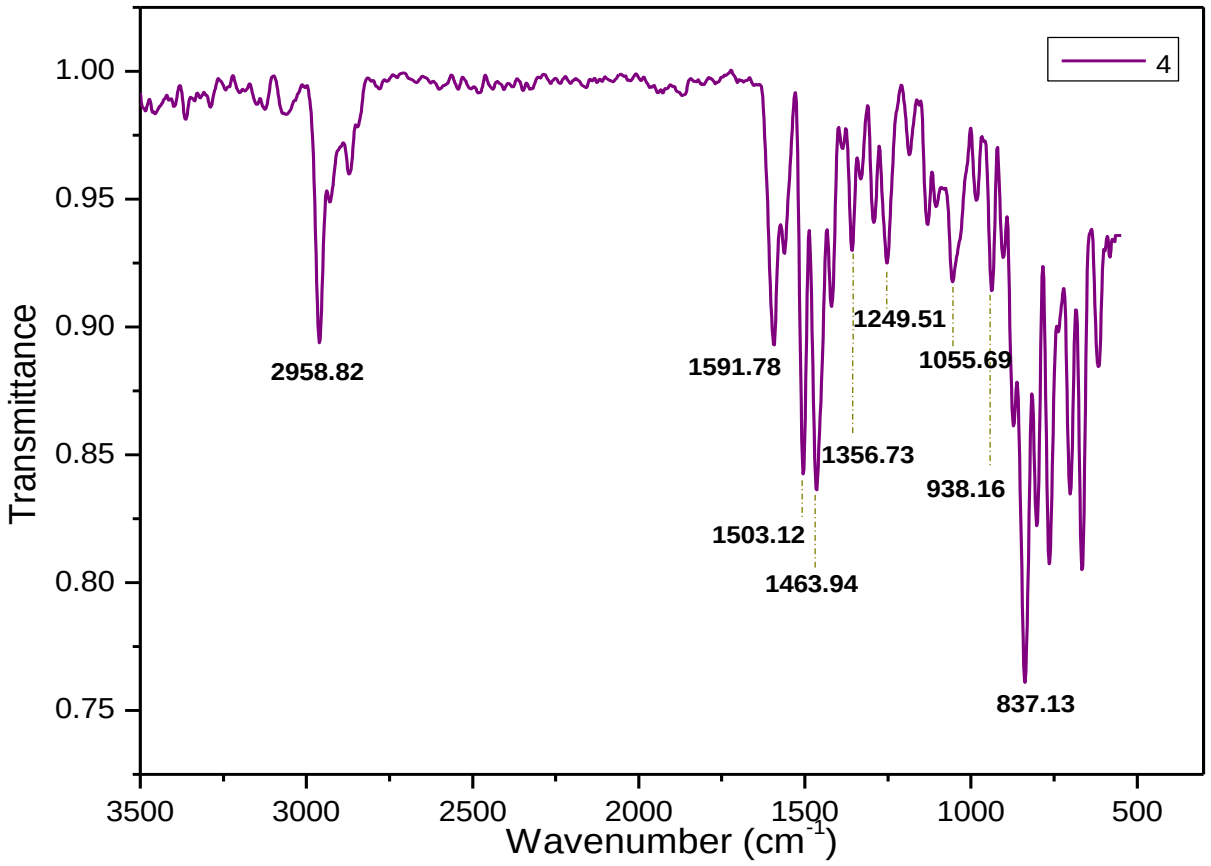


Figure S17: IR (ATR) spectrum of **4**

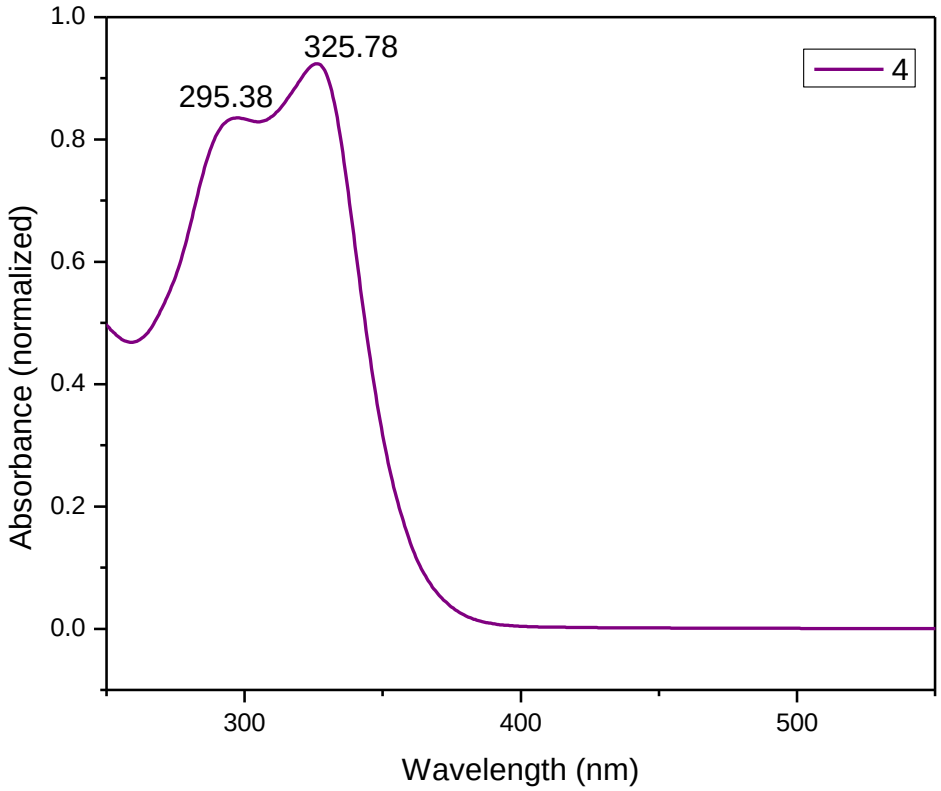


Figure S18: UV-VIS spectrum of **4** in THF

Synthesis of 5:

Method 1: By deprotonation of 5a using bases such as Et_3N or KHMDS

5a (0.350 g, 0.75 mmol) was dissolved in 10 mL THF in a round bottom flask. After that, Et_3N (0.12 mL, 0.82 mmol) was added to it at room temperature, resulting in the immediate formation of $Et_3NH^+Cl^-$ precipitate. The reaction was run for 12 hours. All the volatiles were completely removed to give a white-colored solid. After that, 10 mL toluene was added to it and stirred for 15 min. Filtered the solution using the funnel. All the volatiles were completely removed to afford the pure yellow-colored solid, with a yield of 53%.

Or

4 (0.070 g, 0.15 mmol) was taken in a Schlenk flask and dried for 20 min. After that, **4** and KHMDS (0.032g, 0.16 mmol) were taken together in the Schlenk flask under the Argon atmosphere, and 10 mL THF was added to it at room temperature, resulting in an orange-colored solution. The reaction was run for 12 hours. All the volatiles were completely removed, and 10 mL toluene was added to it and stirred for 15 minutes. Filtered the solution using a funnel. Completely removed all the volatiles to afford the pure yellow-colored solid, **5**.

Method 2: By the one-pot reaction of 5-IPr, $SiMe_3CHN_2$, and water

5-IPr carbene (0.200 g, 0.51 mmol) was dissolved in 8 mL toluene in a Schlenk flask. After that, $SiMe_3CHN_2$ (0.86 mL, 0.51 mmol) and degassed water (0.01 mL, 0.51 mmol) were added to it at room temperature. The reaction was stirred for 12 hours, resulting in a yellow-colored solution. The solution was filtered using a cannula. Completely removed all the volatiles to afford the pure yellow-colored solid, **5**. Suitable crystals of **5** were obtained upon supersaturation in toluene.

Note: The reaction requires the precise addition of water, as excess water can lead to the formation of a mixture of decomposed products of carbene along with **5**.

^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = 1.25 (d, *J* = 7 Hz, 12 H, CH(C***H***$_3$)$_2$), 1.39 (d, *J* = 6.75 Hz, 12 H, CH(C***H***$_3$)$_2$), 3.19 (sept, *J* = 5.75 Hz, 4 H, C***H***(CH$_3$)$_2$), 5.70 (d, 1 H, *J* = 15.01 Hz, NNC***H***$_2$), 5.83 (singlet, 2 H, NC***H***C***H***N), 6.89 (d, 1 H, *J* = 15.01 Hz, NNC***H***$_2$), 7.11 (d, *J* = 7.50 Hz , 4 H, Ar-H), 7.21 (t, *J* = 7.75 Hz, 2 H, Ar-H).

^{13}C{^{1}H} DEPT NMR (101 MHz, 298 K, C_6D_6): 134.92 ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ= 23.13, 23.97 (CH(***C***H$_3$)$_2$, 28.95 (***C***H(CH$_3$)$_2$, 114.56, 117.14 (N***C***H***C***HN), 123.61(Ar-C), 129.03 (Ar-C), 135.35 (***C***NNCH$_2$), 146.08, 146.93 (Ar-C), 151.43 (CNN***C***H$_2$) ppm.

IR (cm^{-1}): 3080, 2960, 2865.33, 1609, 1549.33, 1481.33, 1364, 1260.77,793.33, 681.35.

HRMS: m/z calcd for $[M+H]^+$ $C_{28}H_{39}N_4$, 431.31; found **431.31** for $C_{28}H_{39}N_4$.

Melting point range: 105-110 ˚C.

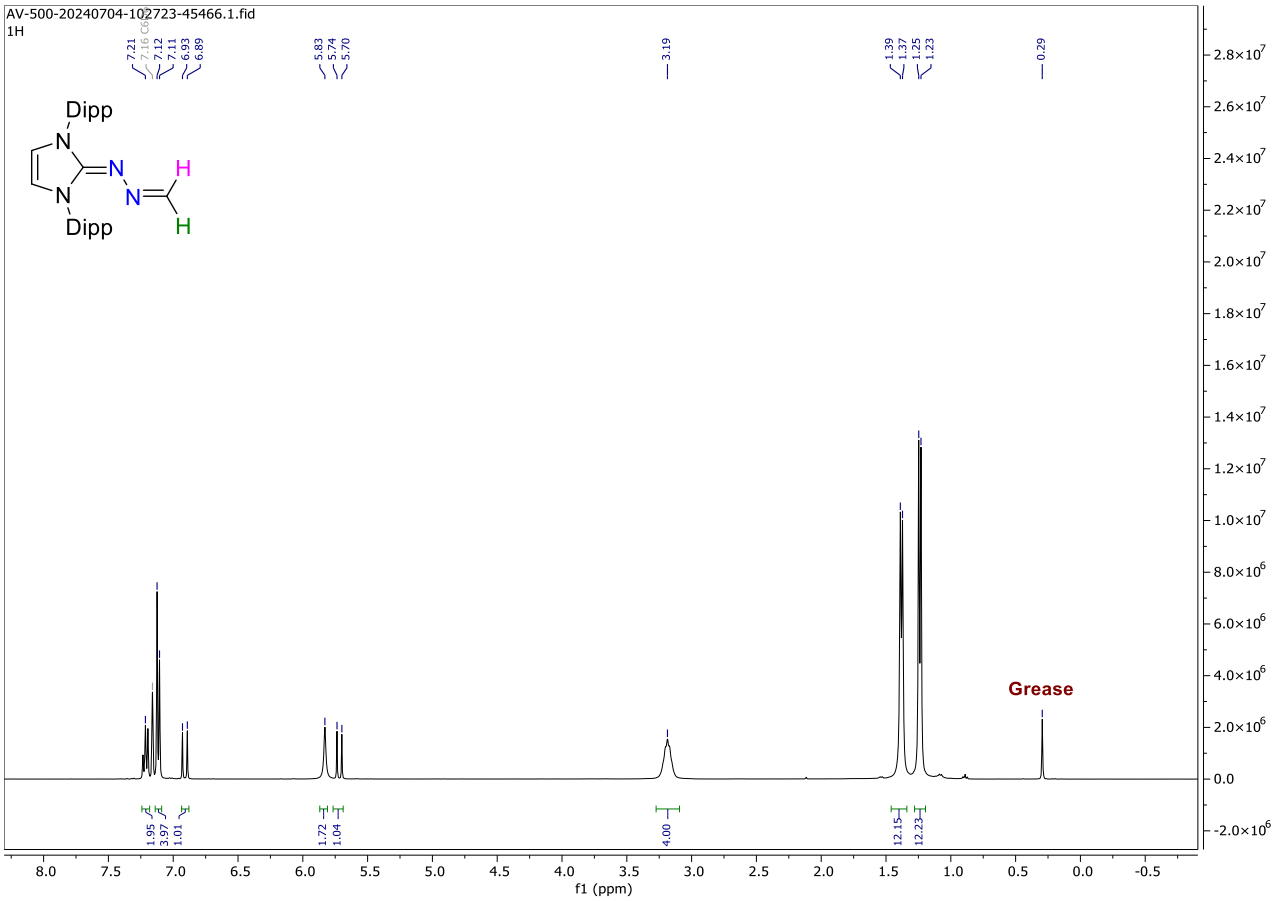


Figure S19: ^{1}H NMR of **5**

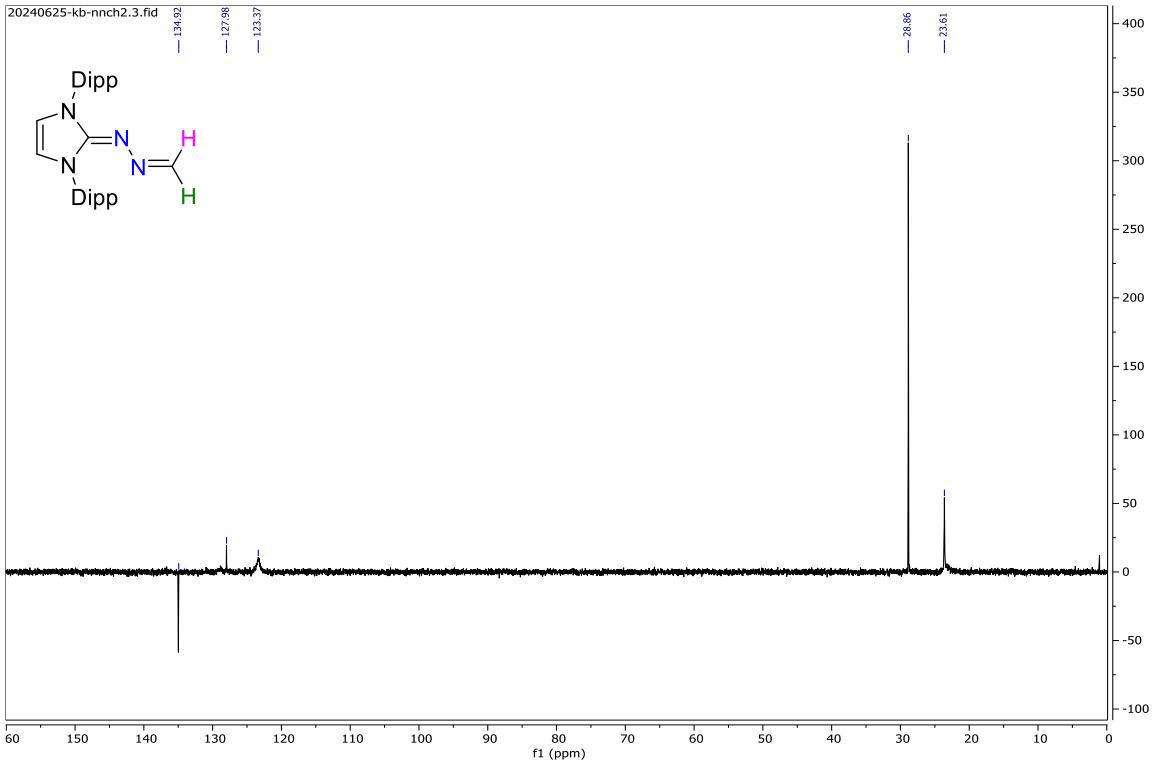


Figure S20: ^{13}C{^{1}H} DEPT NMR of **5**

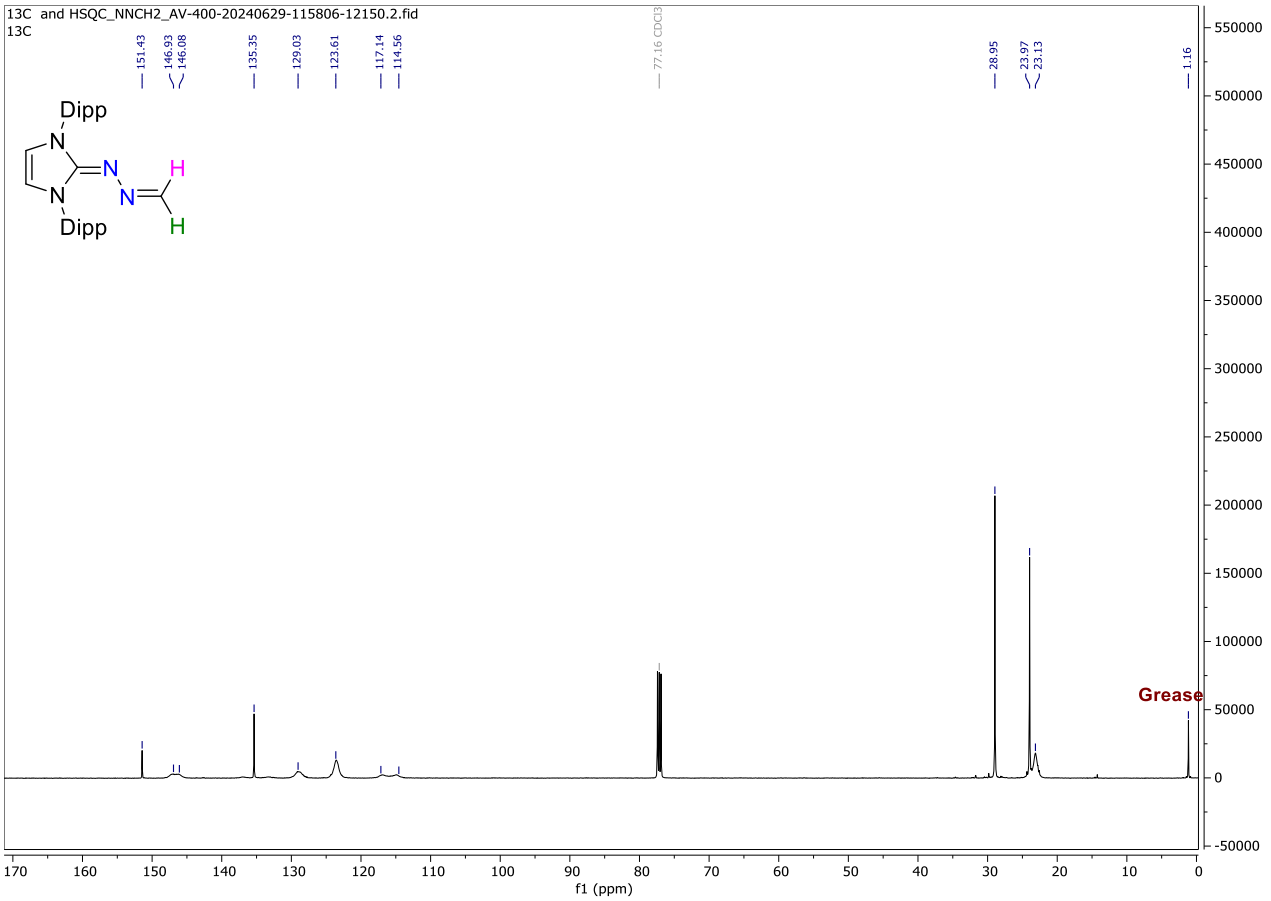


Figure S21: $^{13}C\{^{1}H\}$ NMR of **5**

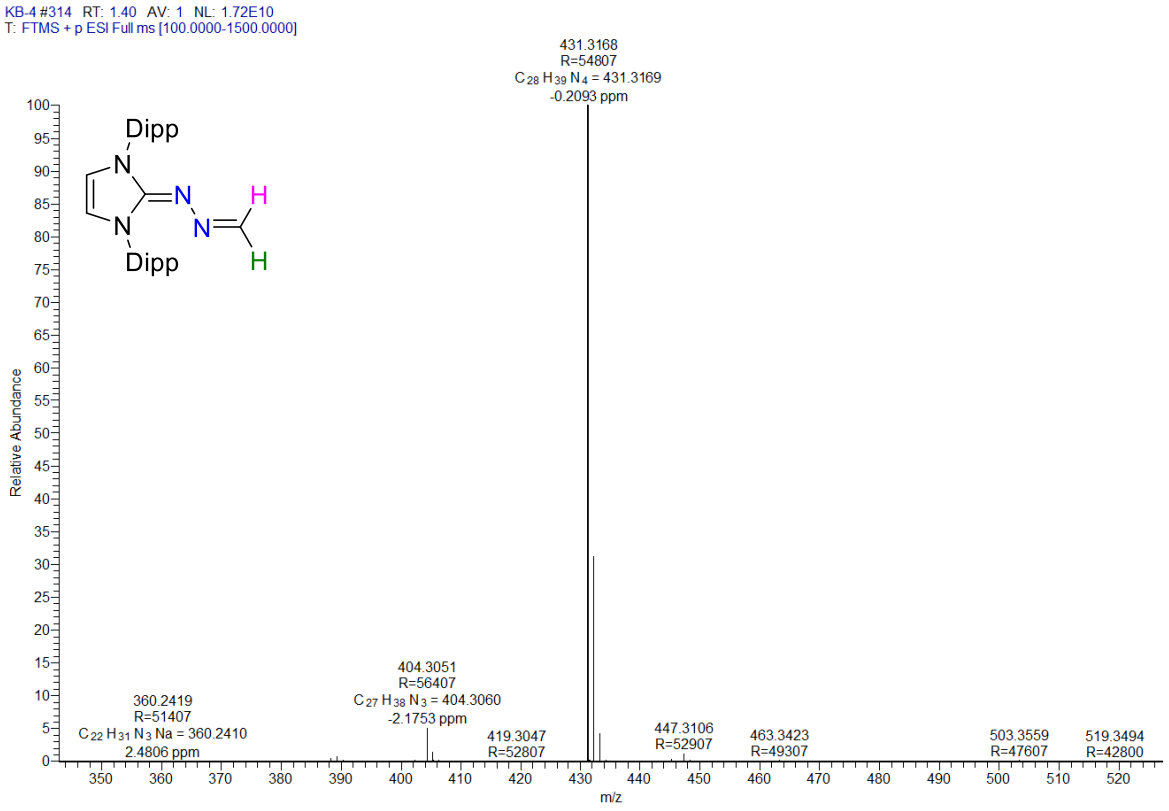


Figure S22: HRMS of **5**

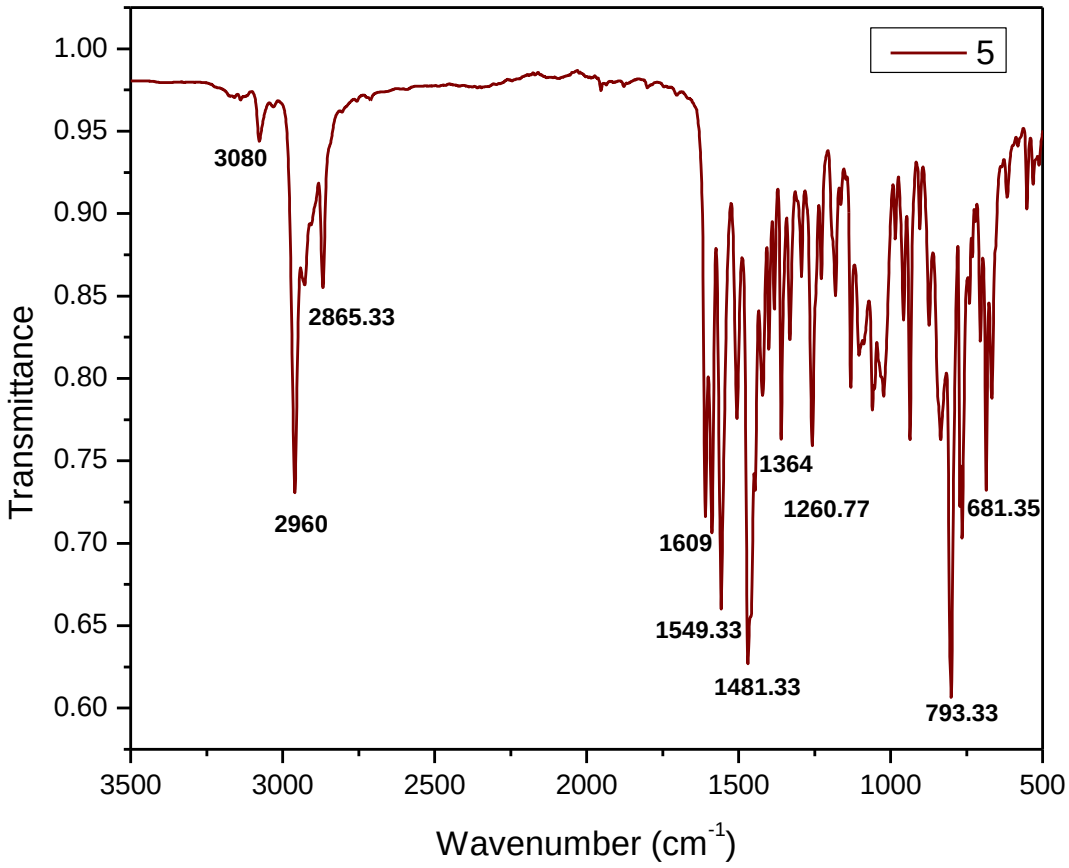


Figure S23: IR spectrum of **5**

Synthesis of 5a:

Method 1: By treating 4 with HCl (0.5 eq.-1.1 eq.)

4 (0.100 g, 0.19 mmol) was dissolved in 12 mL toluene in a round bottom flask. After that, 4 M HCl in dioxane (0.05 mL, 0.21 mmol) was added to it at room temperature, resulting in the formation of precipitate within an hour. The reaction was run for 12 hours. Completely removed all the volatiles to give a white-colored solid. After that, 10 mL hexane was added to it for washing and stirred for 15 min. Decanted the hexane part and completely dried the precipitate part to get pure product, **5a** in 91% yield. Suitable crystals for XRD analysis were grown by slow evaporation of DCM and hexane mixture in air at room temperature.

Method 2: By treating 5 with 1.1 eq. HCl

5 (0.060 g, 0.14 mmol) was dissolved in 7 mL toluene in a round bottom flask. After that, 4 M HCl in dioxane (0.04 mL, 0.15 mmol) was added to it at room temperature. The reaction was run for 12 hours. All the volatiles were completely removed, followed by a hexane wash to give the pure product **5a**.

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.19-1.23 (dd, *J* = 3.88 Hz, 24 H, CH(C***H***$_3$)$_2$), 2.58 (sept, *J* = 6.75 Hz, 4 H, C***H***$(CH_3)_2$), 5.98 (d, 1 H, *J* = 11.26 Hz,

NNC***H***$_2$), 6.78 (singlet, 2 H, NC***H***C***H***N),7.24 (d, 4 H, Ar-H), 7.25 (t, 2 H, Ar-H), 7.94 (d, 1 H, *J* = 11.26 Hz, NNC***H***$_2$),13.88 (N$^+$***H***) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ= 23.04, 24.21 (CH(***C***H$_3$)$_2$, 29.30 (***C***H(CH$_3$)$_2$, 119.41 (N***C***H***C***HN), 124.60 (Ar-C), 130.69 (Ar-C), 131.34 (Ar-C), 141.77 (Ar-C), 144.62 (***C***NNCH$_2$), 145.35 (CNN***C***H$_2$) ppm.

IR (cm^{-1}): 2958.78, 2868.06, 1614.44, 1455.68, 1383.51, 1212.38, 1030.93, 806.19, 698.97.

HRMS: m/z calcd for [M]$^+$[Cl]$^-$ $C_{28}H_{39}N_4Cl$, 466.29; found **431.31** for $C_{28}H_{39}N_4$.

Melting point range: 184-188 ˚C.

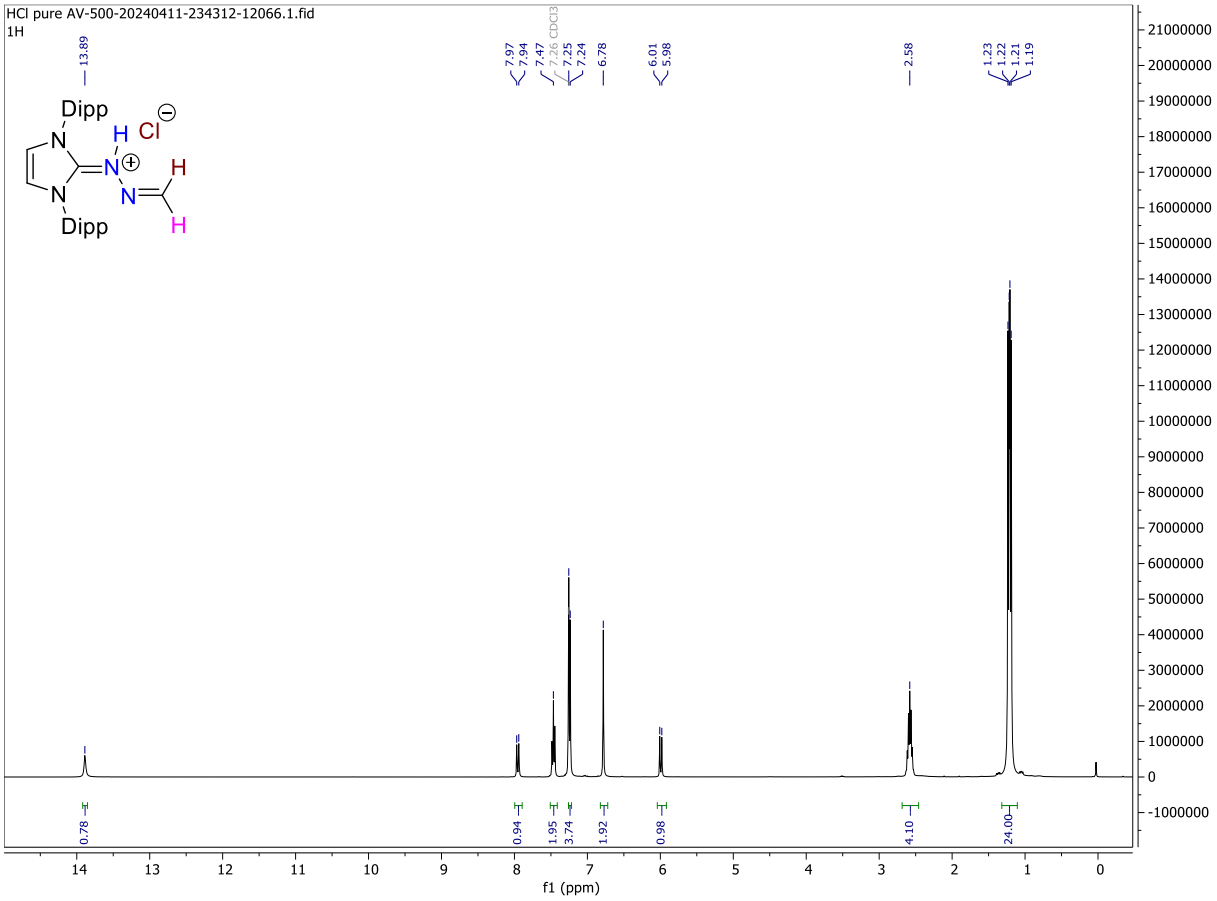


Figure S24: ^{1}H NMR spectrum of **5a**

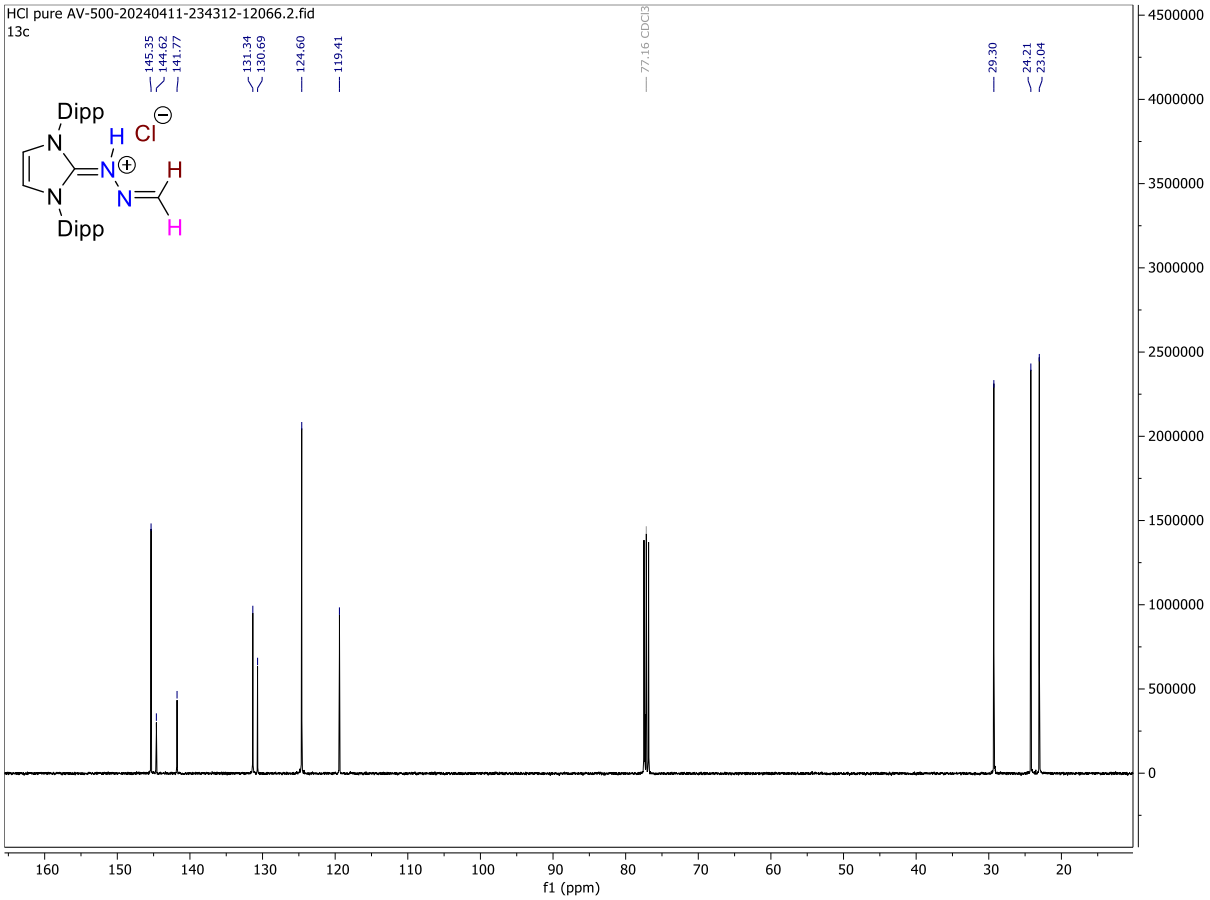


Figure S25: $^{13}C\{^{1}H\}$ NMR spectrum of **5a**

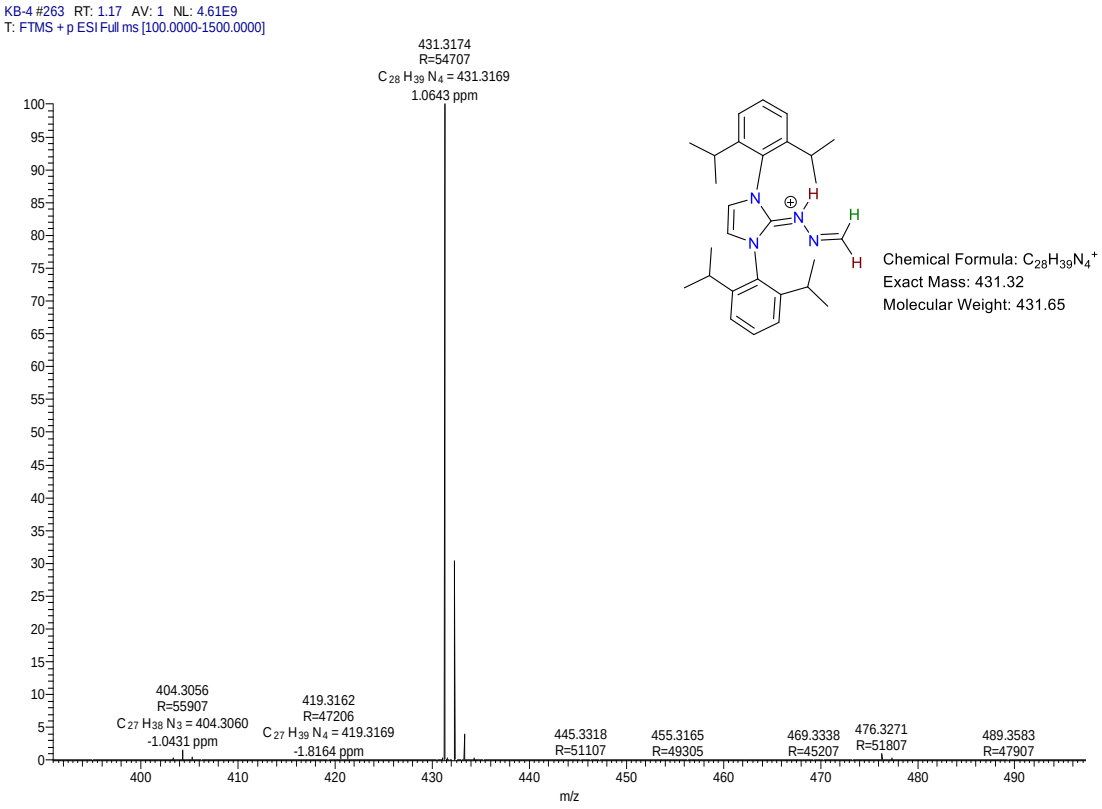


Figure S26: HRMS spectrum of **5a**

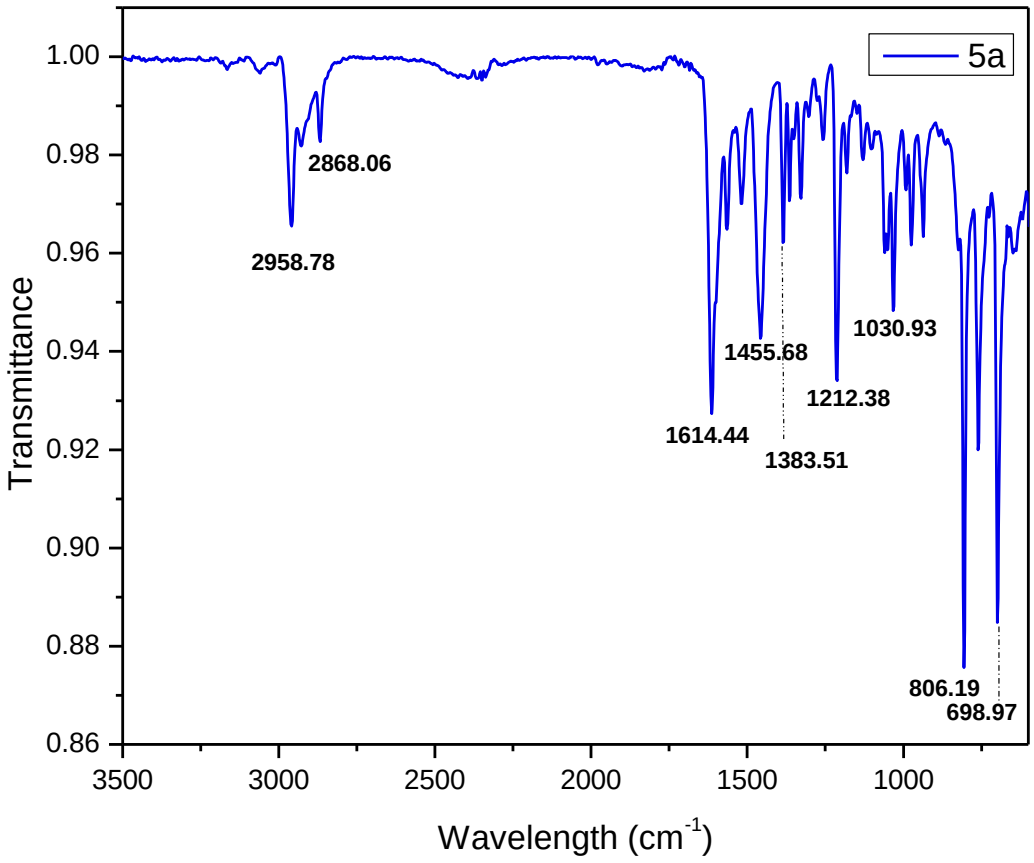


Figure S27: IR (ATR) spectrum of **5a**

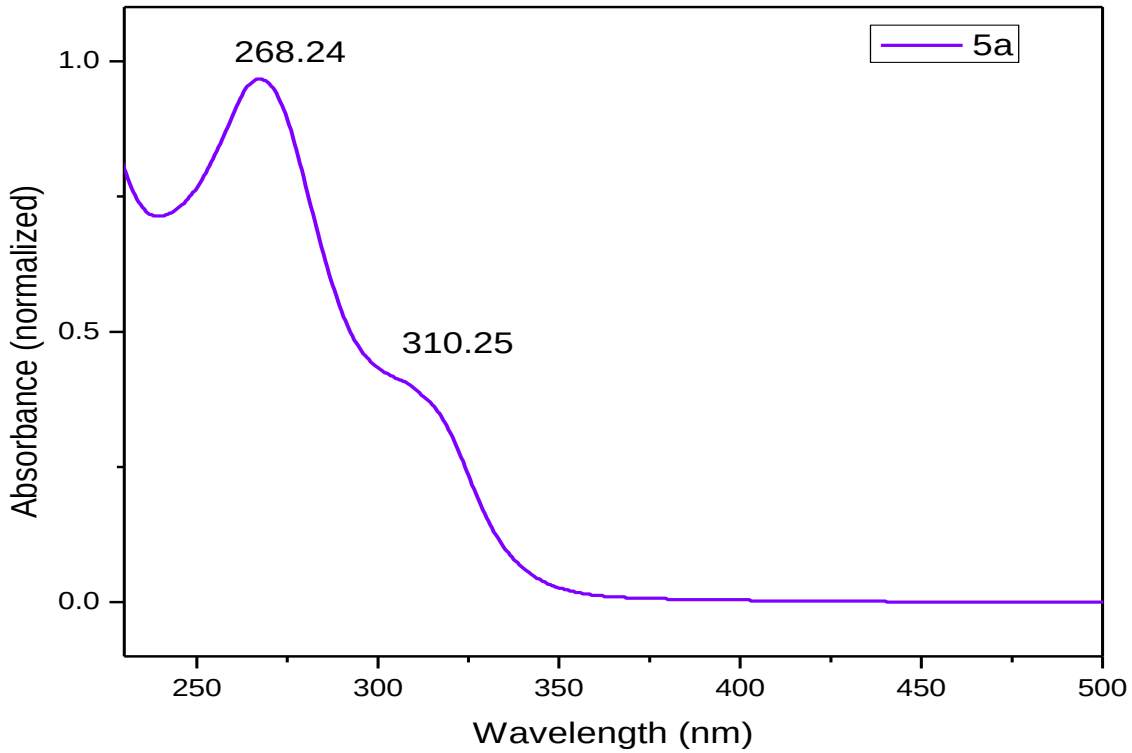


Figure S28: UV-VIS spectrum of **5a** in THF

Synthesis of 6 and **7:** 5-I^{t}Bu (0.200 g, 1.10 mmol) was dissolved in 10 mL hexane in a Schlenk flask and kept at -36 ˚C for 10 min. After that, $SiMe_3CHN_2$ (1.84 mL, 1.10 mmol) was added to the solution resulting in a deep red-colored solution along with the formation of a yellow-colored precipitate. The reaction was run for 12 hours while slowly warming to room temperature. The solution was filtered using a cannula and completely dried the precipitate part followed by toluene wash to get the pure product **6** with a yield of 21%.

Suitable crystals were grown by concentrating the filtrate to 3 mL when the reaction was performed in toluene and stored at room temperature to get red-colored crystals **6** after 2 days.

^{1}H NMR of the filtrate part in C_6D_6 shows the formation of a mixture of products comprising both **6** and **7.** Suitable crystals of **7** for XRD analysis were grown from the NMR tube itself after keeping it at room temperature for a week.

However, compound **7** could not be isolated and well-characterized. Also, it was difficult to predict the yield of **7** as the filtrate part comprised a mixture of both **6** and **7**.

^{1}H NMR of 6 (400 MHz, 298 K, $CDCl_3$): 1.48 (singlet, 18 H, C(C***H***$_3$)$_3$, 7.37 (singlet, 2 H, NC***H***C***H***N), 8.27 (CNC***H***NN) ppm.

^{13}C{^{1}H} NMR of 6 (125.7 MHz, 298 K, $CDCl_3$): 30.21 (C(***C***H$_3$)$_3$), 63.41(***C***(CH$_3$)$_3$, 118.22 (N***C***H***C***HN), 143.99 (N***C***N), 146.09 (***C***NCHNN), 152.50 (CN***C***HNN) ppm.

IR (cm^{-1}) of 6: 3094.91, 2971.19, 1571.16, 1439.20, 1375.28, 1321.67, 1185.59, 981.46, 849.50, 732.72.

HRMS of 6: m/z calcd for $[M+H]^+$ $C_{13}H_{22}N_5$, 248.18; found **248.18**.

Melting point range of 6: 209-214˚C.

^{29}Si of 7 (79.49 MHz, 298 K, C_6D_6): -10.32 ppm

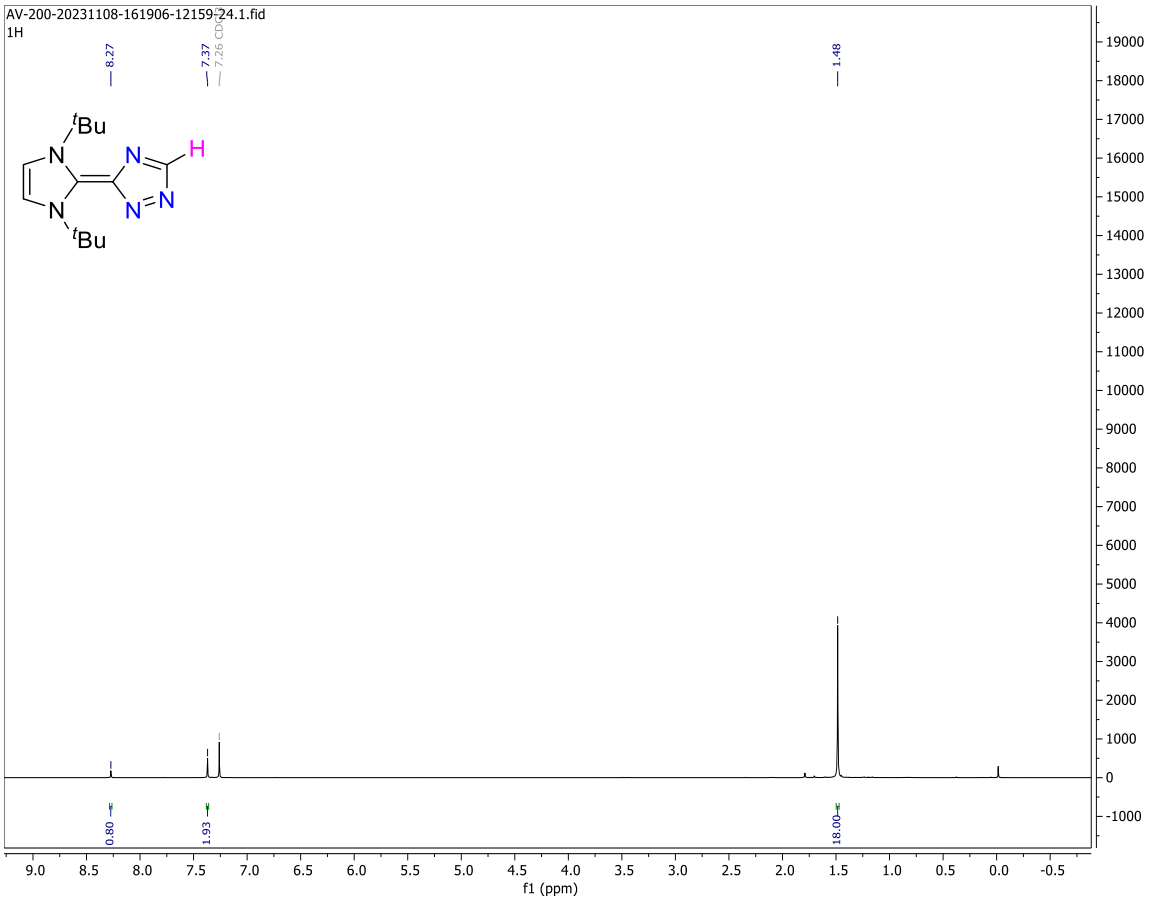


Figure S29: ^{1}H NMR spectrum of **6**

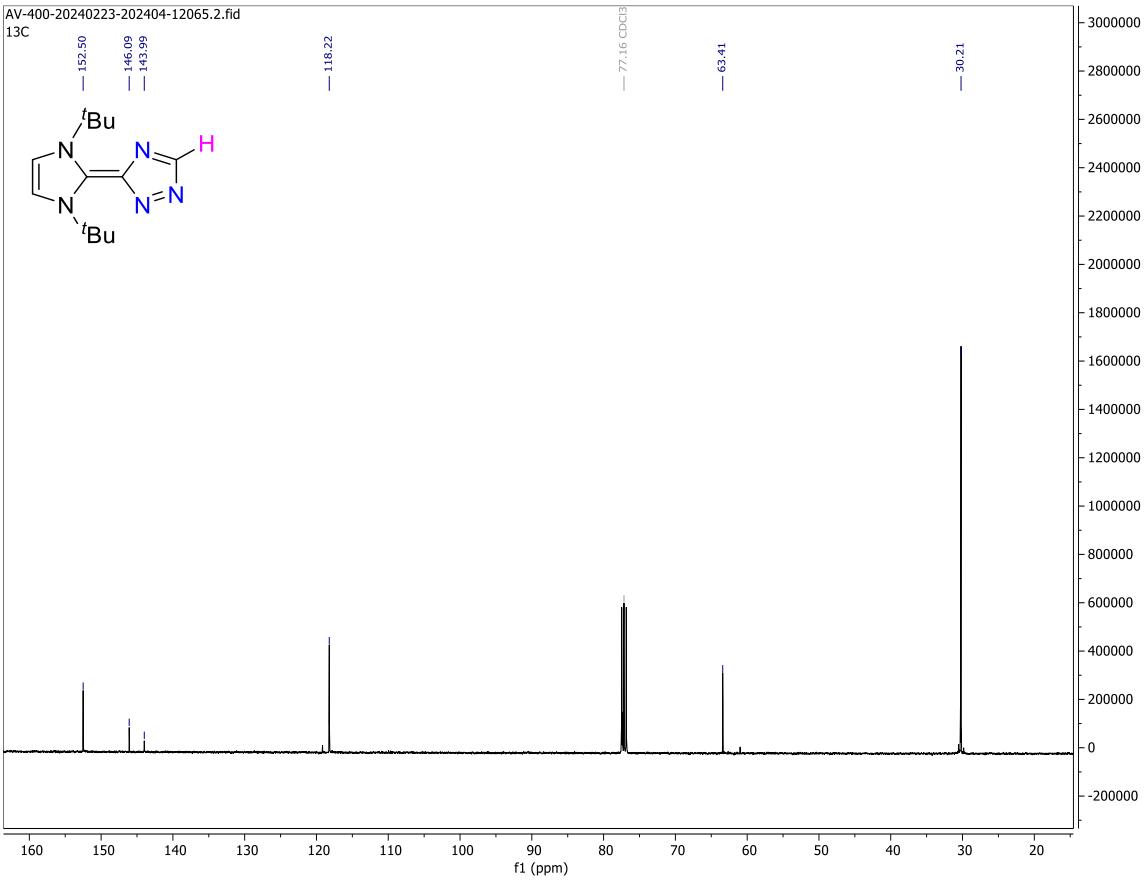


Figure S30: ^{13}C{^{1}H} NMR spectrum of **6**

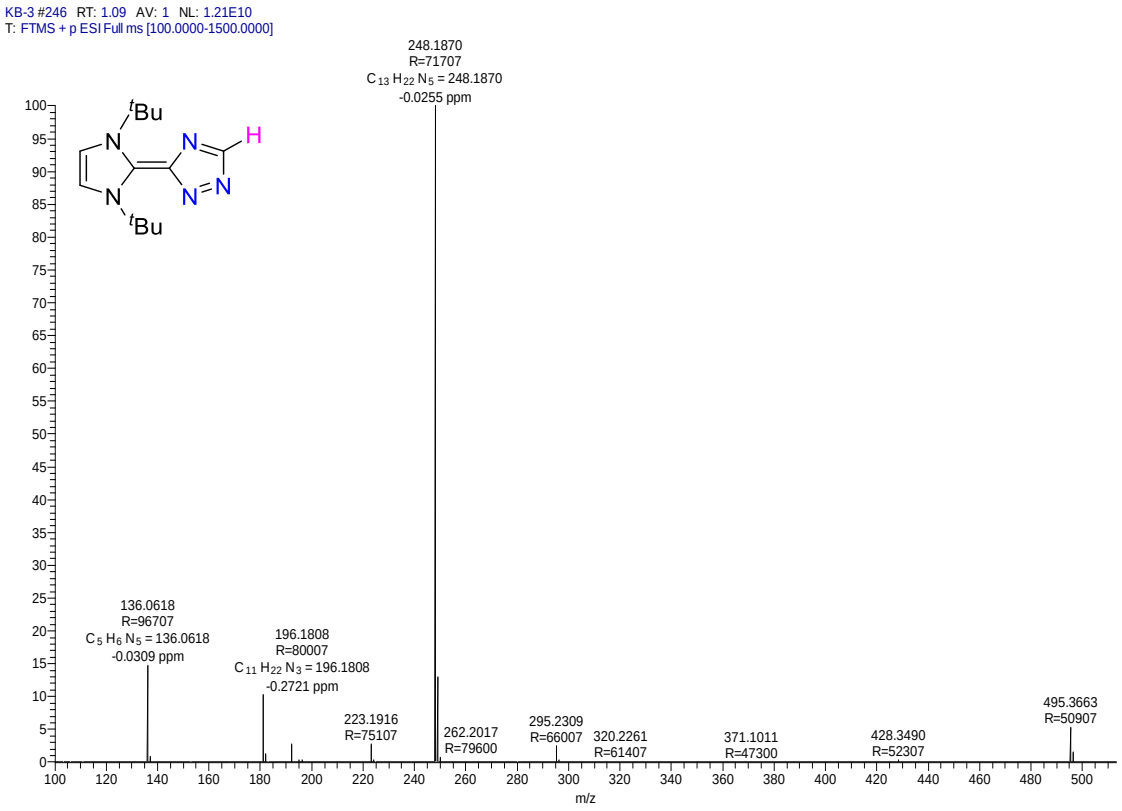


Figure S31: HRMS spectrum of **6**

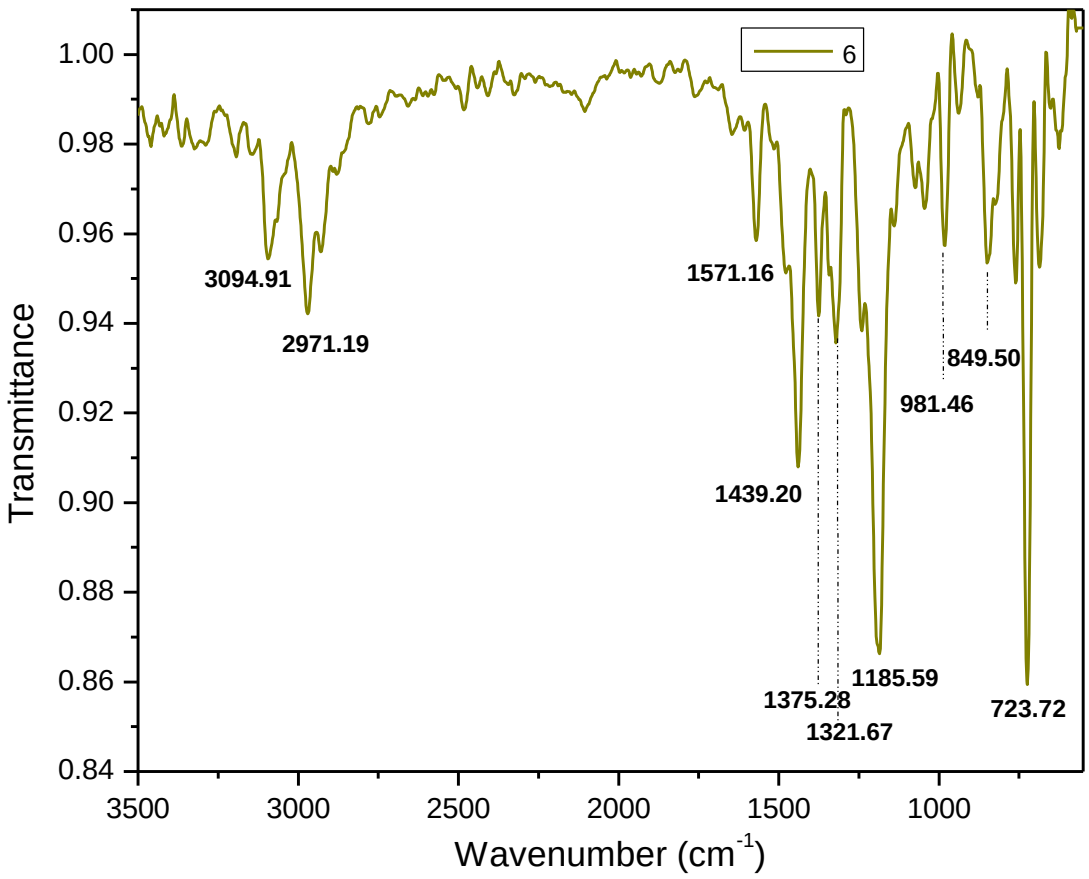


Figure S32: IR (ATR) spectrum of **6**

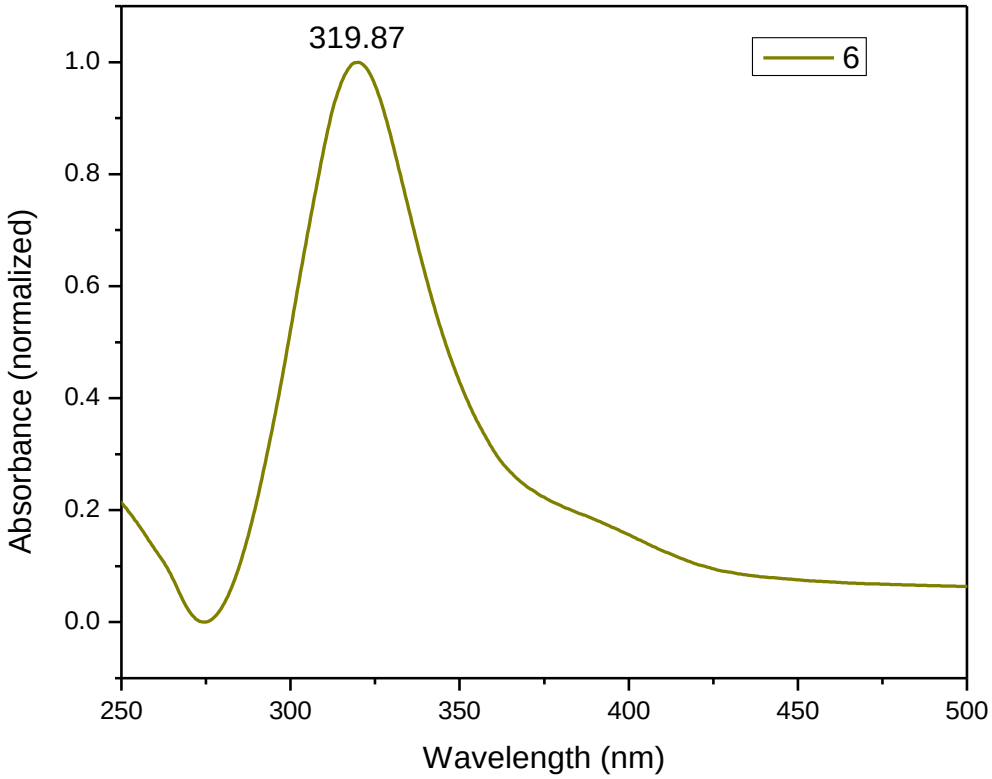


Figure S33: UV-VIS spectrum of **6**

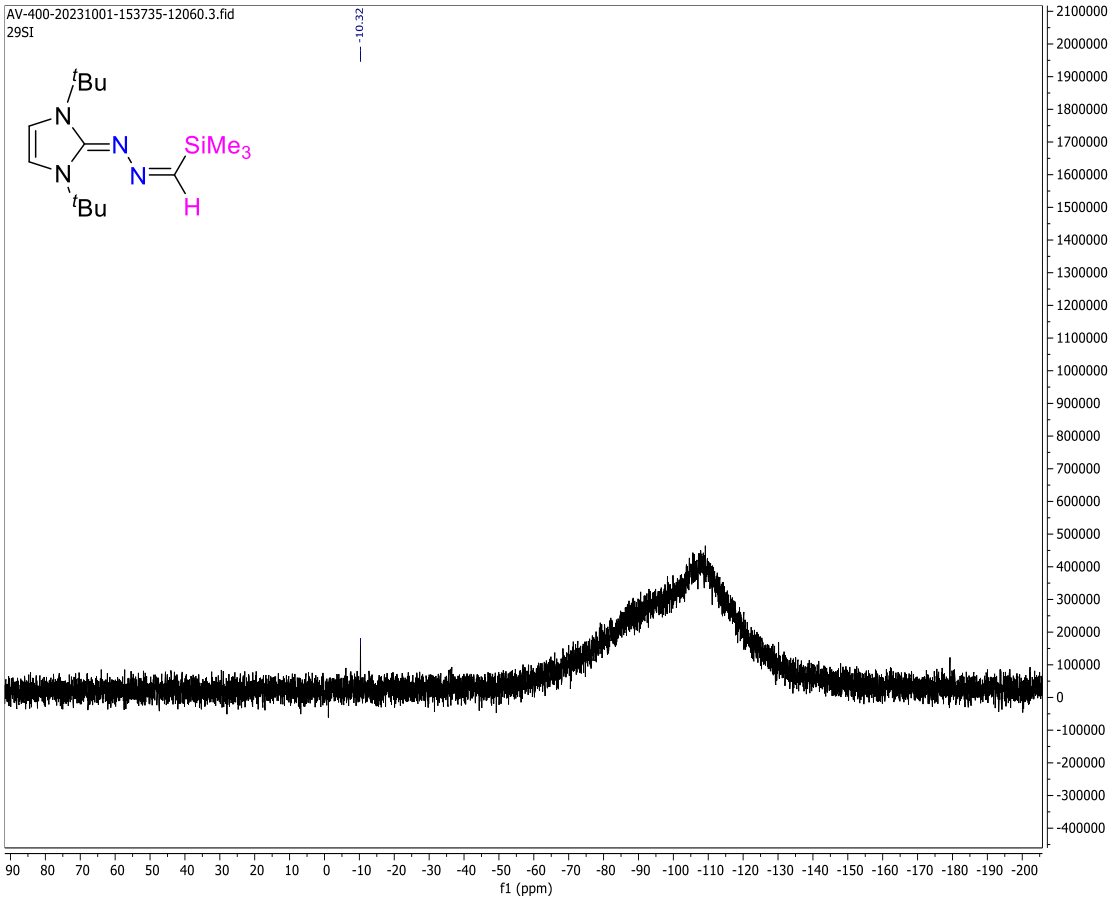


Figure S34: $^{29}Si\{^{1}H\}$ NMR spectrum of **7**

Synthesis of 7a: 5-I^{t}Bu carbene (0.120 g, 0.66 mmol) was dissolved in 8 mL toluene in a Schlenk flask. After that, $SiMe_3CHN_2$ (1.1 mL, 0.66 mmol) and degassed water (0.01 mL, 0.66 mmol) were added to it at room temperature. The reaction was stirred for 12 hours, resulting in a yellow-colored solution. The solution was filtered using a cannula. All the volatiles were completely removed to afford the pure dark yellow-colored sticky solid **7a**, which gets solidified upon keeping the flask in a glovebox within 24 h with a yield of 75%.

Suitable crystals for XRD analysis were grown from the saturated solution of toluene at room temperature.

Note: The reaction requires the precise addition of water, as excess water can lead to the formation of a mixture of decomposed products of carbene and **7a**.

^{1}H NMR (500 MHz, 298 K, C_6D_6): δ = 1.54 (singlet, 18 H, C(C***H***$_3$)$_3$), 6.08 (singlet, 2 H, NC***H***C***H***N), 6.33 (d, 1 H, *J* = 15.13 Hz, NNC***H***$_2$), 7.40 (d, 1 H, *J* = 15.13 Hz, NNC***H***$_2$) ppm.

^{13}C{^{1}H} DEPT NMR (125.7 MHz, 298 K, C_6D_6): 130.35 ppm.

^{13}C{^{1}H} NMR (125.7 MHz, 298 K, C_6D_6): δ= 29.83 (C(***C***H$_3$)$_3$, 57.04 (***C***(CH$_3$)$_3$, 109.42 (N***C***H***C***HN),130.73(CNN***C***H$_2$), 152.71 (***C***NNCH$_2$) ppm.

IR (cm^{-1}): 3177.34, 3057.75, 2962.91,1513.41, 1445.31, 1385.47, 1187.63, 1012.37, 903.09, 643.30.

HRMS: m/z calcd for $[M+H]^+$ $C_{12}H_{23}N_4$, 223.18; found 223.19.

Melting point range: 55-60 ˚C.

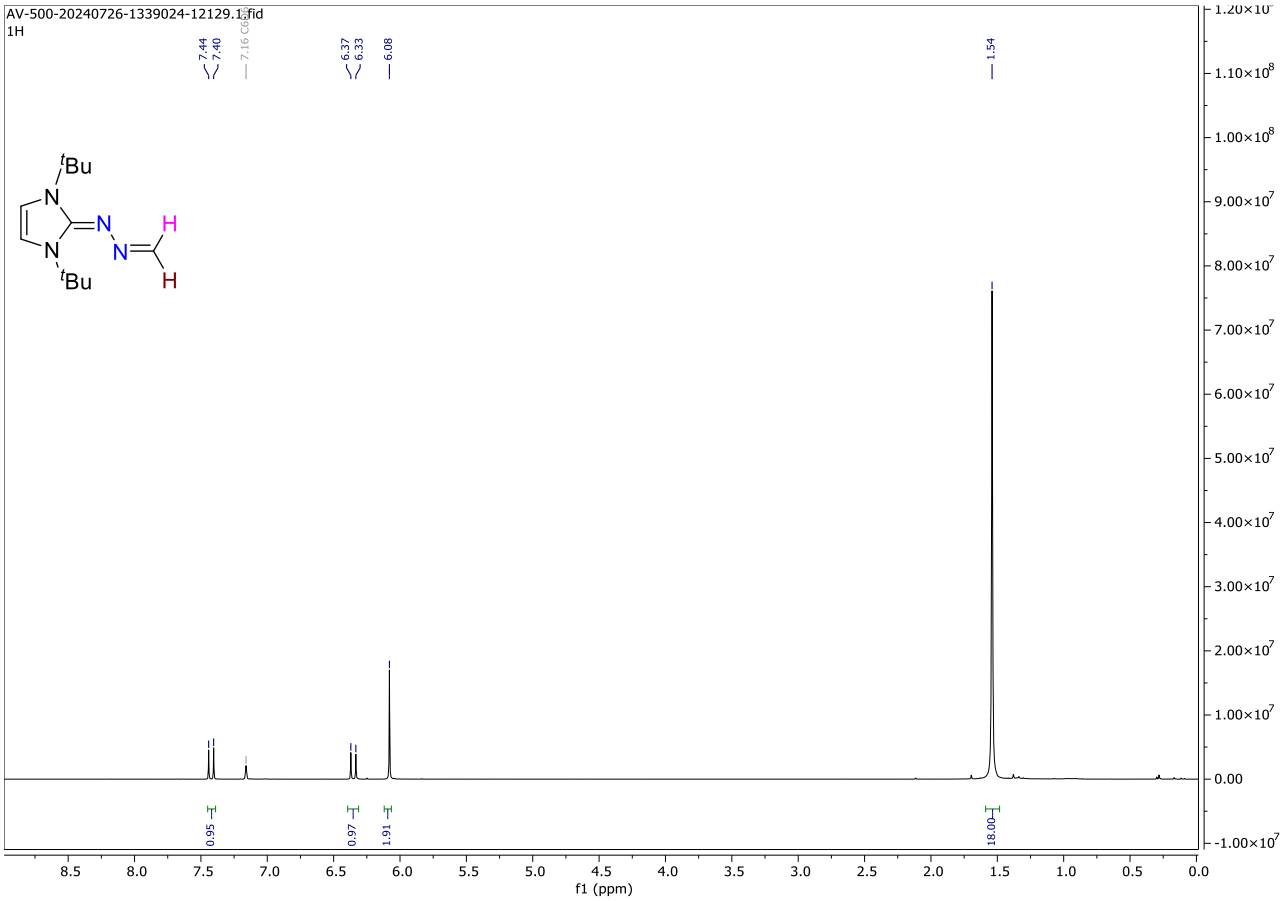


Figure S35: ^{1}H NMR of **7a**

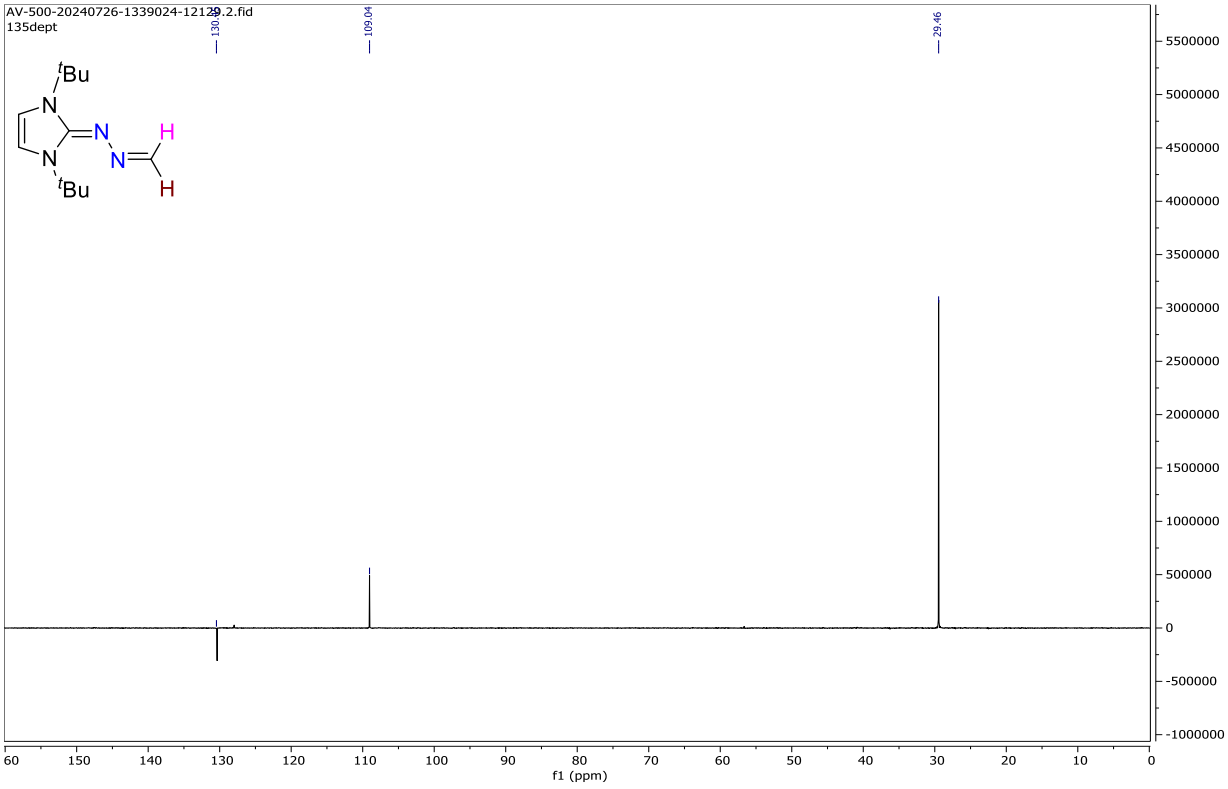


Figure S36: ^{13}C{^{1}H} DEPT NMR of **7a**

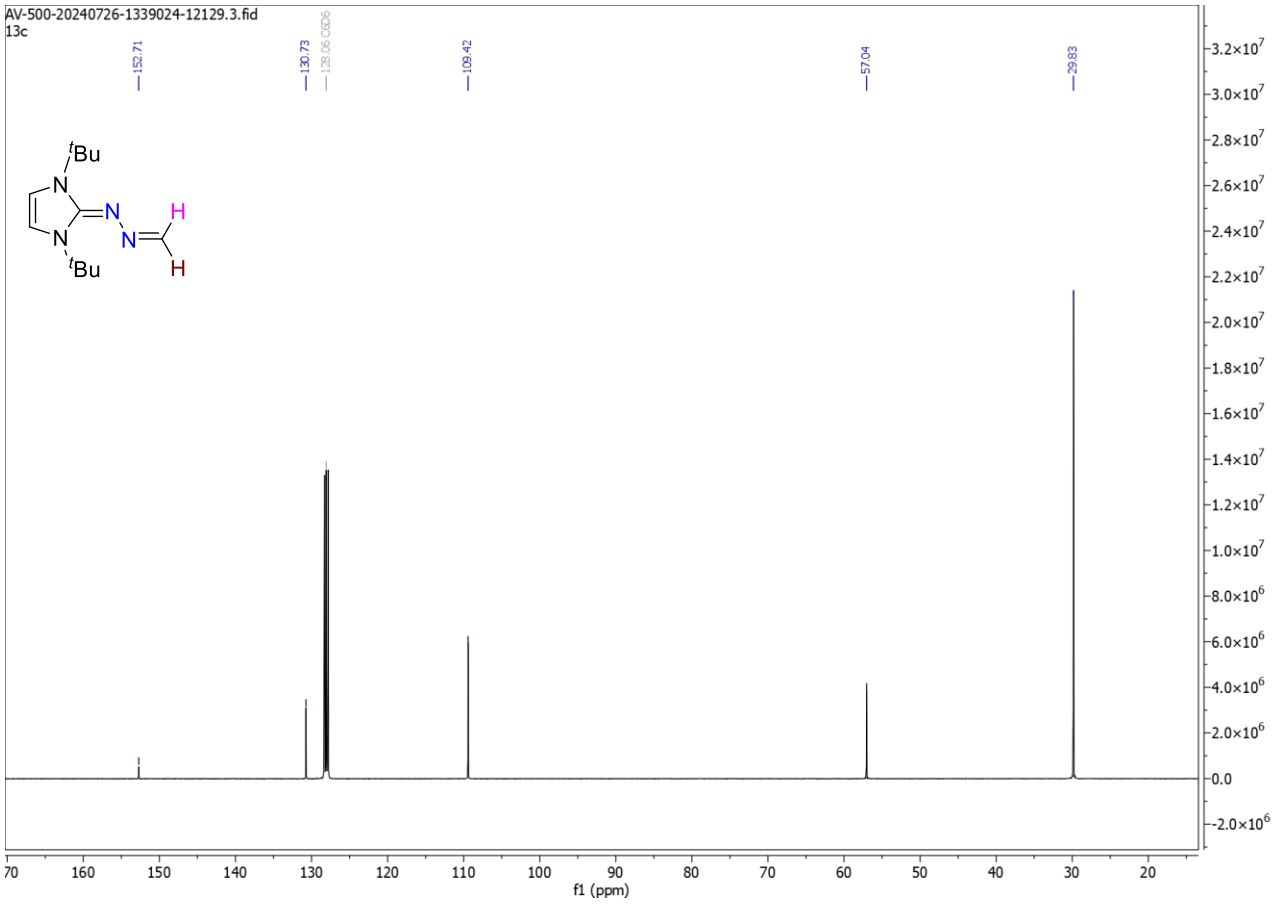


Figure S37: $^{13}C\{^{1}H\}$ NMR of **7a**

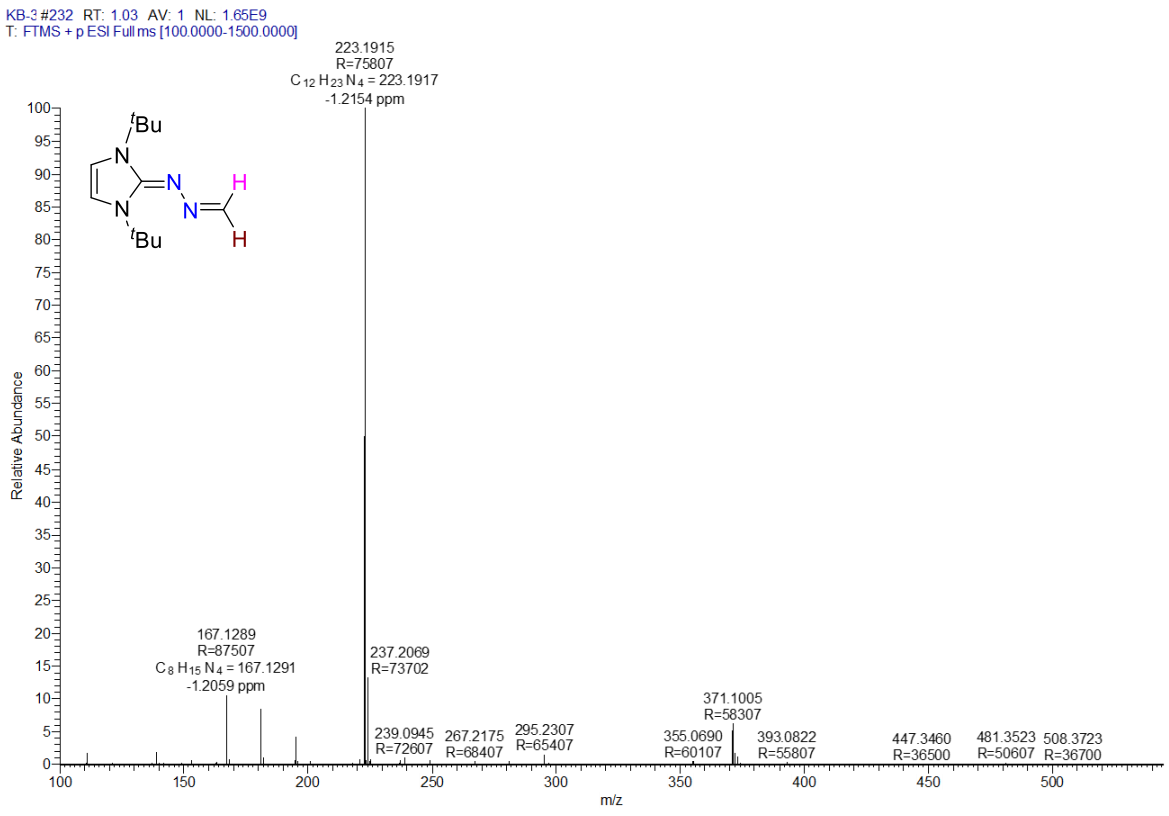


Figure S38: HRMS of **7a**

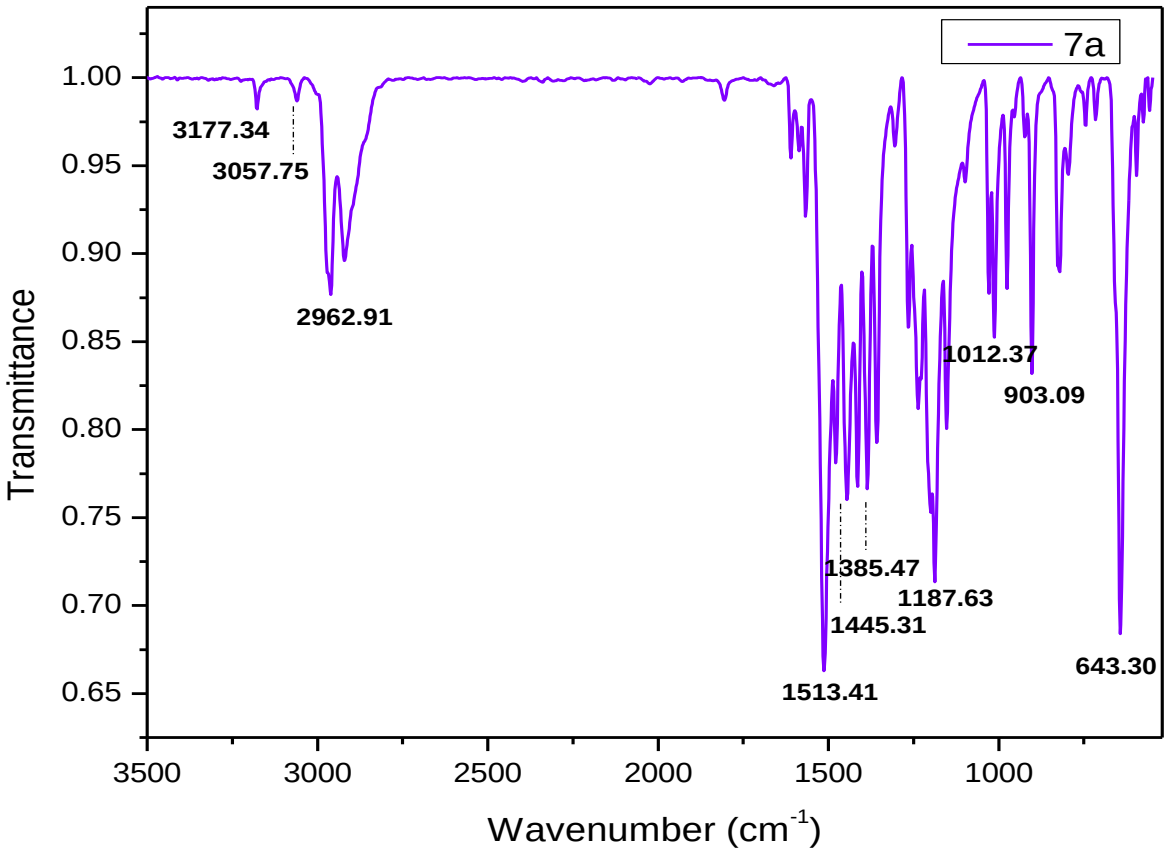


Figure S39: ATR(IR) spectrum of **7a**

Synthesis of 8: DAC.OTf salt (0.300 g, 0.50 mmol) and NaHMDS (0.094 g, 0.51 mmol) were taken together and dissolved in 20 mL toluene at room temperature. The reaction was run for 30 min. Filtered the solution using frit and kept the Schlenk flask at -36 ˚C. $SiMe_3CHN_2$ (1.08 mL, 0.65 mmol) was added to the filtrate at low temperature, resulting in a yellow-colored solution. The reaction was run for 20 hours while slowly warming to room temperature. All the volatiles were removed and the pure product was isolated using column chromatography in 5% ethylacetate and pet ether with a yield of 30%. The suitable crystals for XRD were grown from the crude mixture at room temperature in DCM and hexane mixture in air.

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = -0.24 (singlet, 9 H, $Si(CH_3)_3$), 1.17 (dd merged, *J* = 7.38 Hz, 12 H, $CH(CH_3)_2$), 1.22 (dd, *J* = 3.63 Hz, 12 H, $CH(CH_3)_2$), 1.73 (singlet, 6 H, $(OCC(CH_3)_2$), 2.91 (sept, *J* = 6.50 Hz, 4 H, $CH(CH_3)_2$), 7.14 (d, *J*= 7.75 Hz, 2 H, Ar-H), 7.19 (singlet, 1 H, $NNCHSiMe_3$), 7.23 (d, *J*= 7.75 Hz, 2 H, Ar-H), 7.35 (t, *J*= 7.75 Hz,1 H, Ar-H), 7.41 (t, *J*= 7.75 Hz, 1 H, Ar-H).

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = -2.31 ($Si(CH_3)_3$), 22.30-24.24 ($CH(CH_3)_3$), 25.36 ($CH(CH_3)_3$), 29.28, 29.35 ($OCC(CH_3)_2$), 47.03 ($CO(CH_3)_2$),

123.77 (Ar-C), 128.97 (Ar-C), 129.37 (Ar-C), 132.58(Ar-C), 133.85 (Ar-C), 137.21 (Ar-C), 145.15 (NN***C***HSiMe$_3$), 168.56 (***C***NNCHSiMe$_3$),171.35, 172.08 (***C***OC(CH$_3$)$_2$).

^{29}Si (79.49 MHz, 298 K, CDCl$_3$): -7.63 ppm

HRMS: m/z calcd for $[M+H]^+$ $C_{34}H_{51}N_4O_2Si$, 575.3703; found **575.37**.

IR (cm^{-1}): 2962.11, 2051.56, 1690.73, 1608.23, 1385.57, 1352.58, 1250.49, 841.24, 789.26, 751.94.

Melting point range: 135-140 ˚C.

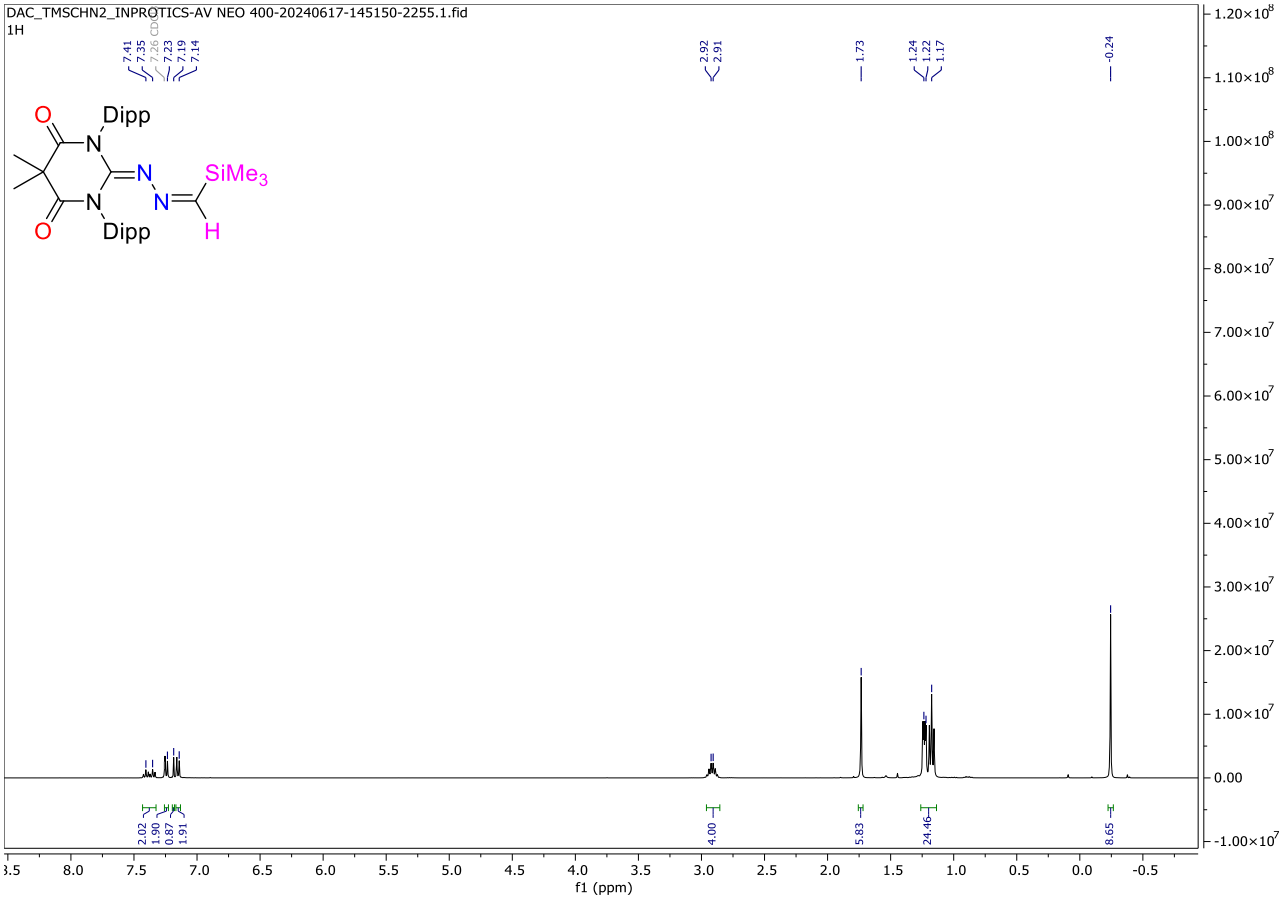


Figure S40: ^{1}H NMR spectrum of **8**

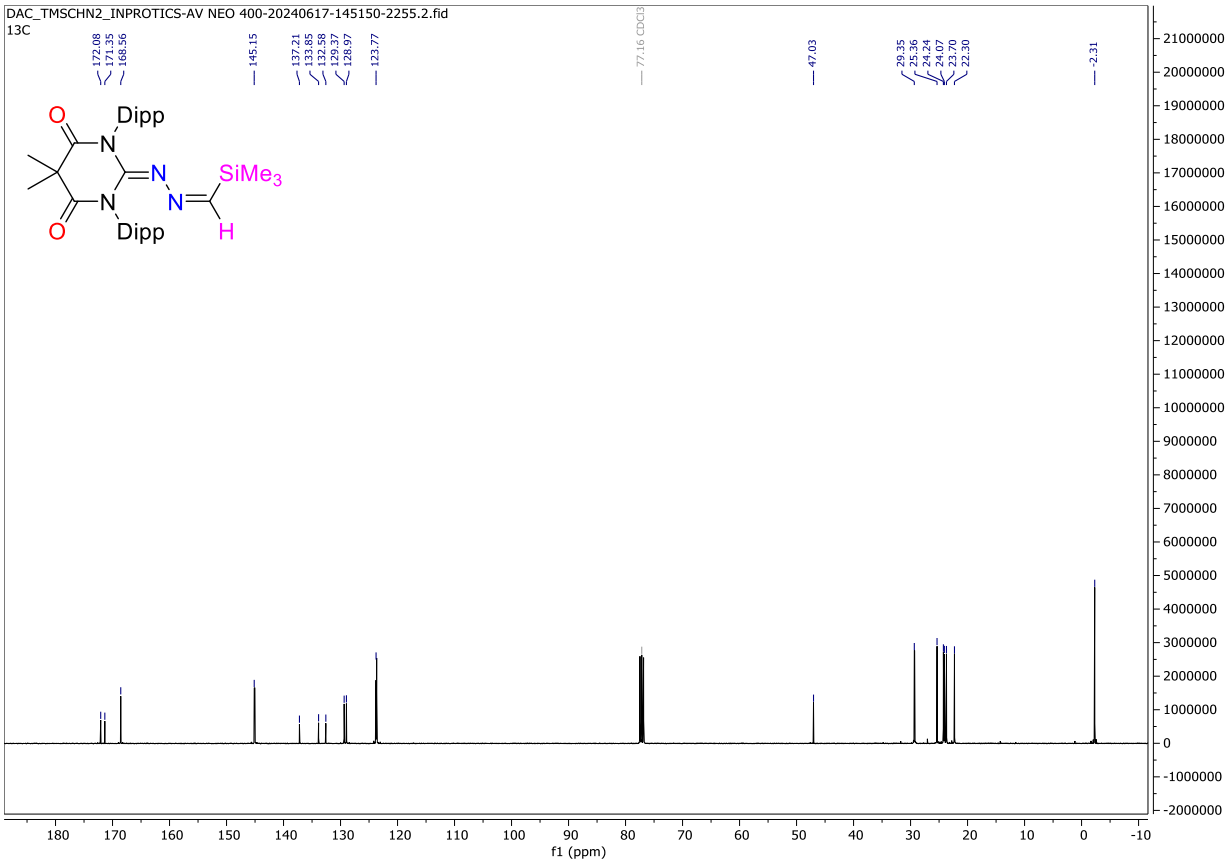


Figure S41: $^{13}C\{^{1}H\}$ NMR spectrum of **8**

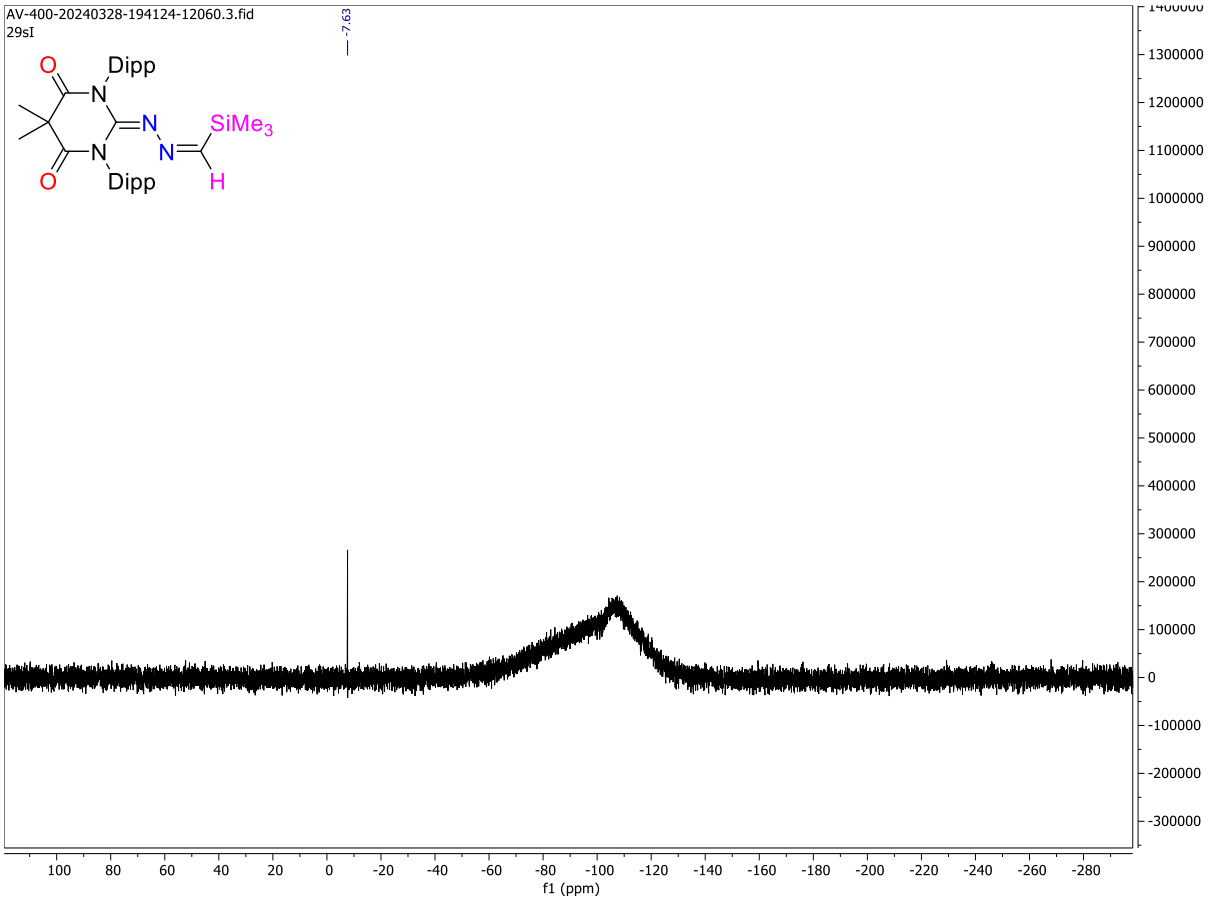


Figure S42: $^{29}Si\{^{1}H\}$ NMR spectrum of **8**

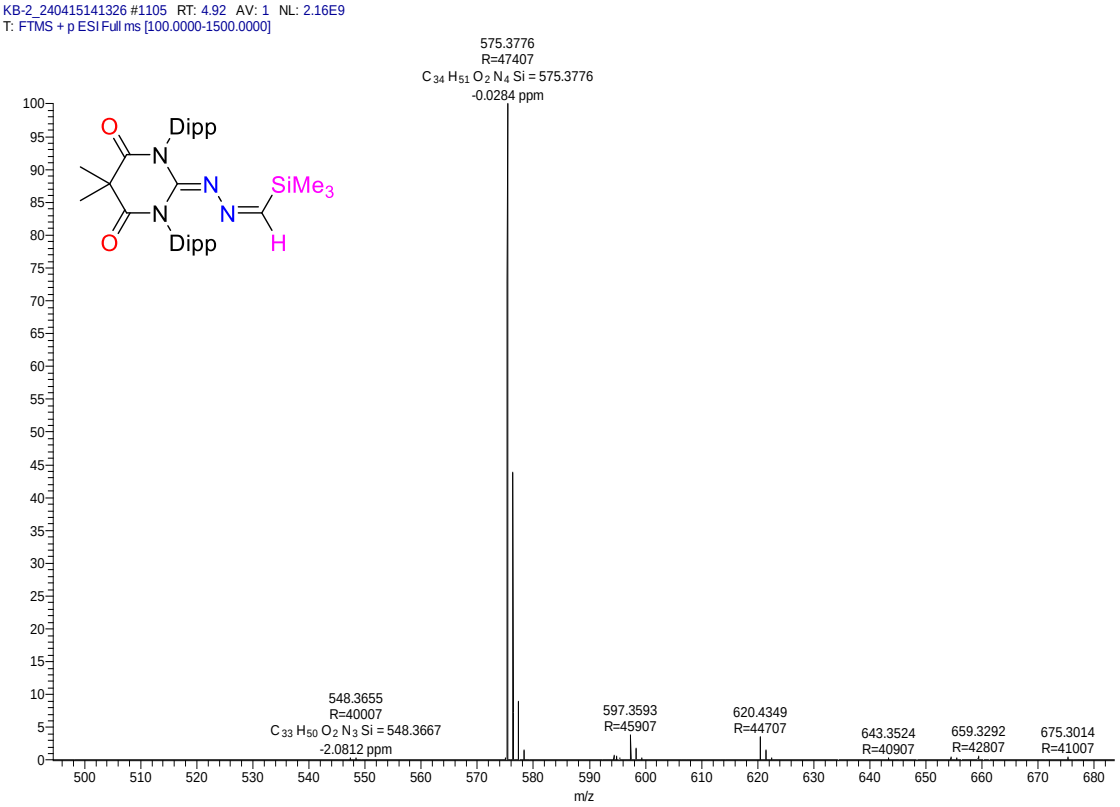


Figure S43: HRMS spectrum of **8**

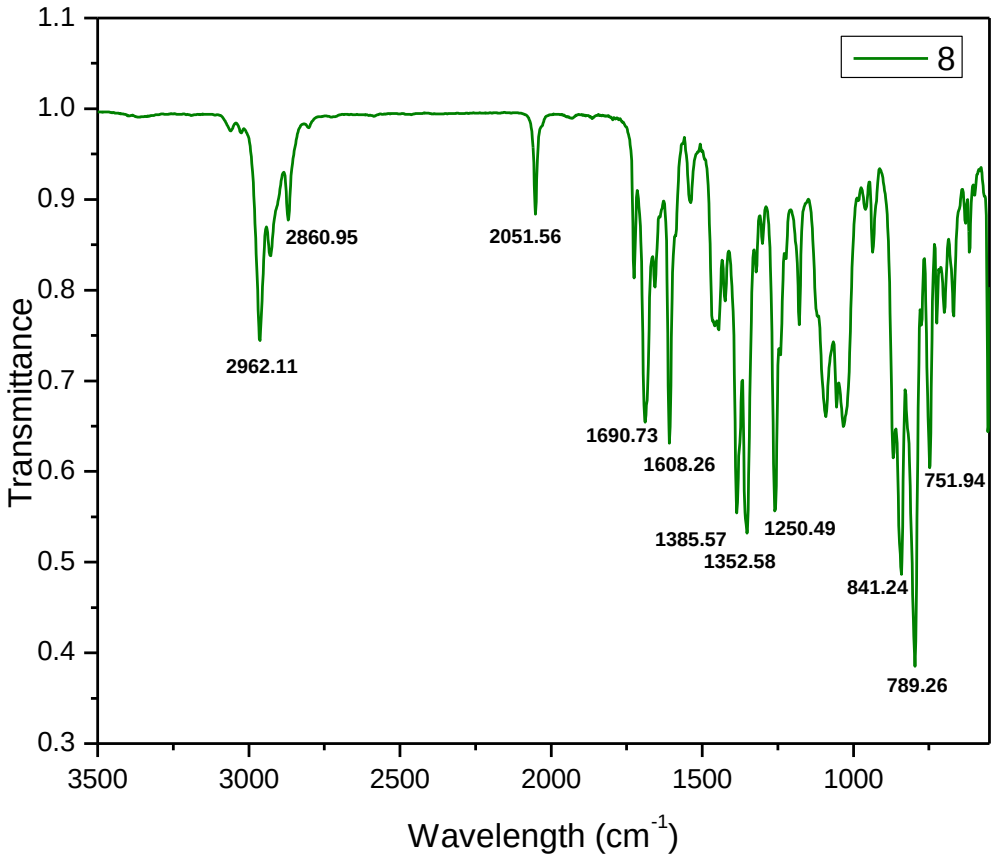


Figure S44: IR (ATR) spectrum of **8**

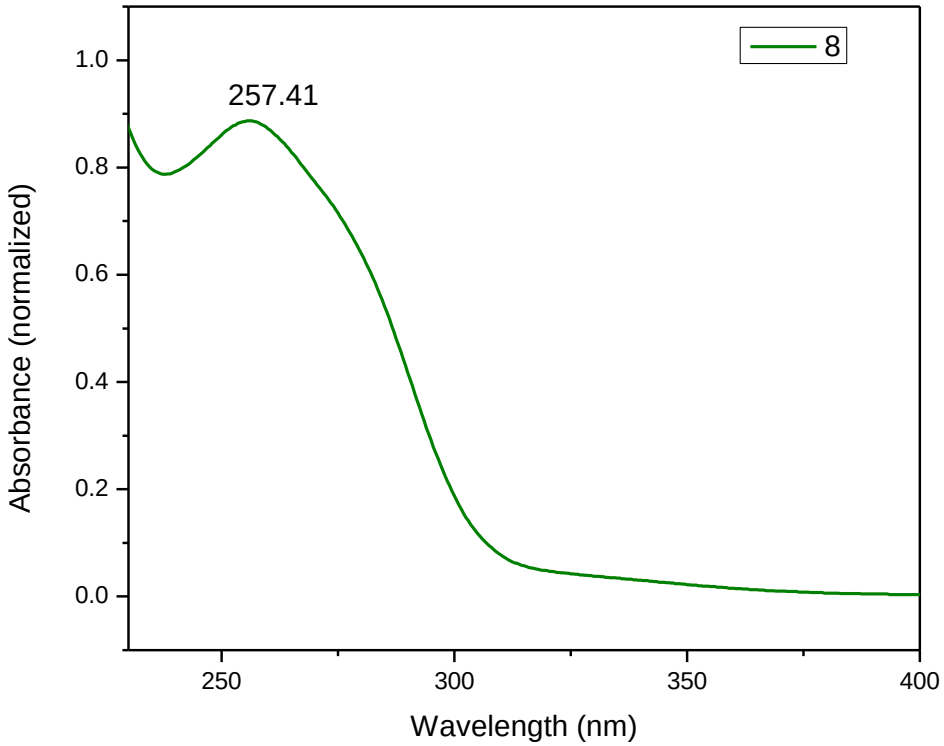


Figure S45: UV-VIS spectrum of **8**

Synthesis of 10: 6-SIPr (0.200 g, 0.49 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C. COO^{t}BuCHN$_2$ (0.071 g, 0.50 mmol) was dissolved in 5 mL toluene in a Schlenk tube and transferred slowly to a pre-cooled solution of 6-SIPr. The reaction was run for 20 hours at room temperature. The solution was filtered using a cannula, concentrated to 3-4 mL, and stored at 4 ˚C to get plate-shaped yellow crystals of **9** after a day with a yield of 60%.

^{1}H NMR (500 MHz, 298 K, CDCl$_3$): δ = 1.18 (d, *J* = 6.75 Hz, 12 H, CH(C***H***$_3$)$_2$), 1.25 (singlet, 9 H, COOC(C***H***$_3$)$_3$), 1.30 (d, *J* = 7 Hz, 12 H, CH(C***H***$_3$)$_2$), 2.27 (quintet, *J* = 6 Hz, 2 H, NCH$_2$C***H***$_2$CH$_2$N), 3.16 (sept, *J* = 6.88 Hz, 4 H, C***H***(CH$_3$)$_2$), 3.58 (t, *J* = 5.88 Hz, 4 H, NC***H***$_2$CH$_2$C***H***$_2$N), 6.68 (singlet, 1 H, NNC***H***COO^{t}Bu), 7.10 (d, 4 H, *J*=7.63 Hz, Ar-H), 7.22 (t, 2 H, *J*=7.13 Hz Ar-H) ppm.

^{13}C{^{1}H} NMR (125.7 MHz, 298 K, CDCl$_3$): δ = 22.90 (NCH$_2$***C***H$_2$CH$_2$N), 23.55 (CH(***C***H$_3$)$_2$), 24.65 (CH(***C***H$_3$)$_2$), 28.35 (COOC(**C**H$_3$)$_3$), 29.02 (**C**H(CH$_3$)$_2$), 51.04 (N***C***H$_2$CH$_2$***C***H$_2$N), 79.33 (COO***C***(CH$_3$)$_3$), 123.82 (Ar-C), 127.50 (Ar-C), 138.59 (Ar-C), 141.22 (Ar-C) ppm, 145.12 (NN***C***HCOO^{t}Bu), 154.13 (***C***NNCHCOO^{t}Bu), 165.25 (NNCH***C***OO^{t}Bu).

HRMS: m/z calcd for [M+H]$^+$ C$_{34}$H$_{51}$N$_4$O$_2$, 547.80; found **547.40**.

IR (cm^{-1}): 2960.88, 1674.26, 1439.20, 1315.49, 1160.84, 1268.08, 1063.94, 797.95, 752.59.

Melting point range: 220-225 ˚C.

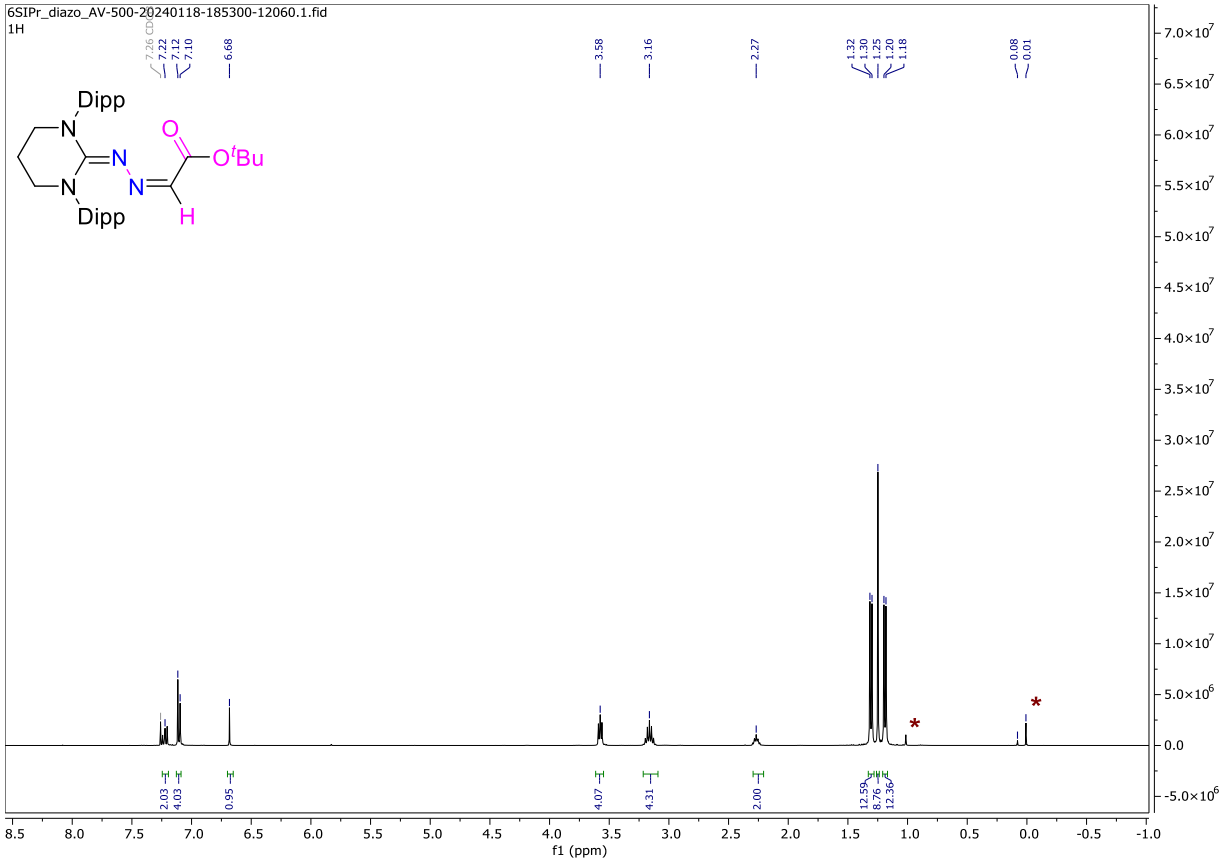


Figure S46: ^{1}H NMR spectrum of **9** (red asterisks belong to minor impurity and 0.08 ppm corresponds to grease)

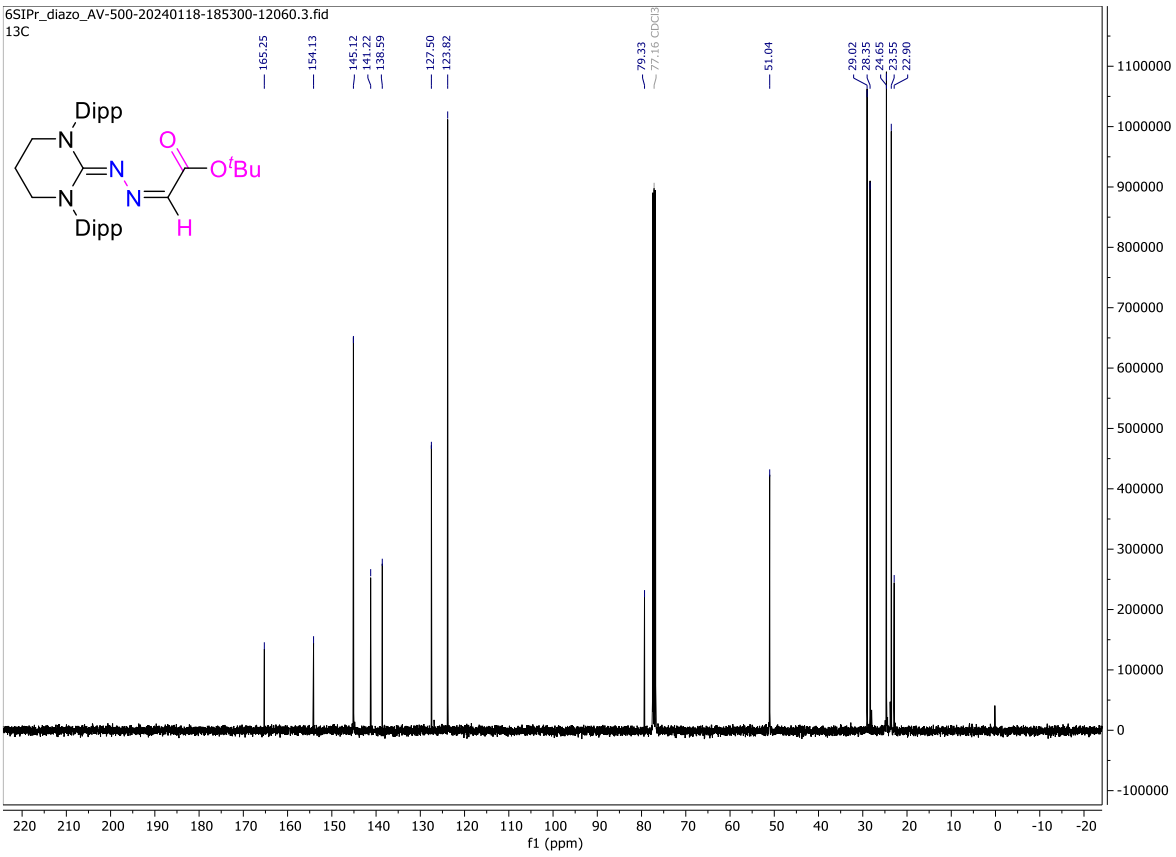


Figure S47: $^{13}C\{^1H\}$ NMR spectrum of **9**

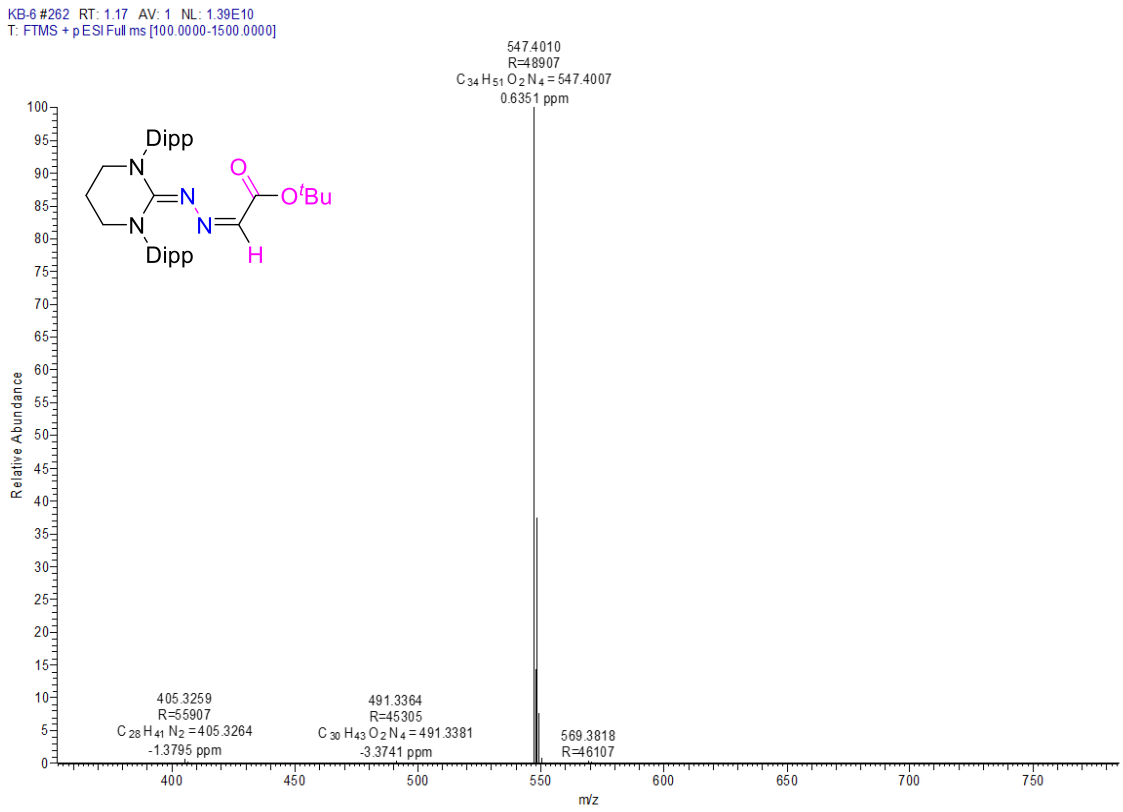


Figure S48: HRMS spectrum of **9**

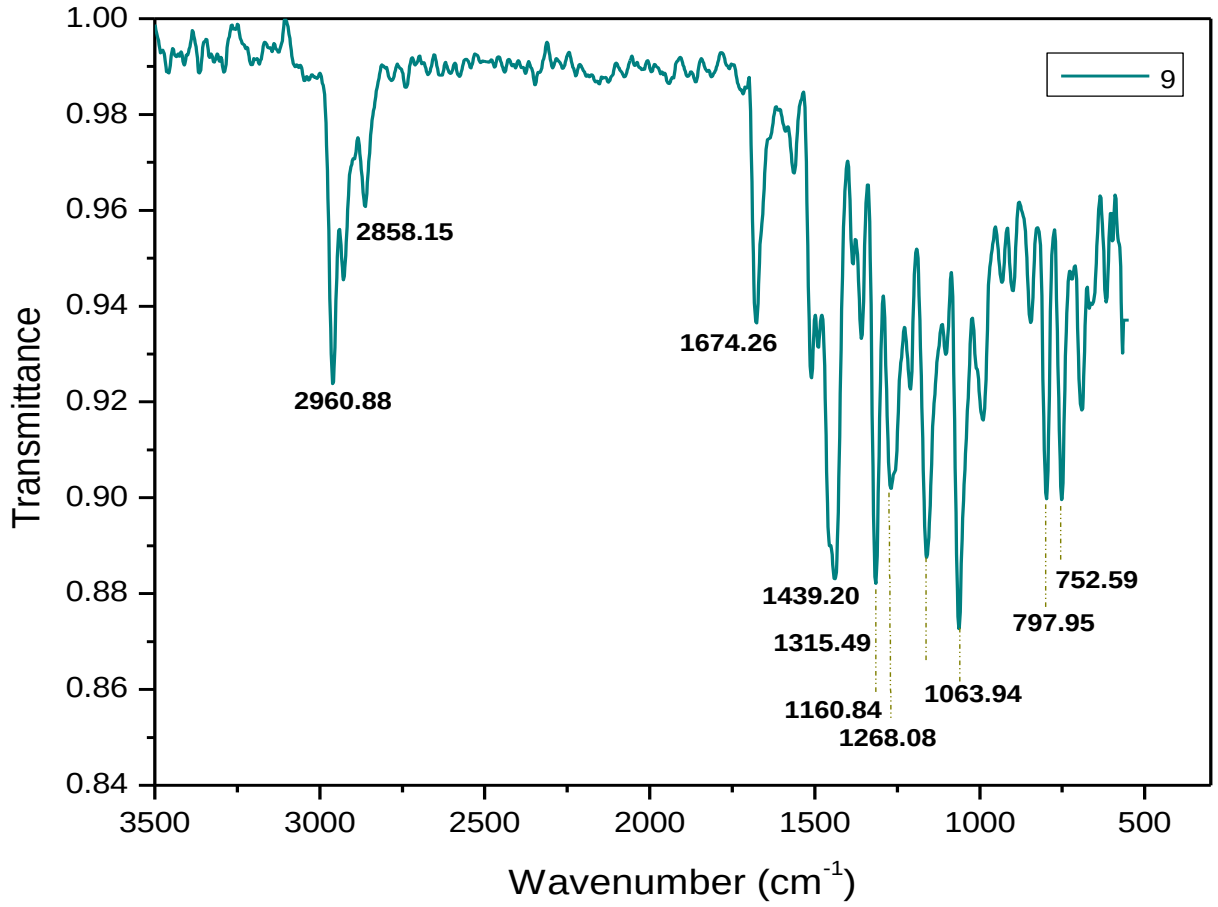


Figure S49: IR (ATR) spectrum of **9**

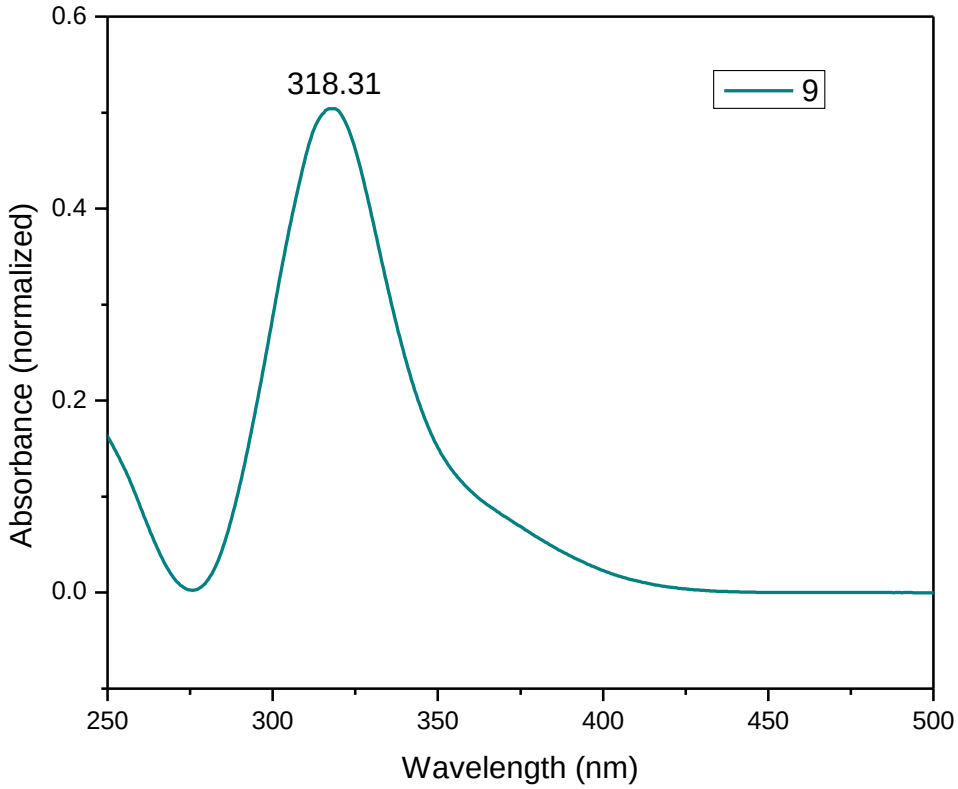


Figure S50: UV-VIS spectrum of **9**

Synthesis of 11: 5-SIPr (0.200 g, 0.51 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C. COO^tBuCHN_2 (0.073 g, 0.51 mmol) was dissolved in 5 mL toluene in a Schlenk tube and transferred slowly to a pre-cooled solution of 5-SIPr. The reaction was run for 18 hours while slowly warming to room temperature. All the volatiles were removed and the residue was dissolved in 6-8 mL of hexane. The solution was filtered using a cannula, concentrated to 3-4 mL, and stored at room temperature to get plate-shaped yellow crystals of **10** after a day with a yield of 62%.

^{1}H NMR (500 MHz, 298 K, C_6D_6): δ = 1.25 (singlet, *J*= 6.48 Hz, 9 H, $COOC(CH_3)_3$), 1.27 (d, *J*= 6.48 Hz, 12 H, $CH(CH_3)_2$), δ = 1.33 (d, *J*= 6.85 Hz,12 H, $CH(CH_3)_2$), 3.23 (broad sept, 4 H, $CH(CH_3)_2$), 3.30 (singlet, 4 H, NCH_2CH_2N), 7.10 (d, *J*= 7.46 Hz, 2 H, Ar-H), 7.20 (t, *J*= 7.58 Hz, 2 H, Ar-H), 7.40 (singlet, 1 H, $NNCHCOO^tBu$), ppm.

$^{13}C\{^1H\}$ NMR (125.7 MHz, 298 K, $CDCl_3$): δ = 24.20 ($CH(CH_3)_2$), 28.23 ($COOC(CH_3)_3$), 29.06 ($CH(CH_3)_2$), 48.96 (NCH_2CH_2N), 51.69 (NCH_2CH_2N), 79.75 ($COOC(CH_3)_3$), 123.98 (Ar-C), 128.70 (Ar-C), 141.10 ($CNNCHCOO^tBu$), 145.91 (Ar-C), 147.90 (Ar-C), 158.63 ($NNCHCOO^tBu$), 165.30 ($NNCHCOO^tBu$).

HRMS: m/z calcd for $[M+H]^+$ $C_{33}H_{49}O_2N_4$, 533.77; found **533.38**.

IR (cm^{-1}): 2960.88, 1690.75, 1597.97, 1517.55, 1453.63, 1313.43, 1263.94, 1156.72, 804.14, 752.59.

Melting point range: 155-160 ˚C.

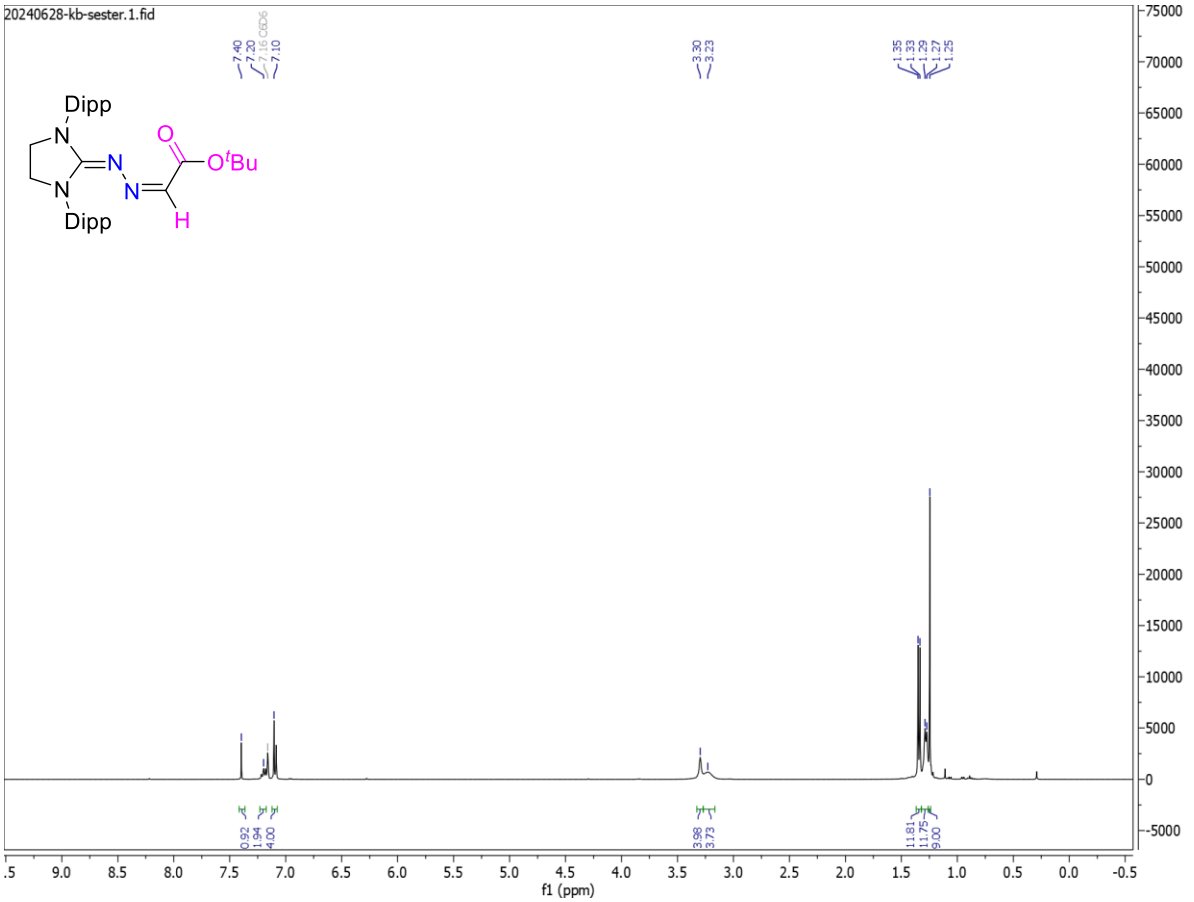


Figure S51: ^{1}H NMR spectrum of **10**

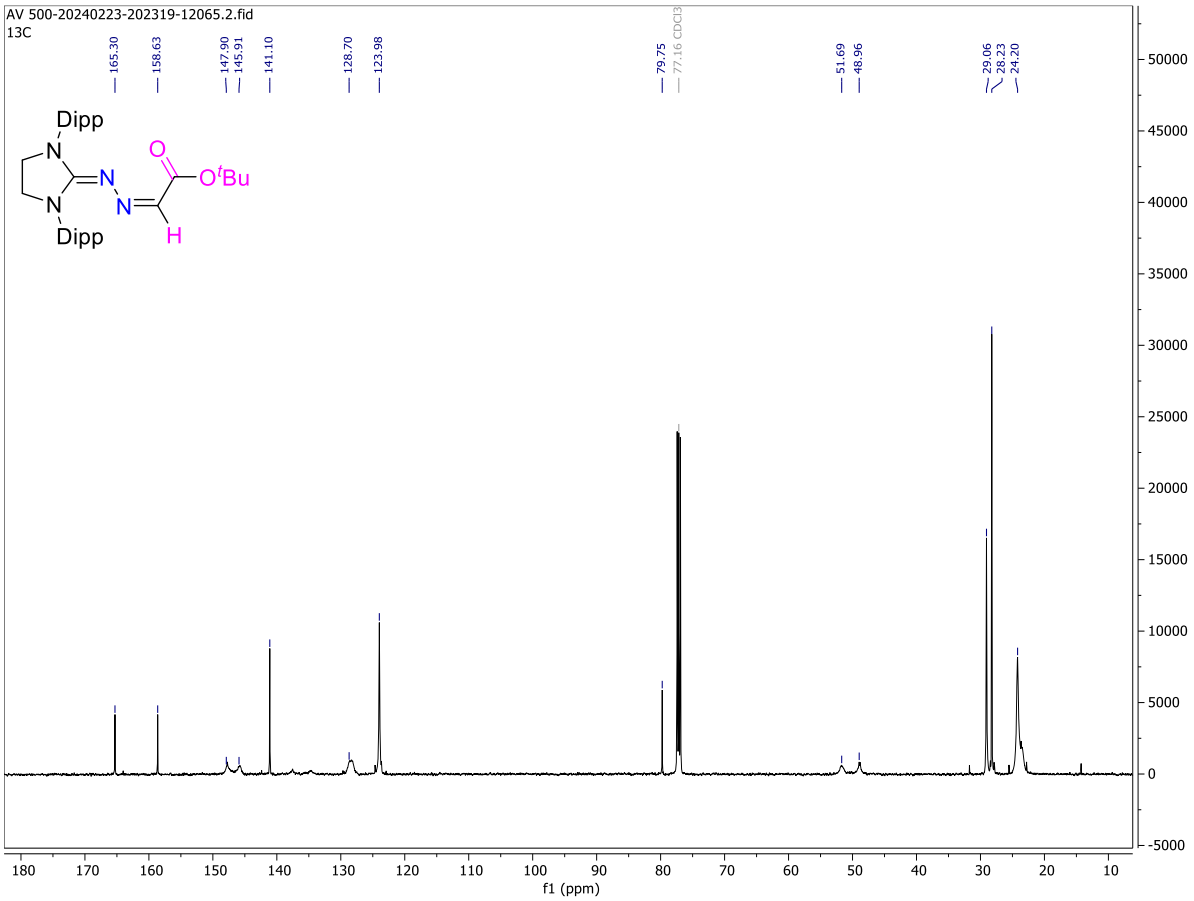


Figure S52: ^{13}C{^{1}H} NMR spectrum of **10**

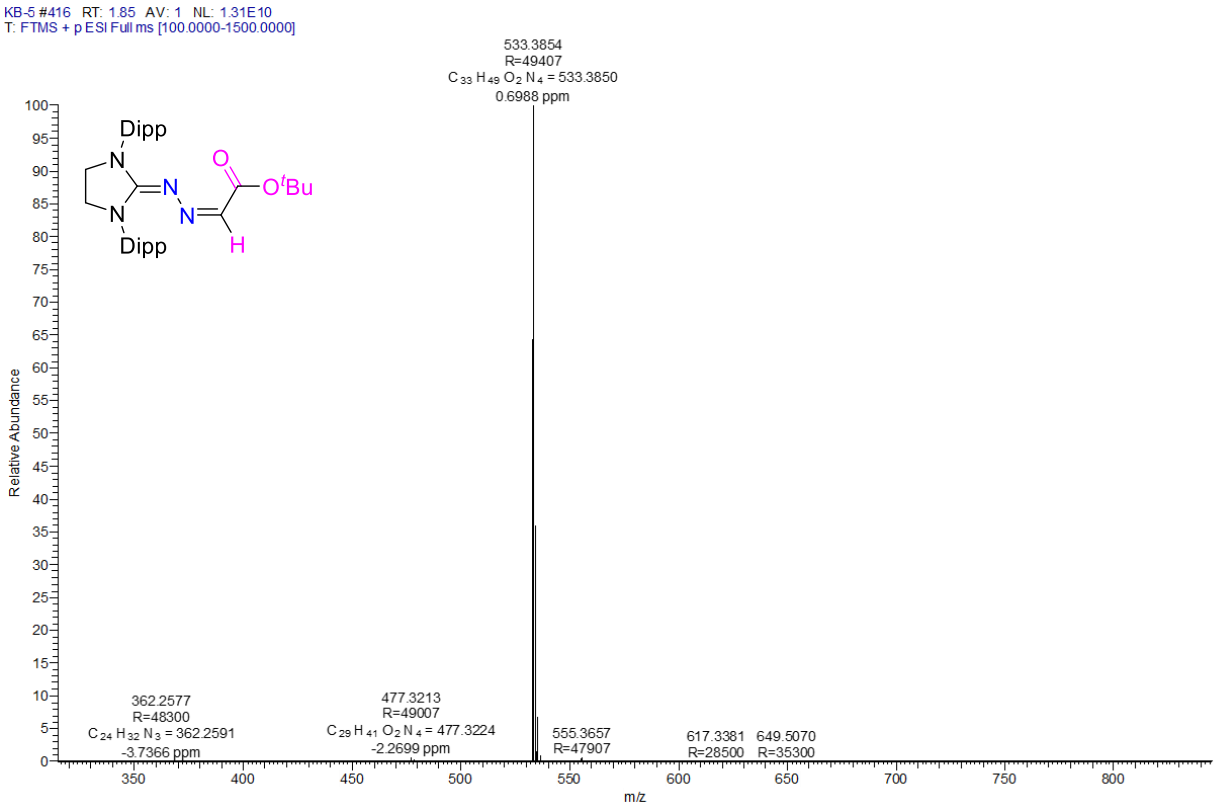


Figure S53: HRMS spectrum of **10**

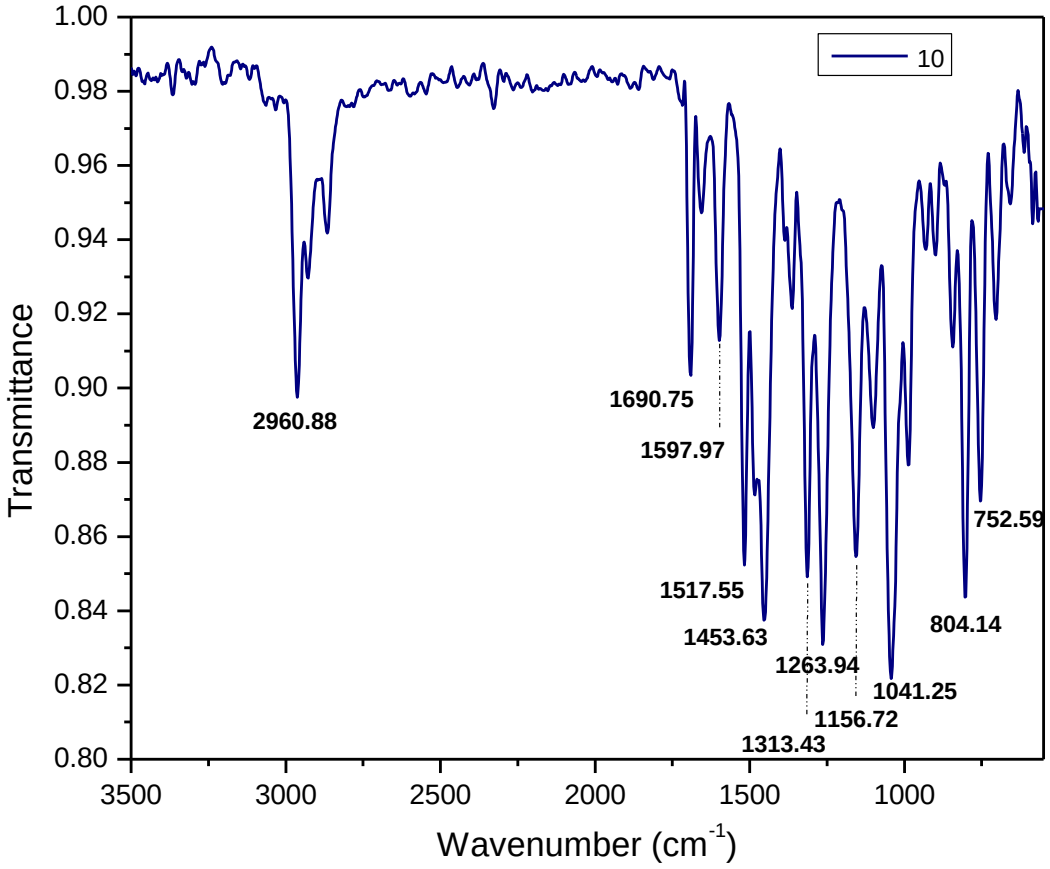


Figure S54: IR (ATR) spectrum of **10**

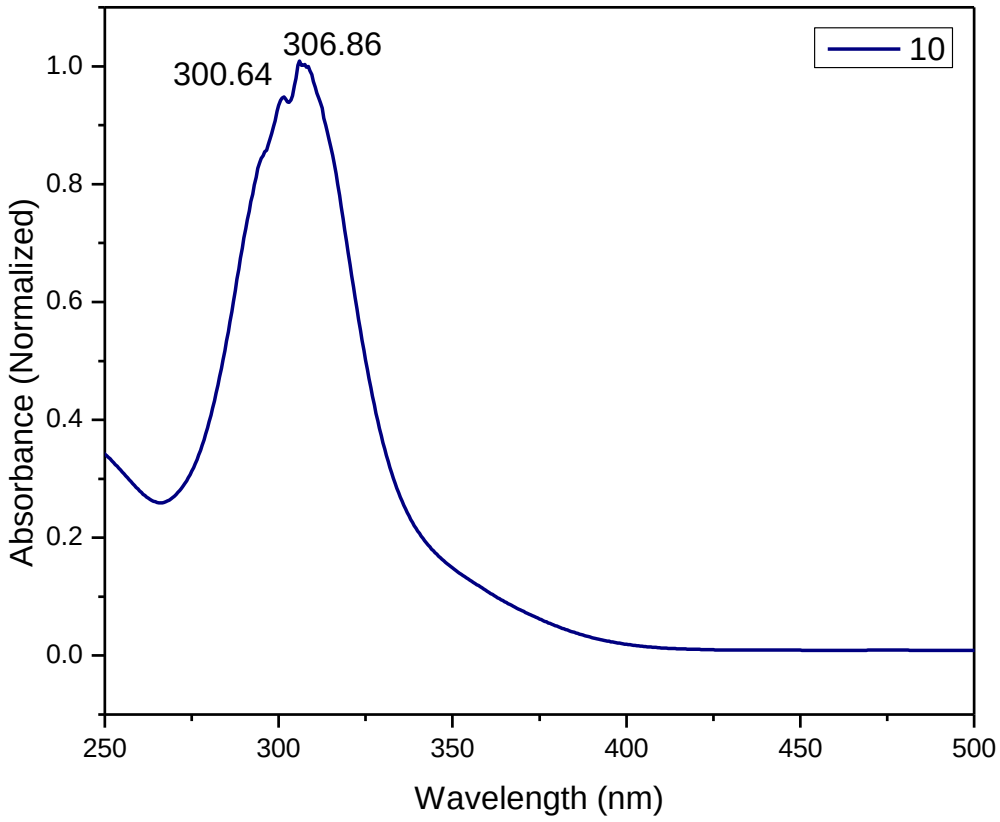


Figure S55: UV-VIS spectrum of **10**

Synthesis of 11: 5-IPr (0.200 g, 0.51 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C. COO^{t}BuCHN$_2$ (0.074 g, 0.52 mmol) was dissolved in 5 mL toluene in a Schlenk tube and transferred slowly to a pre-cooled solution of 5-IPr. The reaction was run for 20 hours while slowly warming to room temperature. The solution was filtered using a cannula, concentrated to 3-4 mL, and stored at -36 ˚C to get block-shaped yellow crystals of **11** after 2 days with a yield of 70%.

^{1}H NMR (400 MHz, 298 K, C$_6$D$_6$): δ = 1.18 (d, *J* = 6.85 Hz, 12 H, CH(C***H***$_3$)$_2$), 1.27 (singlet, 9 H, COOC(C***H***$_3$)$_3$), 1.31 (d, *J* = 6.88 Hz, 12 H, CH(C***H***$_3$)$_2$), 3.01 (sept, *J* = 6.85 Hz, 4 H, C***H***(CH$_3$)$_2$), 5.82 (singlet, 2 H, NC***H***C***H***N), 7.09 (d, 4 H, *J* = 7.70 Hz, Ar-H), 7.22 (t, *J* = 7.46 Hz , 2 H, Ar-H), 7.47 (singlet, 1 H, NNC***H***COO^{t}Bu) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, C$_6$D$_6$): δ = 23.50 (CH(***C***H$_3$)$_2$), 23.88 (CH(***C***H$_3$)$_2$), 28.39 (COOC(***C***H$_3$)$_3$), 29.28 (***C***H(CH$_3$)$_2$), 78.58 (COO***C***(CH$_3$)$_3$), 116.69 (Ar-C), 123.96 (Ar-C), 125.70 (Ar-C), 128.57 (Ar-C), 129.62 (N***C***H***C***HN), 137.89, 138.12 (Ar-C), 146.26 (NN***C***HCOO^{t}Bu), 152.52 (***C***NNCHCOO^{t}Bu), 164.73 (NNCH***C***OO^{t}Bu) ppm.

HRMS: m/z calcd for [M+H]$^+$ C$_{33}$H$_{47}$N$_4$O$_2$, 531.36; found **531.36**.

IR (cm^{-1}): 2962.95, 1678.38, 1579.41, 1463.94, 1327.86, 1278.37, 1072.18, 987.65, 936.10, 756.71.

Melting point range: 99-103 ˚C.

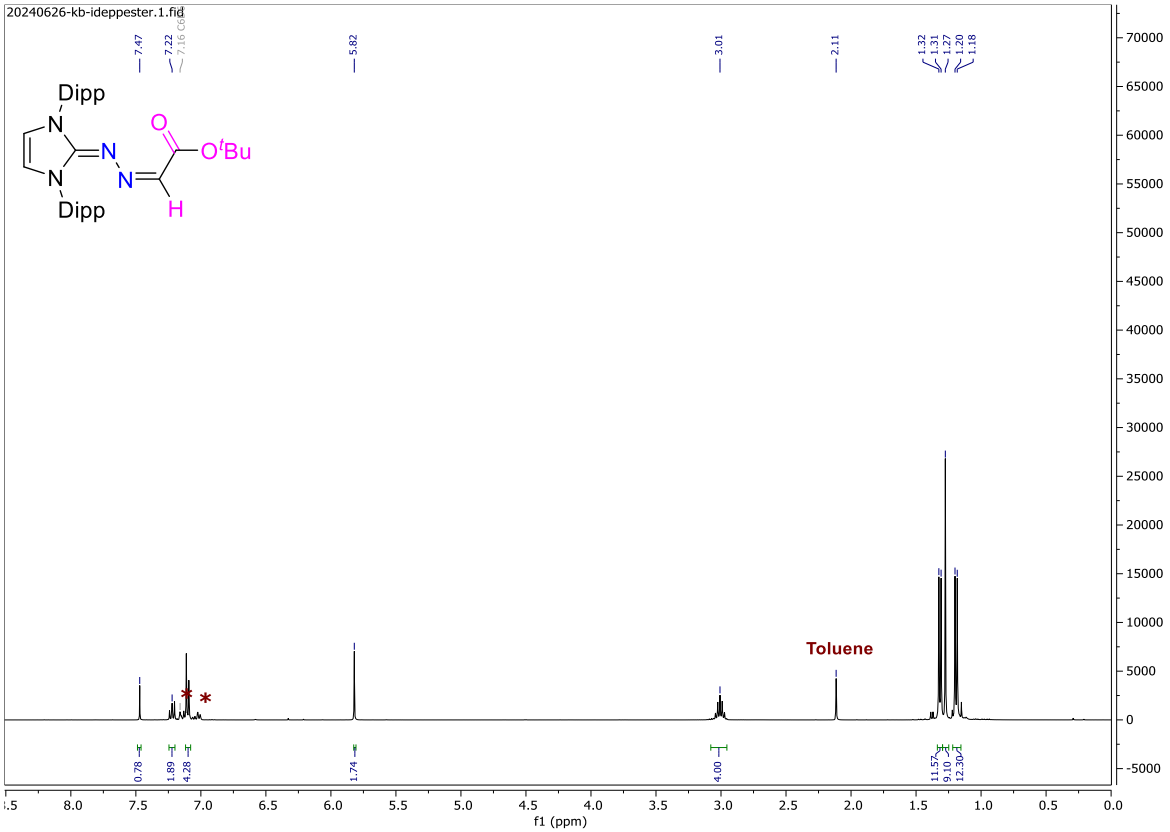


Figure S56: ^{1}H NMR spectrum of **11** (red asterisks belong to toluene)

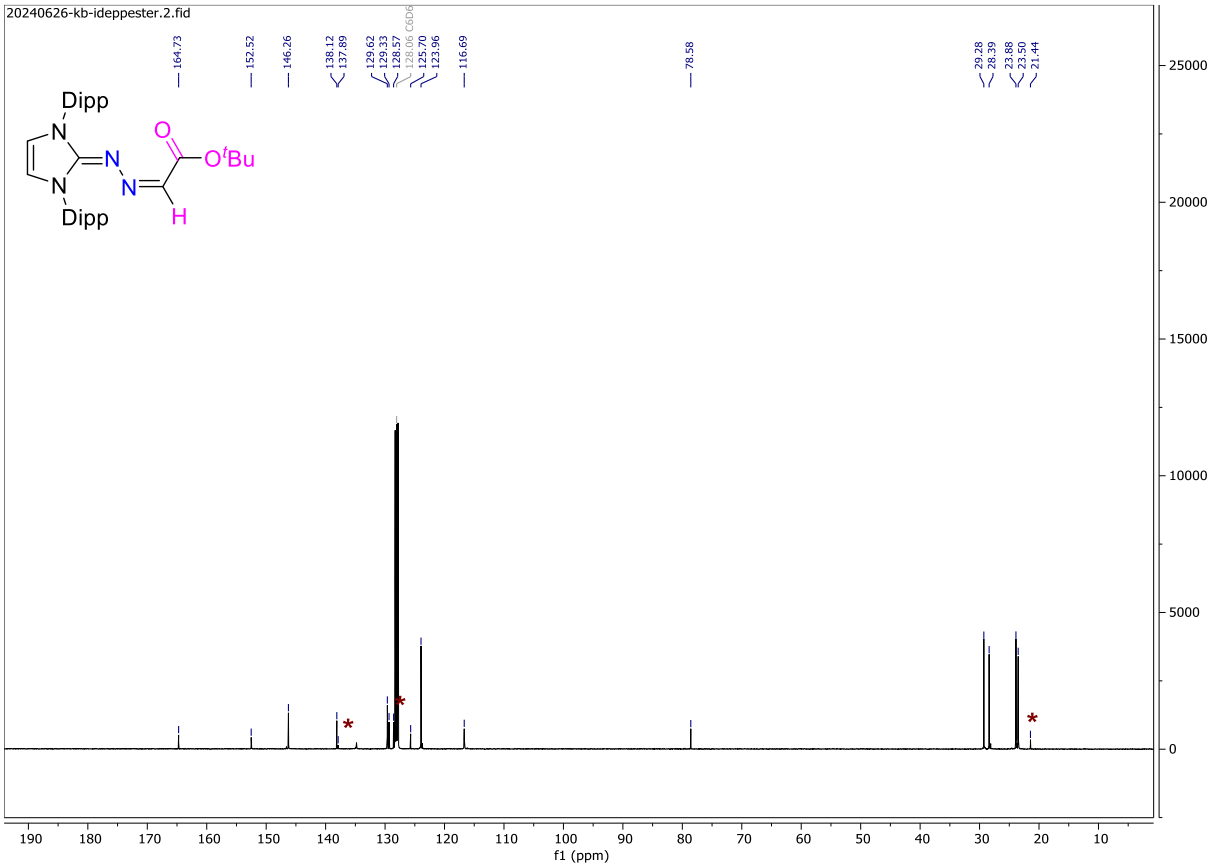


Figure S57: $^{13}C\{^{1}H\}$ NMR spectrum of **11** (red asterisks belong to toluene)

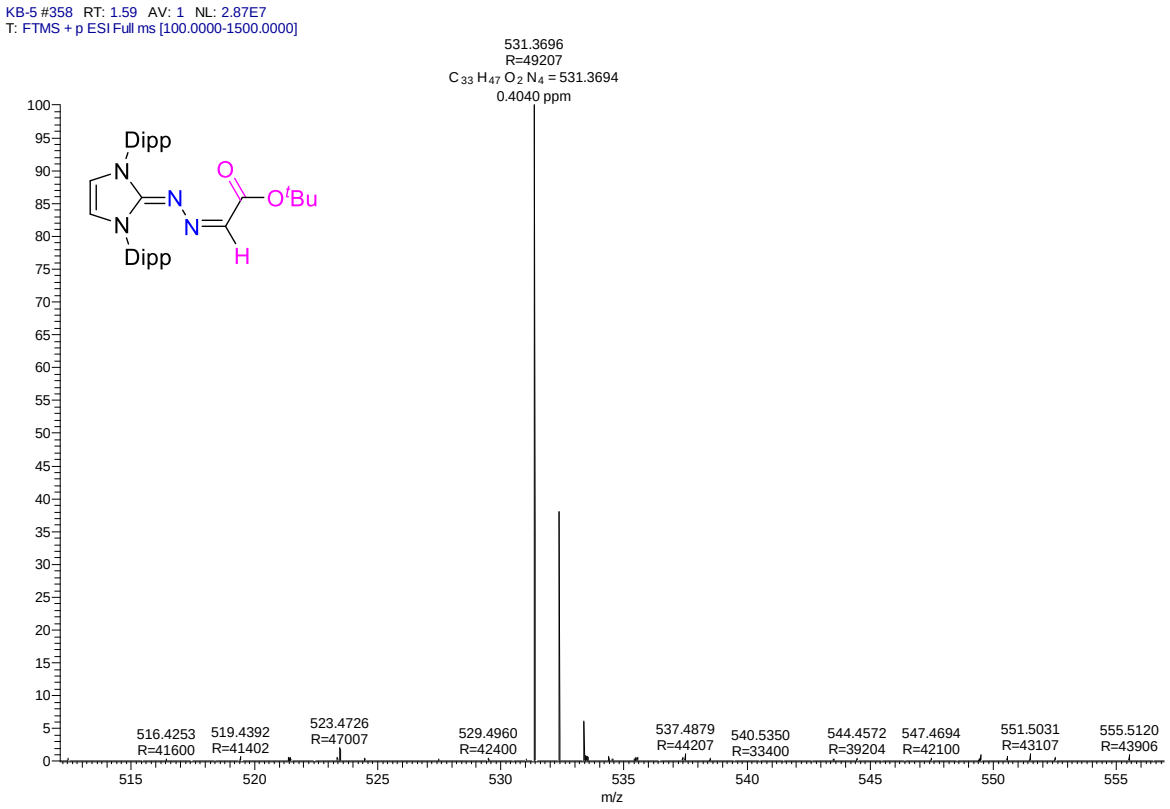


Figure S58: HRMS spectrum of **11**

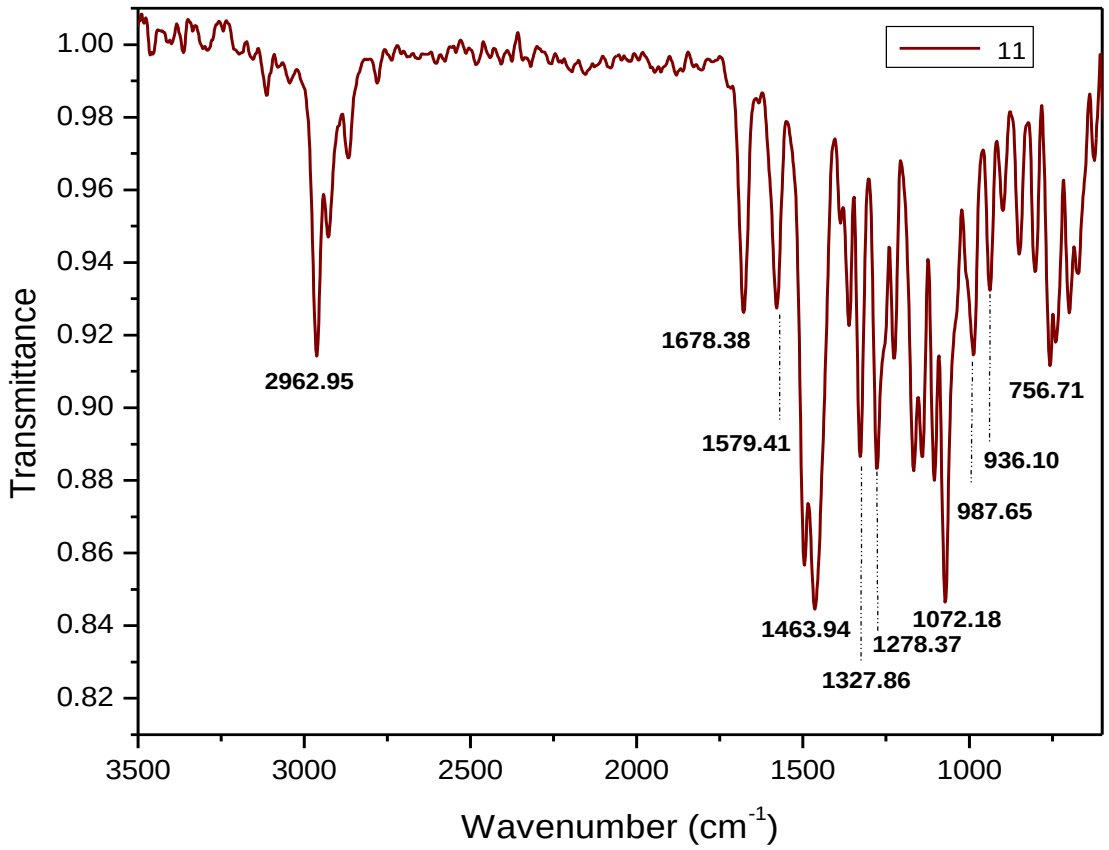


Figure S59: IR (ATR) spectrum of **11**

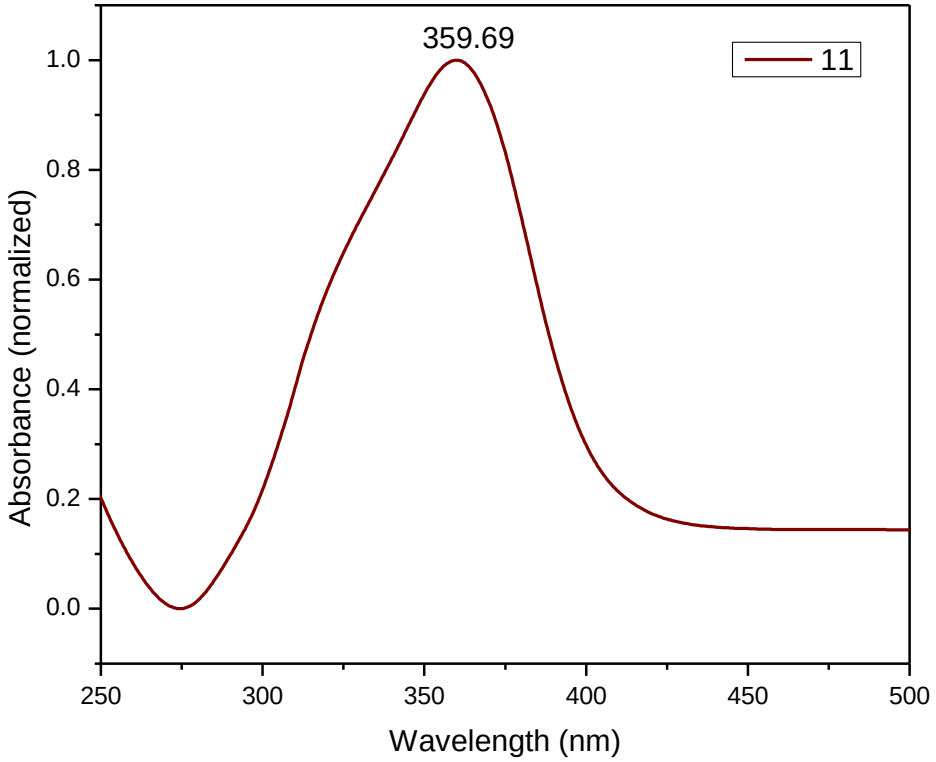


Figure S60: UV-VIS spectrum of **11**

Synthesis of 12: DAC.OTf salt (0.300 g, 0.50 mmol) and NaHMDS (0.094 g, 0.51 mmol) were taken together and 20 mL toluene was added to it. The reaction was

run for 30 min. Filtered the solution using frit and kept the Schlenk flask at -36 ˚C. COO^tBuCHN_2 (0.094 g, 0.66 mmol) was dissolved in 5 mL toluene and transferred to the Schlenk flask resulting in a yellow-colored solution. The reaction was run for 18 hours while slowly warming to room temperature. All the volatiles were removed and the pure product was isolated using column chromatography in 5% ethylacetate and pet ether with a yield of 35%. The suitable crystals for XRD were grown from the crude mixture by slow evaporation at room temperature in the DCM and hexane mixture in air.

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.18 (dd, *J* = 6.50 Hz, 9 H, CH(C***H***$_3$)$_2$), 1.22 (d, *J* = 6.88 Hz, 14 H, CH(C***H***$_3$)$_2$), 1.33 (singlet, 9 H, COOC(C***H***$_3$)$_3$), 1.76 (singlet, 6 H, (OCC(C***H***$_3$)$_2$), 2.89 (sept, *J* = 6.13 Hz, 4 H, C***H***(CH$_3$)$_2$), 6.56 (singlet, 1 H, NNC***H***COO^{t}Bu), 7.13 (d, *J* = 7.50 Hz , 2 H, Ar-H), 7.22 (d, *J* = 7.38 Hz , 2 H, Ar-H), 7.34 (t, *J* = 7.63 Hz , 1 H, Ar-H), 7.40 (t, *J* = 7.38 Hz , 1 H, Ar-H) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ = 22.15-24.37 (CH(***C***H$_3$)$_3$), 25.33 (***C***H(CH$_3$)$_3$), 27.87 (COOCC(***C***H$_3$)$_2$), 29.36 (COOC(***C***H$_3$)$_3$), 47.20 (COO***C***(CH$_3$)$_2$, 81.42 (OC***C***(CH$_3$)$_2$), 123.49-132.31 (Ar-C), 137.47(N***C***NNCOO^{t}Bu), 145.03 (Ar-C), 145.34 (***C***HCOO^{t}Bu), 145.71 (Ar-C), 161.93 (***C***OOC(CH$_3$)$_3$), 171.01, 171.93 (O***C***C(*C*H$_3$)$_2$) ppm.

HRMS: m/z calcd for $[M+H]^+$ $C_{36}H_{51}N_4O_4$, 603.38; found **603.39**.

IR (cm^{-1}): 2962.91, 1692.79, 1608.20, 1577.33, 1453.61, 1383.51, 1335.14, 1255.83, 1158.77, 983.51.

Melting point range: 155-158 ˚C.

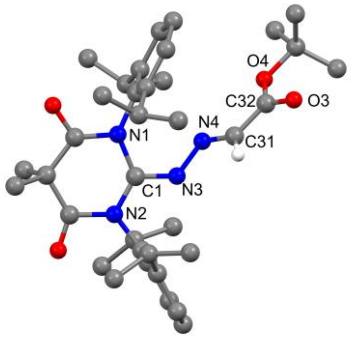


Figure S61: The solid-state structure of **12**

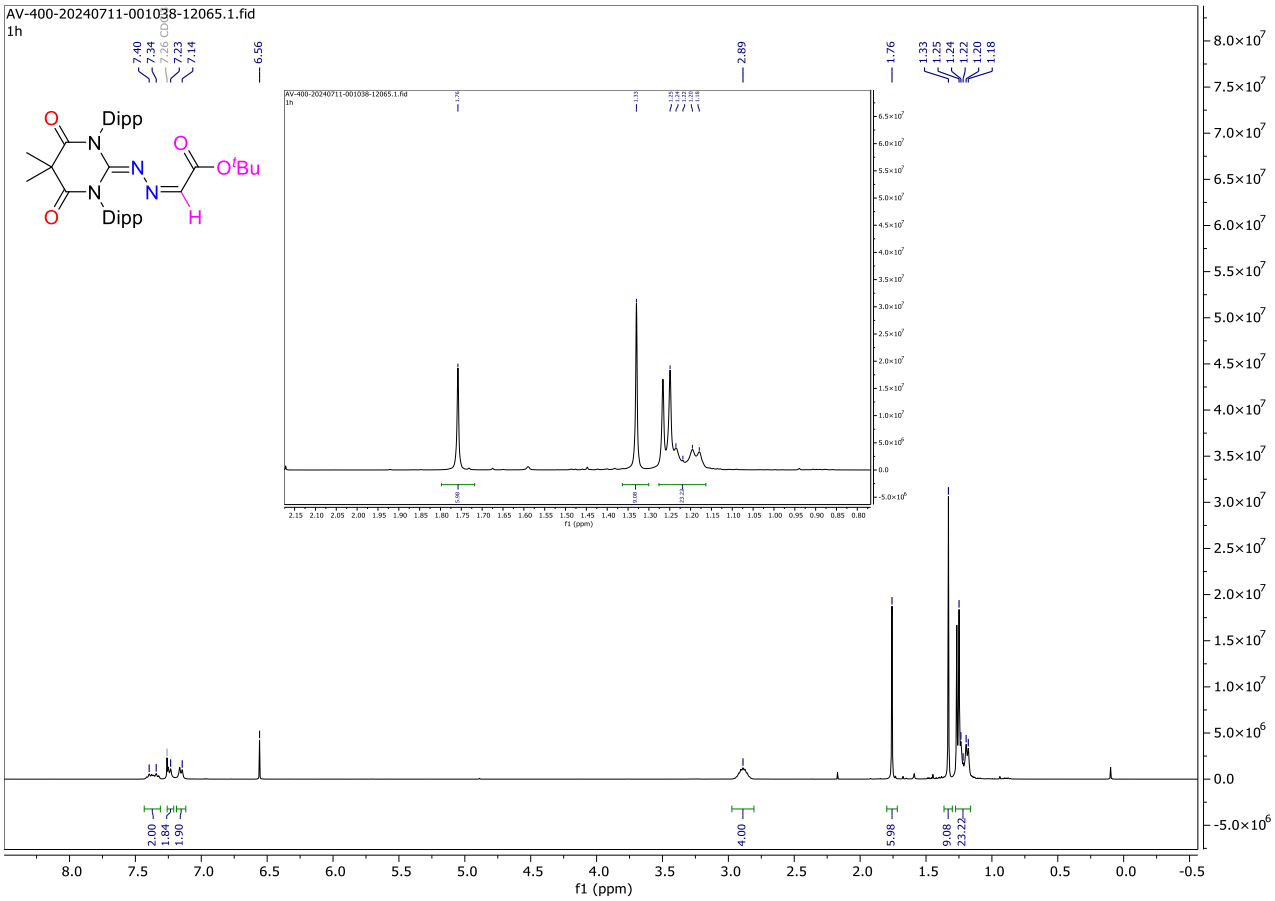


Figure S62: ^{1}H NMR spectrum of **12** (very small extra peaks in the region 0-2 ppm belong to minor impurities)

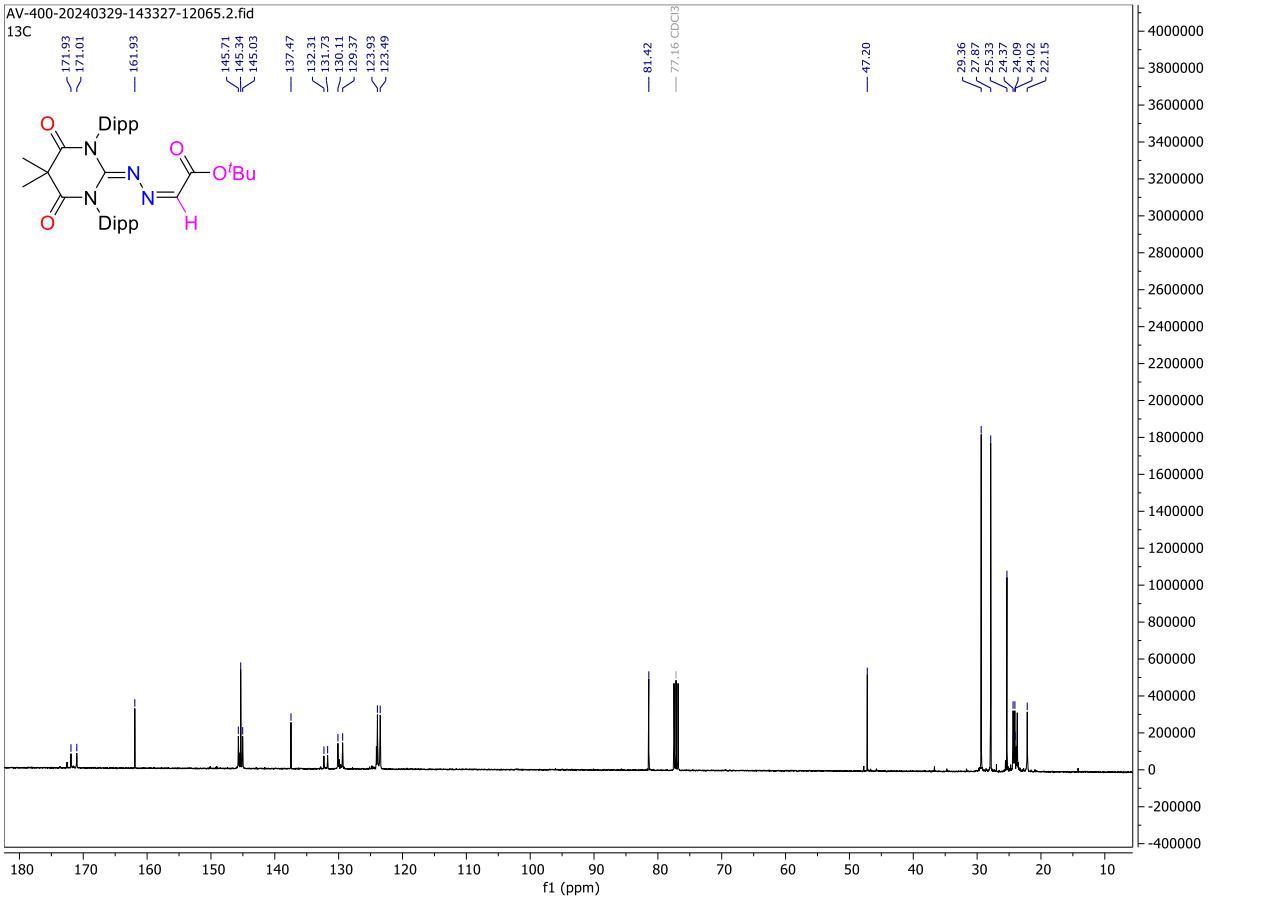


Figure S63: $^{13}C\{^{1}H\}$ NMR spectrum of **12**

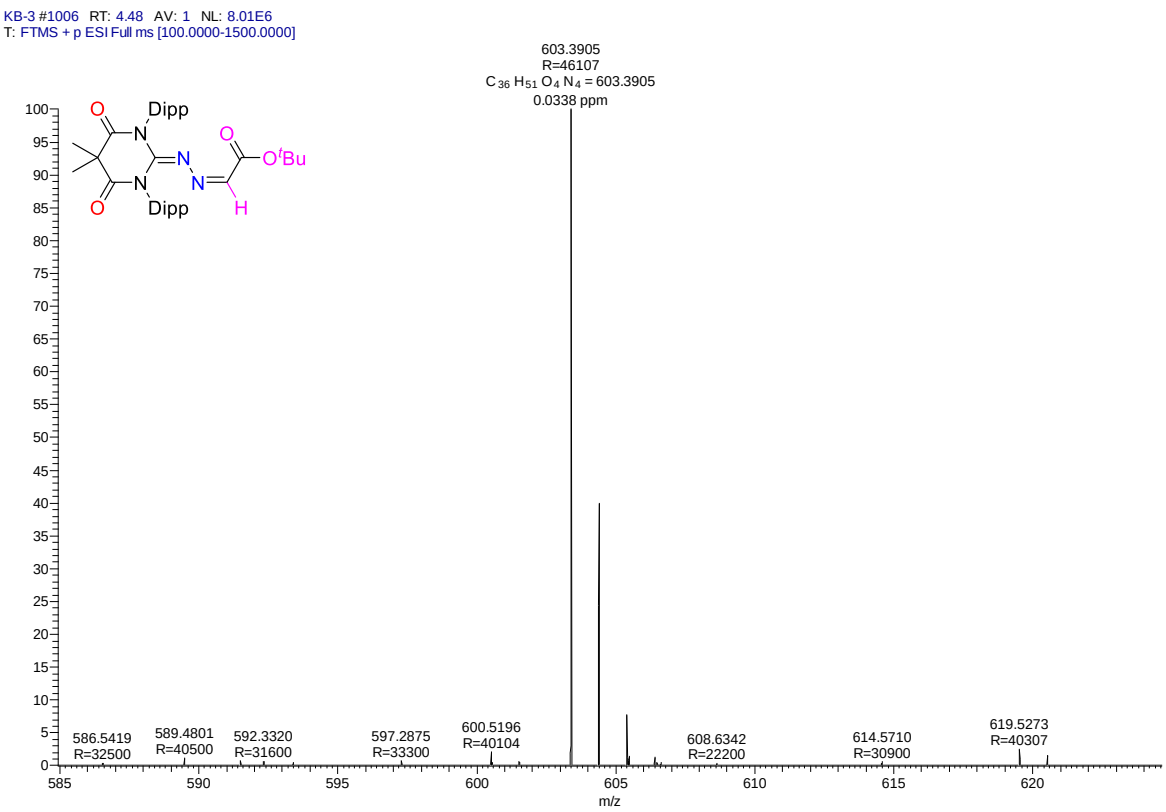


Figure S64: HRMS spectrum of **12**

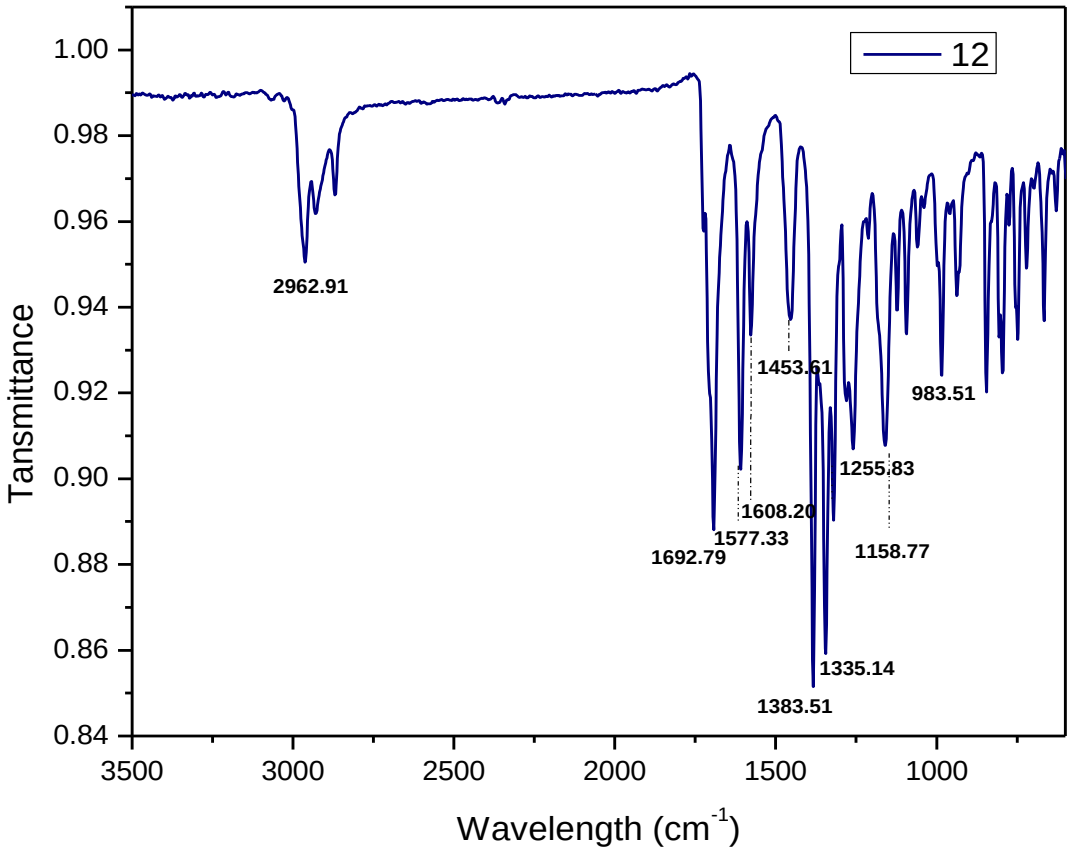


Figure S65: IR (ATR) spectrum of **12**

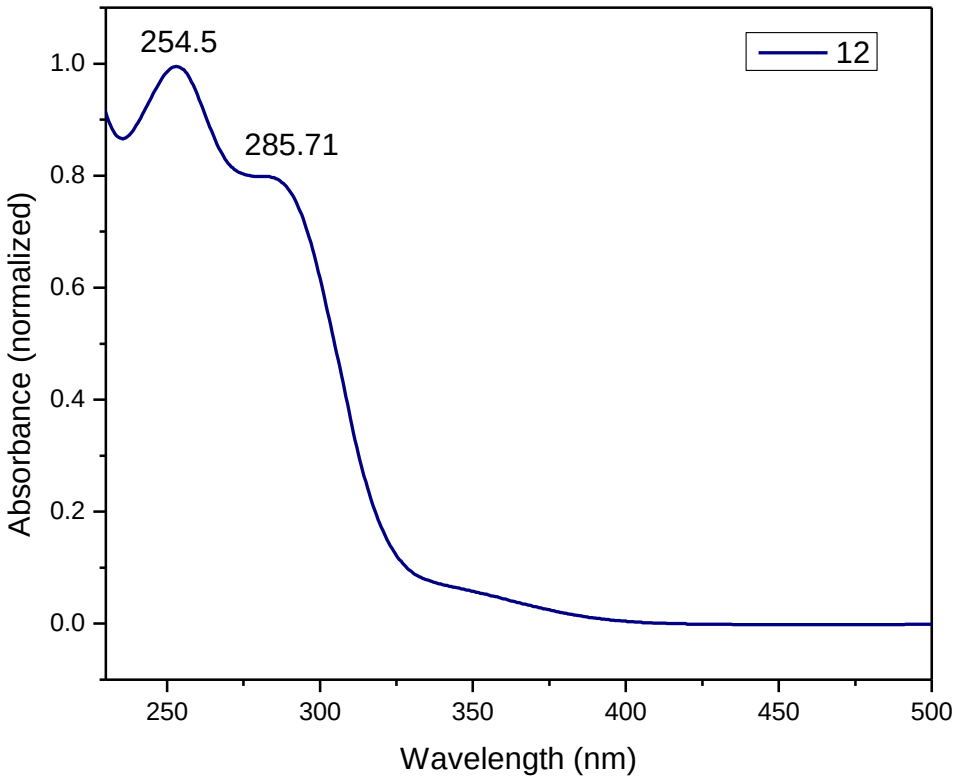


Figure S66: UV-VIS spectrum of **12**

Synthesis of 13 and **14:** 5-I^{t}Bu (0.300 g, 1.66 mmol) was dissolved in 10 mL toluene in a Schlenk flask and kept at -36 ˚C for 10 min. After that, COO^{t}BuCHN$_2$ (0.241 g, 1.7 mmol) solution in toluene was added to the solution of 5-I^{t}Bu resulting in an orange-colored solution with the immediate formation of a yellow-colored precipitate. The reaction was run for 6 hours while slowly warming to room temperature. The solution was filtered using a cannula and all the volatiles were removed to yield a yellow-colored sticky liquid product, **14** with a yield of 35%. Suitable crystals were obtained upon supersaturation by dissolving the product in DCM and hexane mixture after leaving the vial exposed to air for a month to afford yellow-colored crystals of **14**.

The precipitate part was completely dried, and 8 mL toluene was added to it and stirred for 15 minutes. Decanted the toluene part and dried the precipitate to get pure product **13** with a yield of 32%. Dissolved **13** in 20 mL THF and filtered using a cannula, concentrated to 3 mL, and kept at -36 ˚C for crystallization to afford block-shaped yellow crystals after a day.

^{1}H NMR (500 MHz, 298 K, THF-d_8) of 13: δ = 1.51, 1.54 (singlet, 18 H, COO^{t}***Bu***), 1.62 (singlet, 18 H, C(C***H***$_3$)$_3$), 1.63 (singlet, 1 H, NNC***H***(COO^{t}Bu)NN), 7.91 (singlet, 2 H, NC***H***C***H***N), 10.09 (singlet, 1 H, imidazolium ***H***) ppm.

^{13}C{^{1}H} NMR DEPT (101 MHz, 298 K, THF-d_8): 27.60, 28.08 (COO(***C***H$_3$)$_3$), 29.02 (C(***C***H$_3$)$_3$), 90.44 (imidazolium ***C***), 120.12 (N***C***H***C***HN),135.04 (NN***C***H(COO^{t}Bu)NN) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ= 28.27, 28.63 (COO(***C***H$_3$)$_3$), 29.98 (C(***C***H$_3$)$_3$), 60.38 (***C***(CH$_3$)$_3$, 79.05, 80.61 (***C***OO(CH$_3$)$_3$), 89.84 (NN***C***(COO^{t}Bu)NN), 119.91 (N***C***H***C***HN),151.69 (NN***C***H(COO^{t}Bu)NN), 165.30, 171.66 (***C***OO(CH$_3$)$_3$) ppm.

HRMS: m/z calcd for **13**: $C_{22}H_{40}N_6O_4$, 452.31; found **180.31** for imidazolium part.

IR (cm^{-1}): 2975.28,1735.24, 1682.48, 1364.95, 1204.13, 1129.90, 1032.99, 928.21, 919.59, 715.2.

Melting point range: 96-100 ˚C.

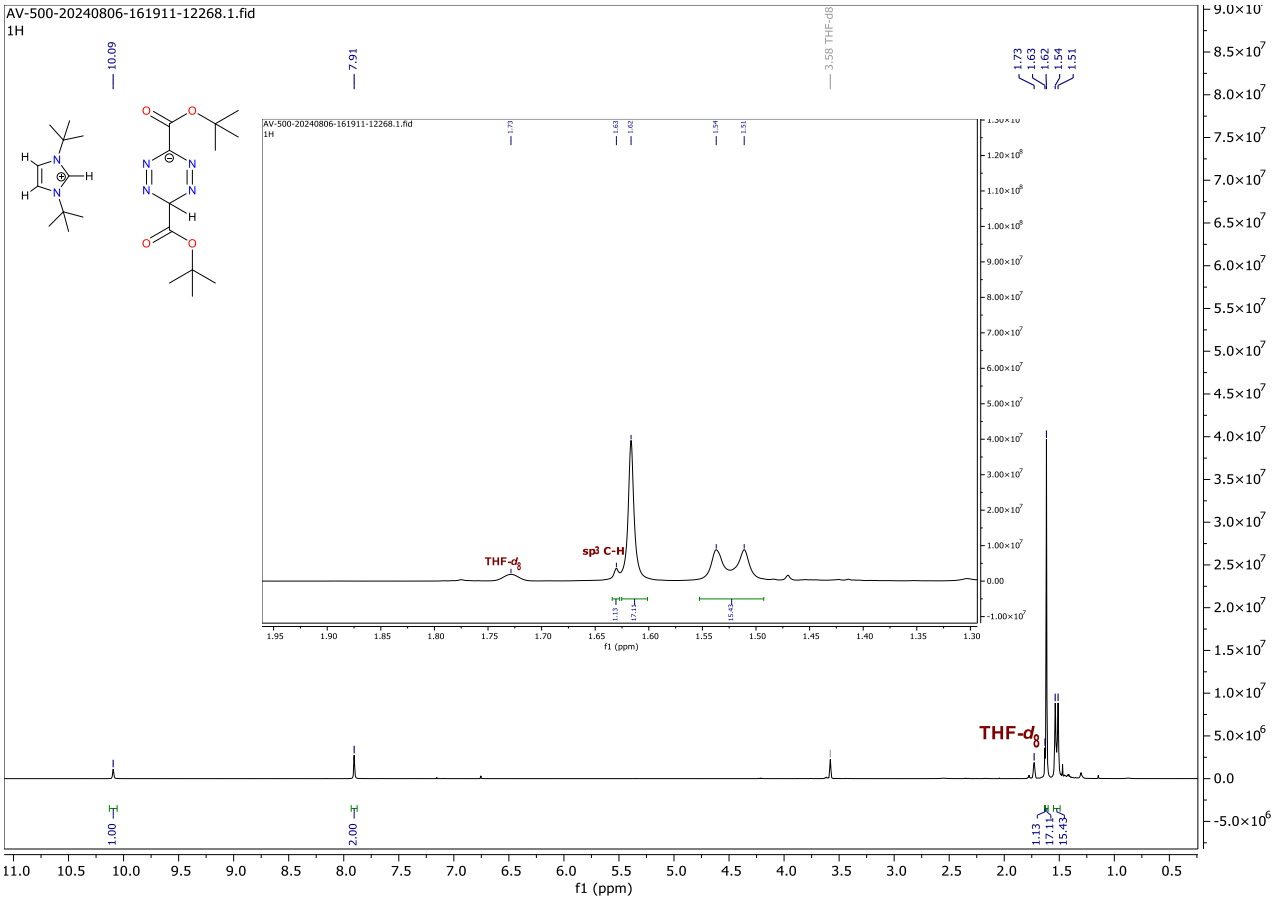


Figure S67: ^{1}H NMR spectrum of **13** in **THF-d_8**

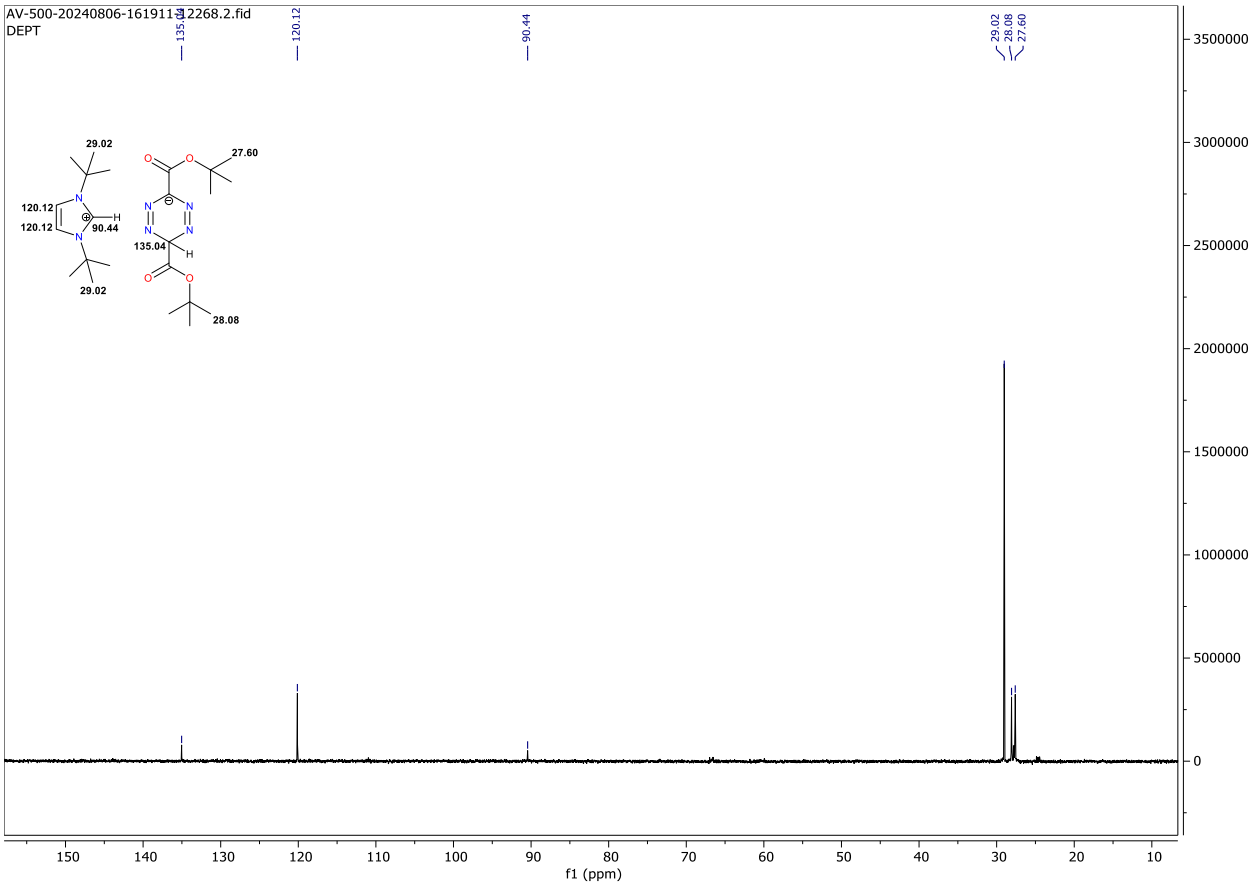


Figure S68: $^{13}C\{^{1}H\}$ DEPT NMR spectrum of **13** in **THF-*d*$_8$**

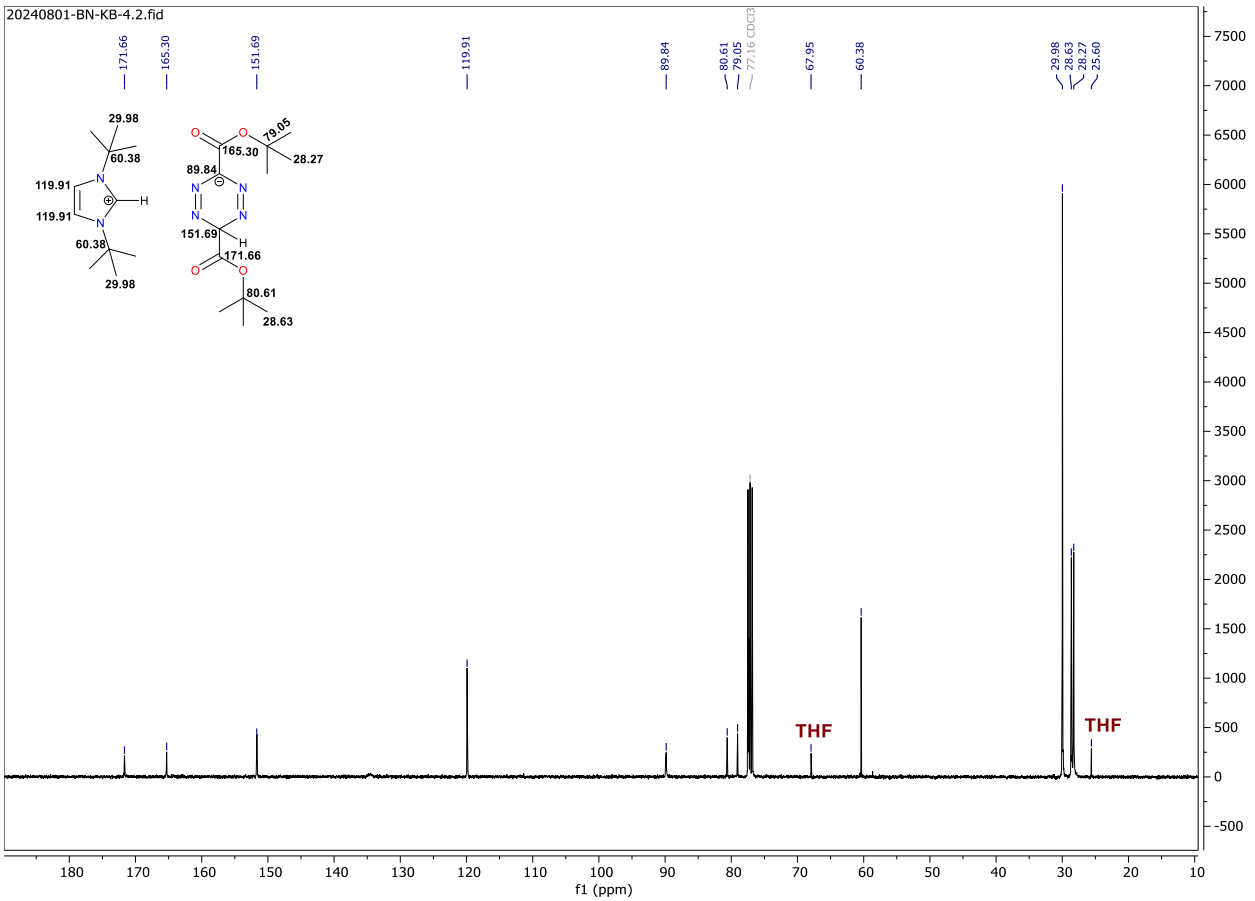


Figure S69: $^{13}C\{^{1}H\}$ NMR spectrum of **13** in **$CDCl_3$**

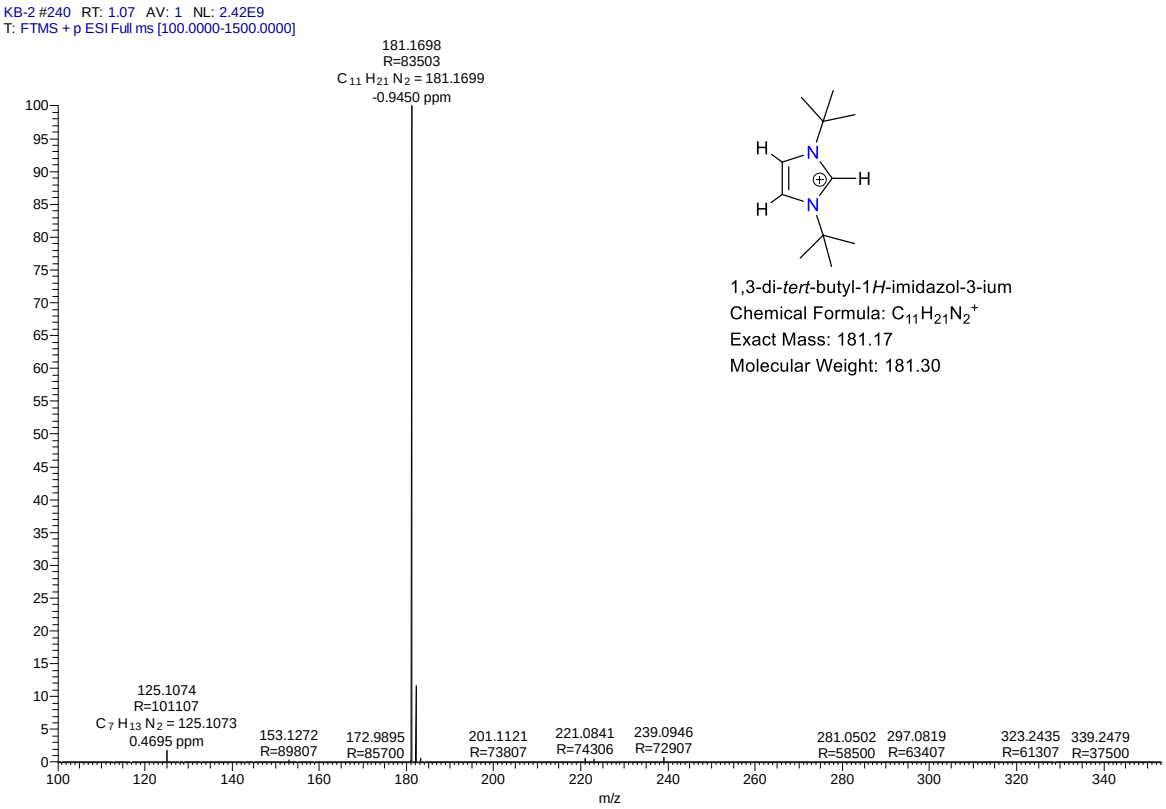


Figure S70: HRMS spectrum of **13**

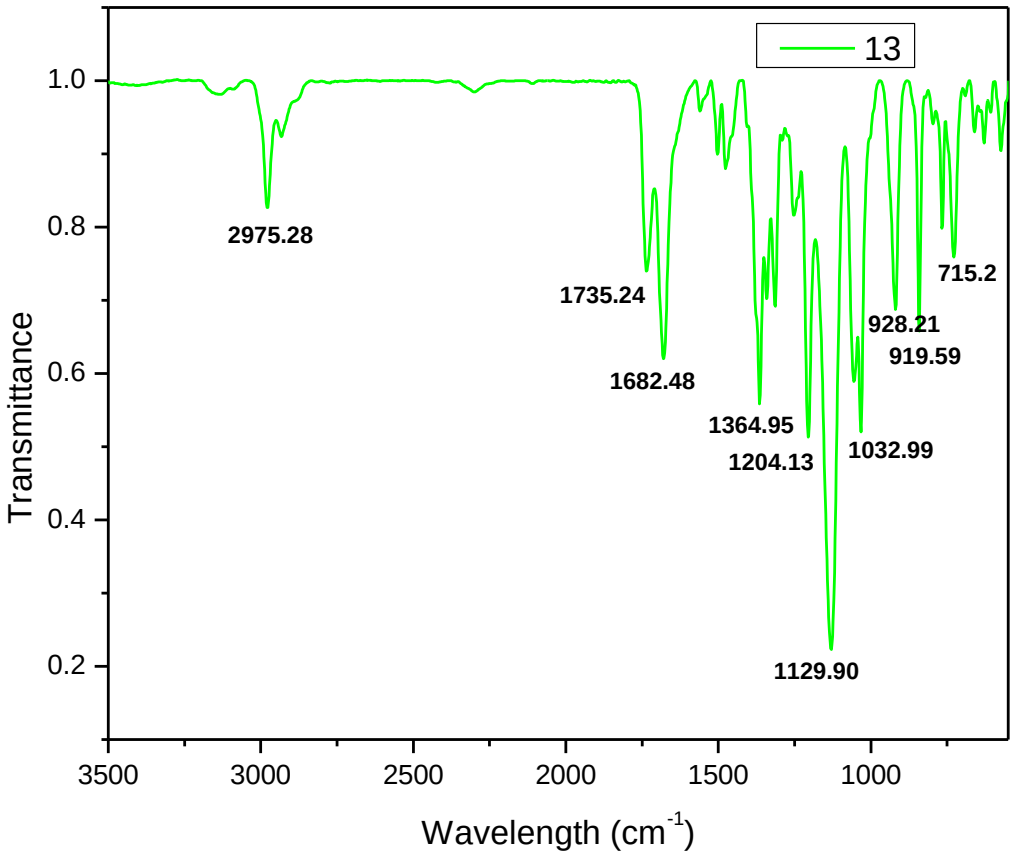


Figure S71: IR (ATR) spectrum of **13**

^{1}H NMR (500 MHz, 298 K, C_6D_6) of 14: δ=1.48 (singlet, 18 H, C(C***H***$_3$)$_3$), 1.54 (singlet, 18 H, COO^t***Bu***), 6.14 (singlet, 2 H, NC***H***C***H***N), 7.88 (C***H***COO^{t}Bu) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, C_6D_6) of 14: δ= 28.74 (COO(***C***H$_3$)$_3$), 29.82 (C(***C***H$_3$)$_3$), 58.51 (***C***(CH$_3$)$_3$, 78.39 (***C***OO(CH$_3$)$_3$), 111.25 (N***C***H***C***HN), 131.56 (***C***HCOO^{t}Bu),153.91(N***C***N), 166.27(***C***OO^{t}Bu) ppm.

HRMS: m/z calcd for **[M+H}$^+$**: $C_{17}H_{31}N_4O_2$, 323.45; found 323.24.

IR (cm^{-1}): 2975.28, 1676.30, 1548.46, 1441.24, 1364.95, 1107.22, 983.88, 661.86.

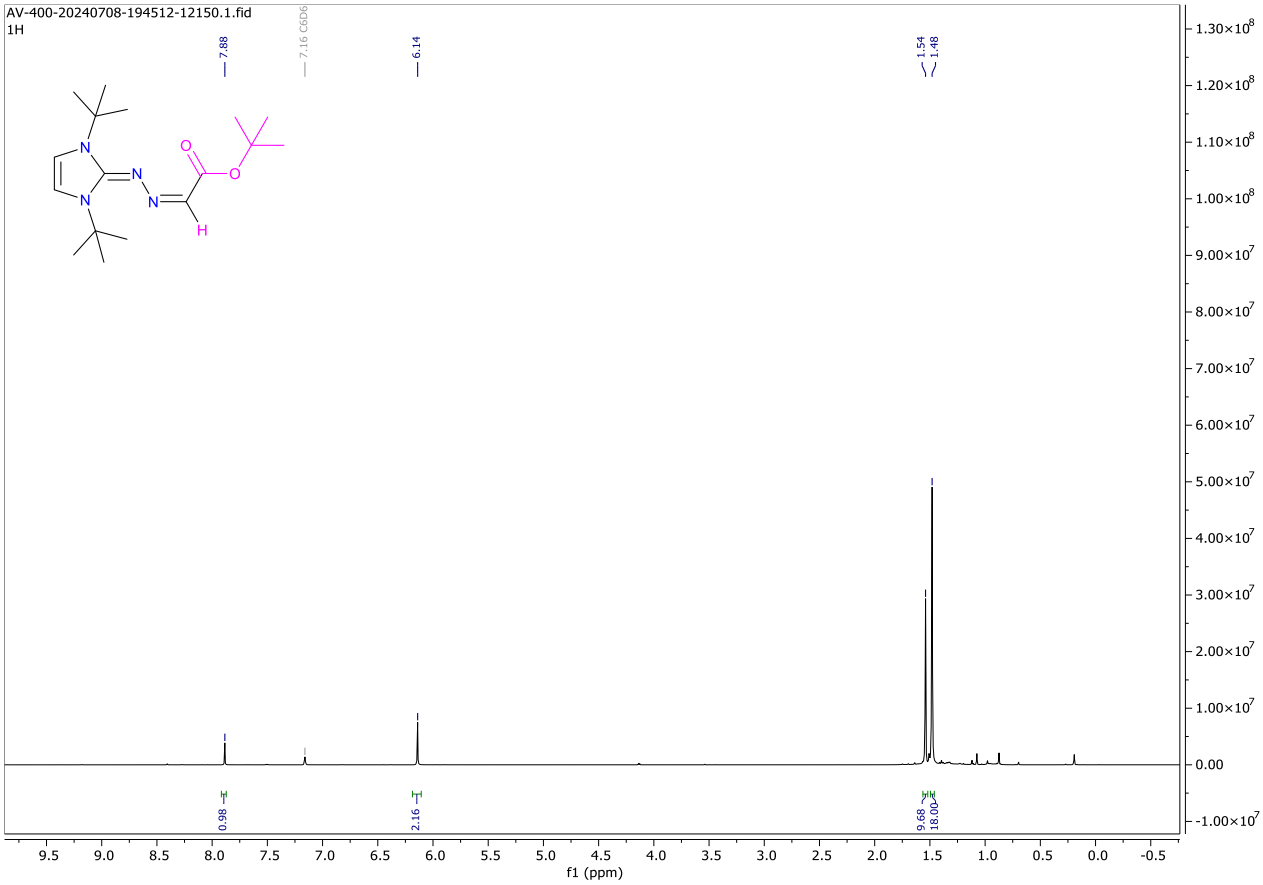


Figure S72: ^{1}H NMR spectrum of **14** (smaller peaks in the region 1.5-0 ppm belong to little impurities)

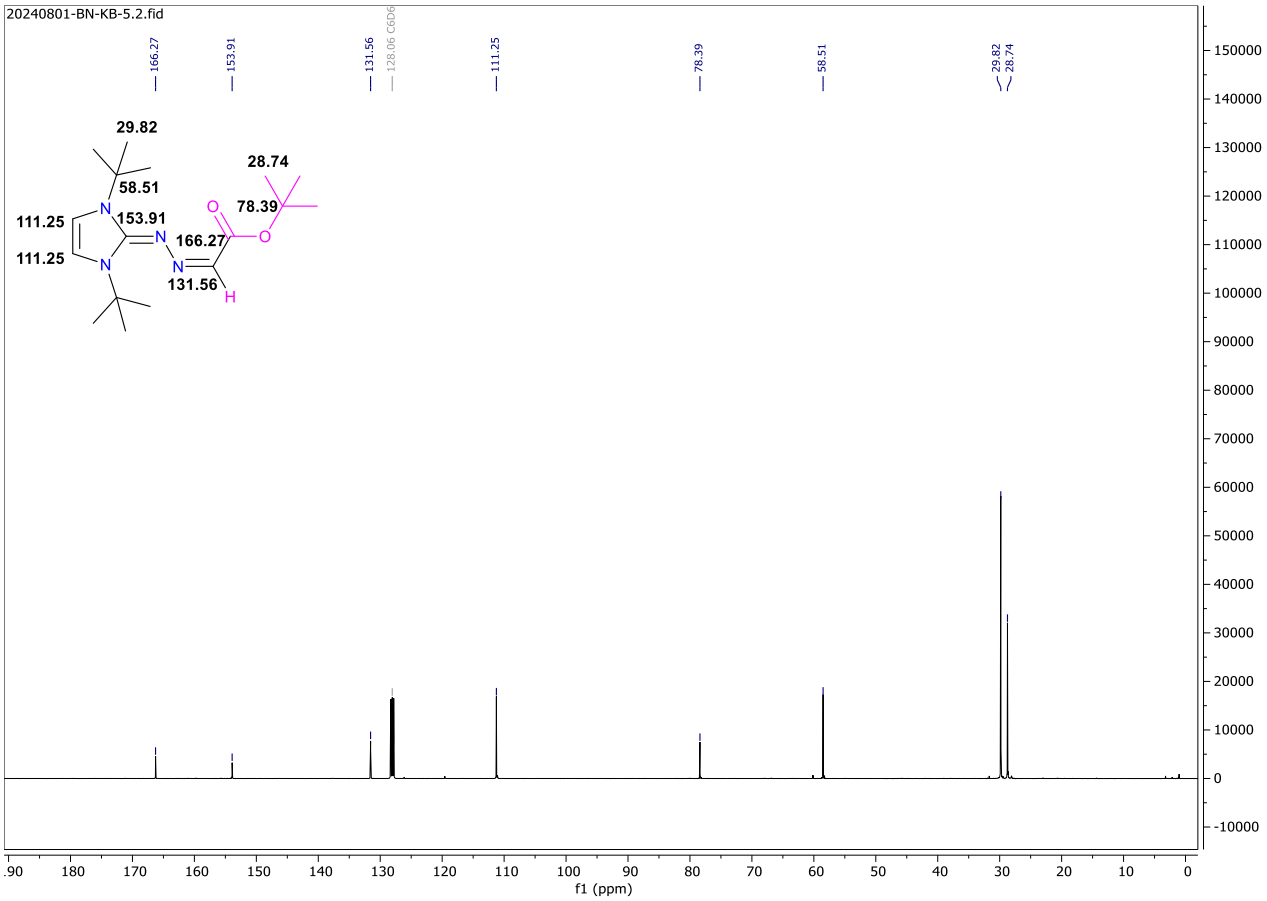


Figure S73: $^{13}C\{^{1}H\}$NMR spectrum of **14**

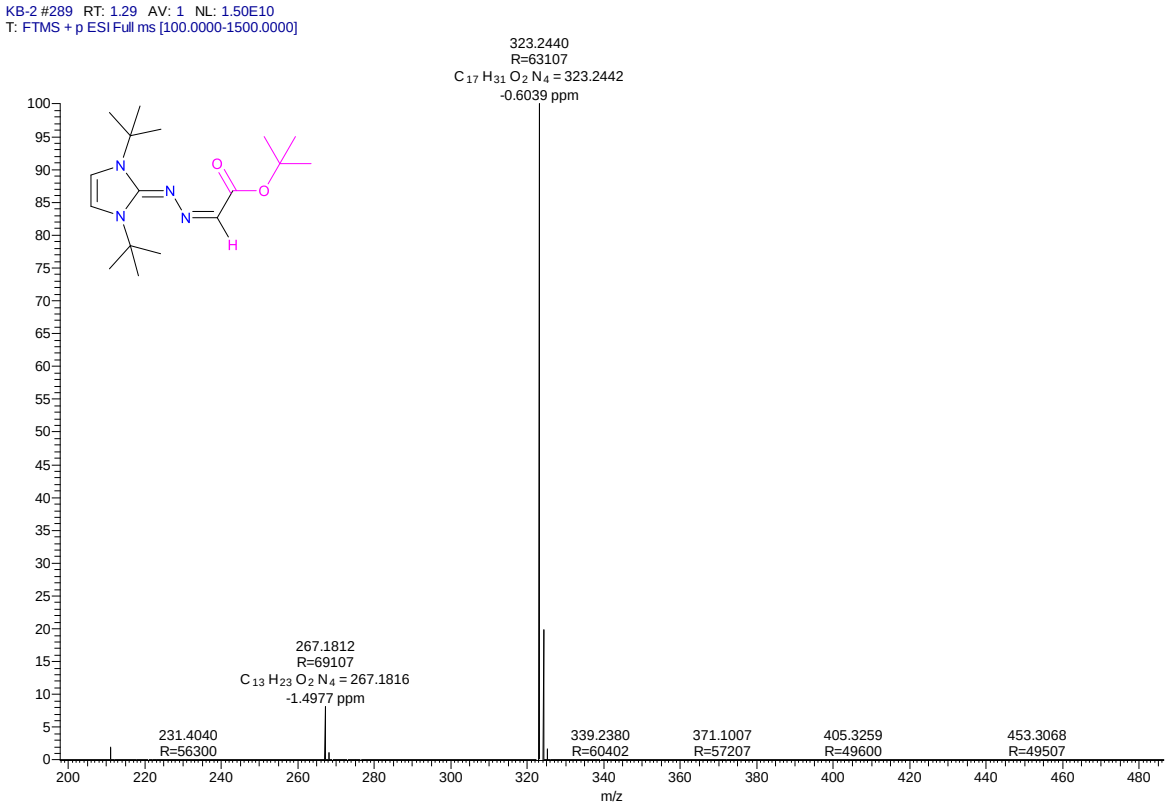


Figure S74: HRMS spectrum of **14**

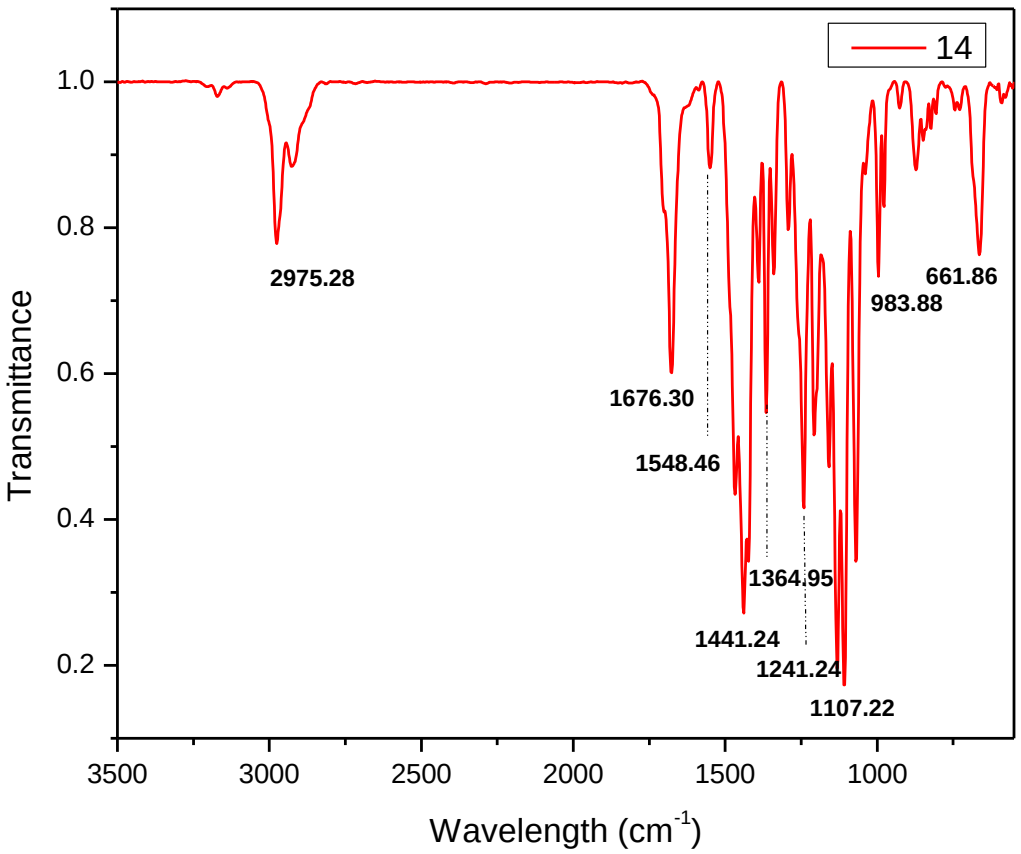


Figure S75: IR (ATR) spectrum of **14**

3. Miscellaneous Information

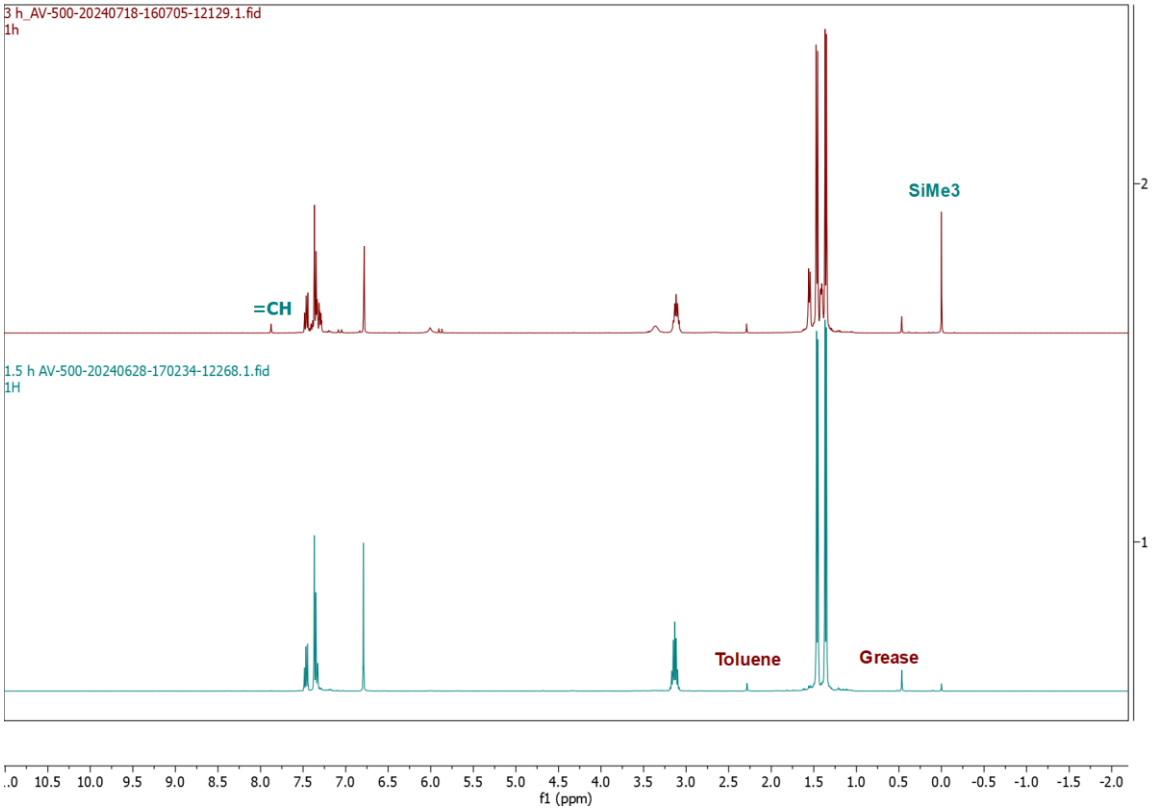


Figure MS1: Time dependents NMR recorded after reaction at low T for 1.5 h and after 3 h respectively.

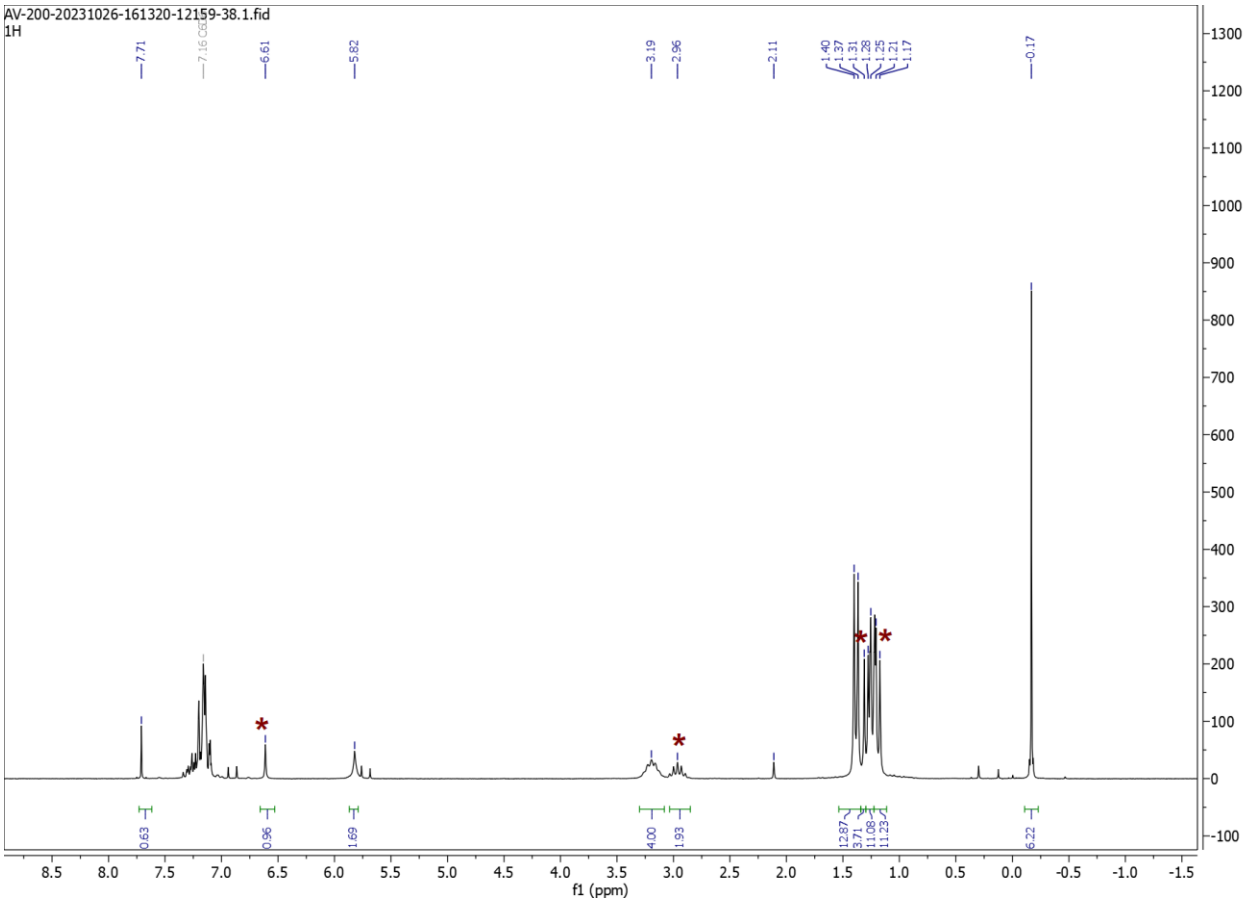


Figure MS2: ^{1}H NMR of the reaction mixture recorded after 10 h (Red asterisks belong to unreacted 5-IPr indicating around 53% conversion)

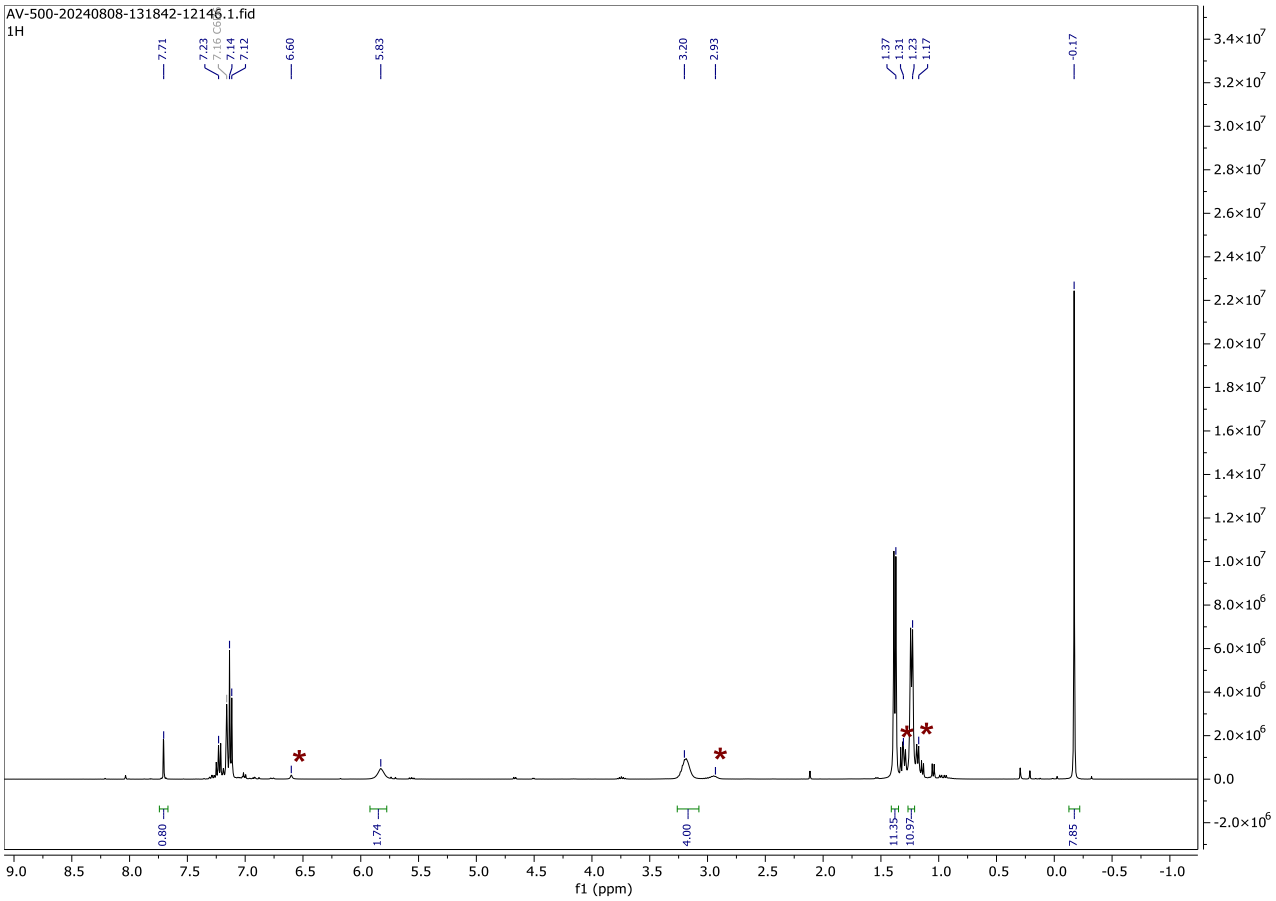
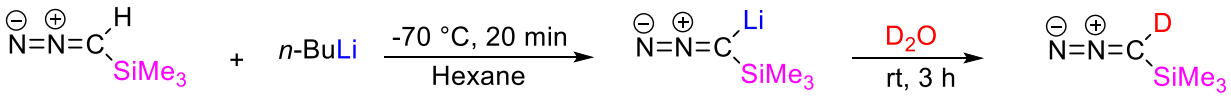


Figure MS3: ^{1}H NMR of the reaction mixture recorded after 15 h (red asterisks belong to unreacted 5-IPr indicating around 95% conversion)



Scheme MS1: Synthesis of $SiMe_3CDN_2$ using a modified procedure[2]

To confirm the source of triazole at the H, we have synthesized $SiMe_3CDN_2$ using a slightly modified procedure. When we performed the NMR tube reaction of 5-I*t*Bu (0.010g, 0.055 mmol) with 0.36 M $SiMe_3CDN_2$ (0.15 mL, 0.055 mmol) in C_6D_6, a color change from yellow to red was observed after 12 h, along with the formation of a red-colored precipitate. But, we consistently ended up with the hydrolyzed product **7a**, due to the presence of the adventitious amount of water ($SiMe_3CDN_2$ preparation requires D_2O which may always contain some amount of H_2O).

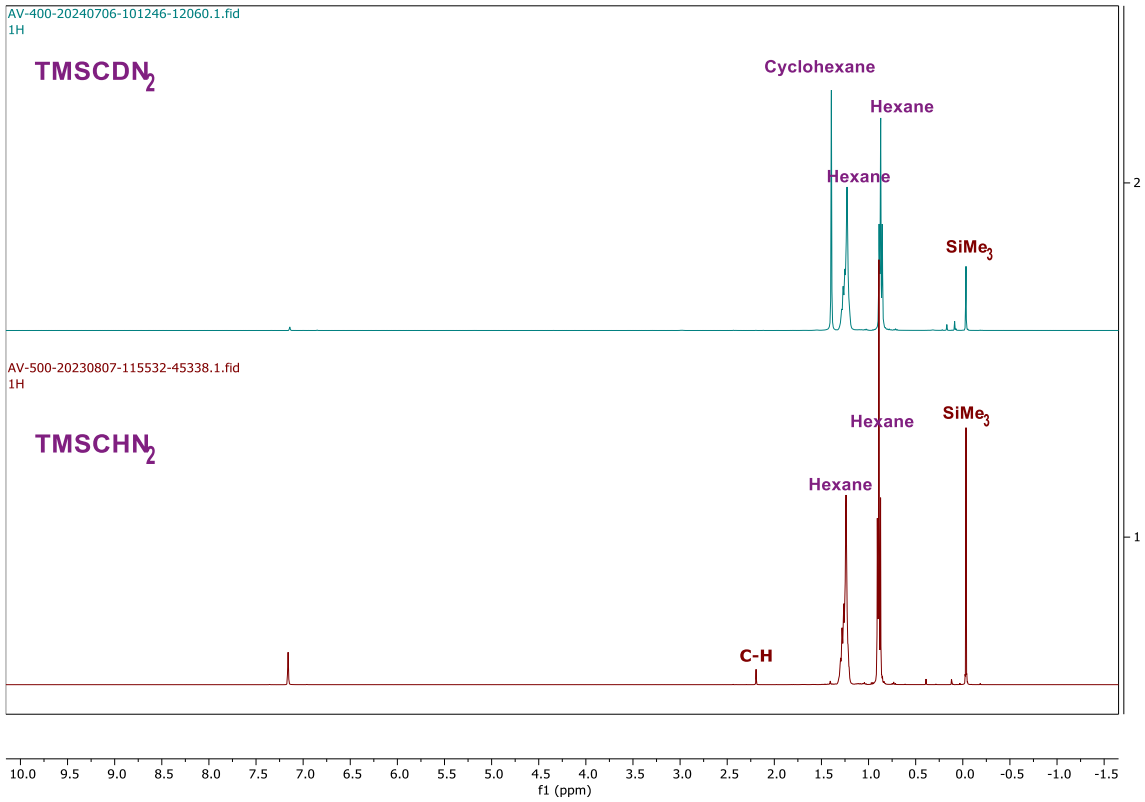


Figure MS4: ^{1}H NMR of $SiMe_3CDN_2$ (0.36 M in hexane), Peak corresponding to C-H at 2.19 ppm disappeared

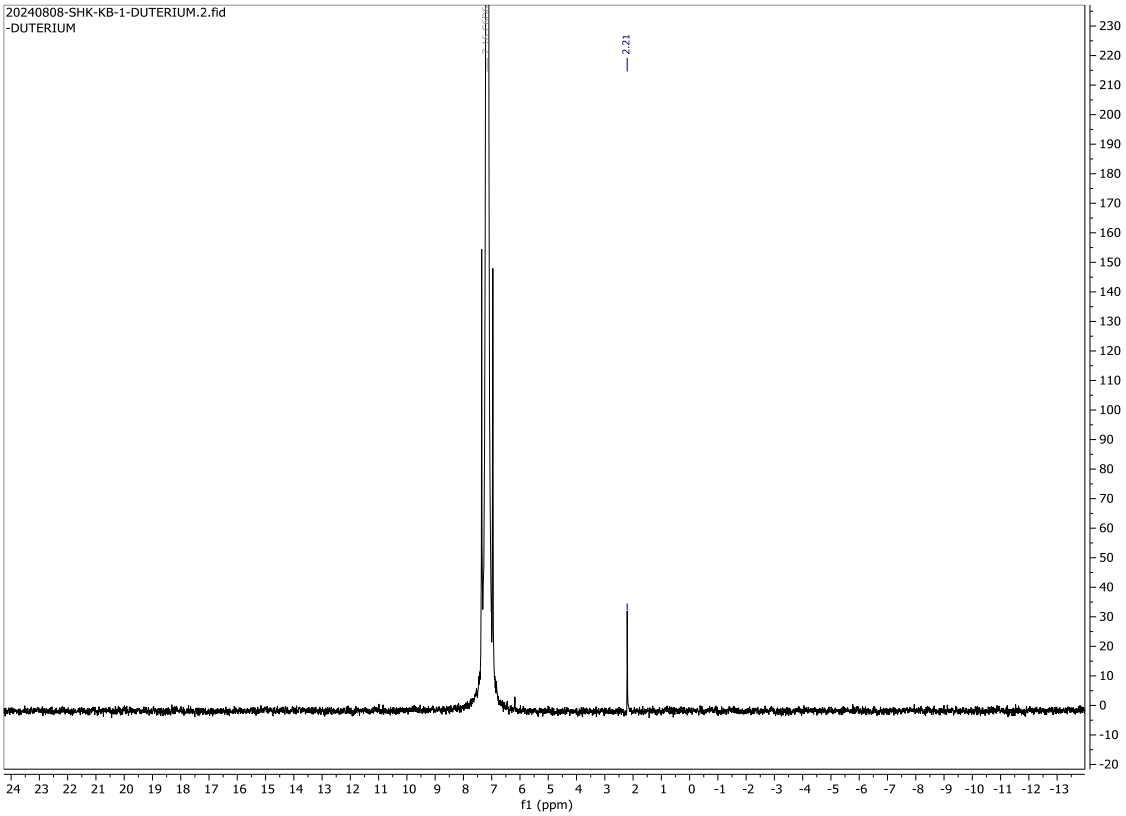


Figure MS5: ^{2}H NMR of $SiMe_3CDN_2$ (0.36 M in hexane), Peak corresponding to C-D appears at 2.21 ppm.

4. Crystallographic data for the structural analysis

X-ray intensity data measurements were carried out on a Bruker SMART APEX II single crystal X-ray CCD diffractometer with graphite-monochromatized (Mo-Kα = 0.71073 Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5 ° at different settings of ϕ and 2θ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by the APEX3 program (Bruker, 2006).[3] All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full-matrix least-squares refinement on F2.[4] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. All the hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms. An ORTEPIII[5] view was drawn with 50% probability displacement ellipsoids and H atoms omitted for clarity.

Identification code	**5_SIPr_TMSCHN2 (1)**	**mo_KB_6TMSCHN2_1_0m _a(3)**
CCDC Number	2347293	2347305
Empirical formula	$C_{31}H_{48}N_4Si$	$C_{32}H_{50}N_4Si$
Formula weight	504.82	518.85
Temperature/K	100(2)	100(2)
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a/Å	8.281(4)	12.2095(15)
b/Å	10.126(5)	16.906(2)
c/Å	19.388(8)	17.394(2)
α/°	86.625(9)	102.647(4)
β/°	85.739(10)	102.612(4)
γ/°	72.015(11)	109.020(4)
Volume/Å^3	1541.0(13)	3144.5(7)
Z	2	4
ρ_{calc}g/cm^3	1.088	1.096
μ/mm^{-1}	0.101	0.100

F(000)	552.0	1136.0
Crystal size/mm^3	0.36 × 0.24 × 0.22	0.35 × 0.22 × 0.12
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.216 to 51.998	4.226 to 55.998
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, 0 ≤ l ≤ 23	-16 ≤ h ≤ 15, -20 ≤ k ≤ 22, -22 ≤ l ≤ 22
Reflections collected	6079	64237
Independent reflections	6079 [R_{int} = 0.108, R_{sigma} = 0.0449]	15012 [R_{int} = 0.0569, R_{sigma} = 0.0480]
Data/restraints/parameters	6079/0/338	15012/12/716
Goodness-of-fit on F^2	1.121	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0713, wR_2 = 0.1624	R_1 = 0.0752, wR_2 = 0.2309
Final R indexes [all data]	R_1 = 0.0842, wR_2 = 0.1726	R_1 = 0.0872, wR_2 = 0.2393
Largest diff. peak/hole / e Å^{-3}	0.48/-0.40	0.83/-0.41

Identification code	**4_mo_IdippTMSCHN2_07_06_0ma_a (4)**	**mo_IDippCHN2TMS_0ma_a (5)**
CCDC Number	2363380	2347306
Empirical formula	$C_{31}H_{46}N_4Si$	$C_{28}H_{38}N_4$
Formula weight	502.81	430.62
Temperature/K	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	10.2595(8)	19.9625(12)
b/Å	19.2221(14)	6.8258(4)
c/Å	16.2971(13)	19.8501(12)
α/°	90	90
β/°	107.065(3)	105.828(2)
γ/°	90	90
Volume/Å^3	3072.4(4)	2602.2(3)
Z	4	4
ρ_{calc}g/cm^3	1.087	1.099

μ/mm^{-1}	0.101	0.065
F(000)	1096.0	936.0
Crystal size/mm^3	0.35 × 0.19 × 0.05	0.2 × 0.13 × 0.05
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.712 to 55.998	5.13 to 60.052
Index ranges	-13 ≤ h ≤ 13, -25 ≤ k ≤ 25, -21 ≤ l ≤ 21	-28 ≤ h ≤ 23, -9 ≤ k ≤ 9, -25 ≤ l ≤ 27
Reflections collected	162231	31733
Independent reflections	7424 [R_{int} = 0.1501, R_{sigma} = 0.0466]	7569 [R_{int} = 0.1105, R_{sigma} = 0.1155]
Data/restraints/parameters	7424/0/356	7569/0/297
Goodness-of-fit on F^2	1.039	1.011
Final R indexes [I>=2σ (I)]	R_1 = 0.0517, wR_2 = 0.1161	R_1 = 0.0748, wR_2 = 0.1565
Final R indexes [all data]	R_1 = 0.0839, wR_2 = 0.1385	R_1 = 0.1640, wR_2 = 0.2014
Largest diff. peak/hole / e Å^{-3}	0.37/-0.38	0.58/-0.28

Identification code	**mo_kb_hcl1_ 0ma_a (5a)**	**mo_ItBu_TMSCHN2_ 0m_a (6)**
CCDC Number	2347322	2347308
Empirical formula	$C_{28}H_{39.5}ClN_4O_{0.25}$	$C_{13}H_{21}N_5$
Formula weight	471.58	247.35
Temperature/K	298(2)	100(2)
Crystal system	triclinic	orthorhombic
Space group	*P*-1	*P*bca
a/Å	9.461(3)	12.1510(4)
b/Å	11.622(4)	11.9324(5)
c/Å	12.759(4)	18.7244(8)
α/°	82.729(9)	90
β/°	82.161(9)	90
γ/°	89.987(9)	90
Volume/Å^3	1378.4(7)	2714.86(19)
Z	2	8

ρ_{calc}g/cm^3	1.136	1.210
μ/mm^{-1}	0.161	0.077
F(000)	509.0	1072.0
Crystal size/mm^3	0.15 × 0.11 × 0.05	0.23 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.346 to 50	5.256 to 60.136
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 13, -14 ≤ l ≤ 15	-17 ≤ h ≤ 17, -16 ≤ k ≤ 16, -26 ≤ l ≤ 26
Reflections collected	32894	52191
Independent reflections	4849 [R_{int} = 0.2524, R_{sigma} = 0.1770]	3968 [R_{int} = 0.0693, R_{sigma} = 0.0400]
Data/restraints/parameters	4849/0/314	3968/0/169
Goodness-of-fit on F^2	0.843	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0563, wR_2 = 0.1145	R_1 = 0.0474, wR_2 = 0.1268
Final R indexes [all data]	R_1 = 0.1284, wR_2 = 0.1320	R_1 = 0.0626, wR_2 = 0.1350
Largest diff. peak/hole / e Å^{-3}	0.25/-0.28	0.36/-0.30

Identification code	**mo_KB_ItBuNNCHTMS_0m_a (7)**	**7a_mo_KB_ItBuNNCH2_0ma_a (7a)**
CCDC Number	2347310	2386081
Empirical formula	$C_{15}H_{30}N_4Si$	$C_{12}H_{22}N_4$
Formula weight	294.52	222.33
Temperature/K	100(2)	100(2)
Crystal system	triclinic	monoclinic
Space group	*P*-1	P2$_1$/c
a/Å	10.1752(12)	11.0142(5)
b/Å	18.596(3)	10.0702(4)
c/Å	19.949(3)	12.5419(6)
α/°	105.886(4)	90
β/°	94.060(5)	110.769(2)
γ/°	91.388(4)	90
Volume/Å^3	3617.7(8)	1300.69(10)

Z	8	4
ρ_{calc}g/cm^3	1.081	1.135
μ/mm^{-1}	0.128	0.071
F(000)	1296.0	488.0
Crystal size/mm^3	0.32 × 0.24 × 0.19	0.34 × 0.27 × 0.11
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.468 to 50.998	5.332 to 60.21
Index ranges	-12 ≤ h ≤ 12, -22 ≤ k ≤ 22, -24 ≤ l ≤ 24	-15 ≤ h ≤ 15, -14 ≤ k ≤ 14, -17 ≤ l ≤ 17
Reflections collected	106350	87928
Independent reflections	13424 [R_{int} = 0.0725, R_{sigma} = 0.0417]	3806 [R_{int} = 0.0577, R_{sigma} = 0.0185]
Data/restraints/parameters	13424/0/757	3806/0/153
Goodness-of-fit on F^2	1.222	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.1004, wR_2 = 0.2341	R_1 = 0.0378, wR_2 = 0.1066
Final R indexes [all data]	R_1 = 0.1098, wR_2 = 0.2382	R_1 = 0.0412, wR_2 = 0.1104
Largest diff. peak/hole / e Å^{-3}	0.74/-0.50	0.36/-0.19

Identification code	**mo_KB_090320 24_0m_a (8)**	**mo_KB_6diazoester _0ma_a (9)**
CCDC Number	2347311	2347313
Empirical formula	$C_{34}H_{50}N_4O_2Si$	$C_{34}H_{50}N_4O_2$
Formula weight	574.87	546.78
Temperature/K	296(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a/Å	9.8892(6)	10.5986(12)
b/Å	15.8752(11)	14.3442(17)
c/Å	21.8134(13)	21.841(3)
α/°	90	90

β/°	95.043(2)	100.144(3)
γ/°	90	90
Volume/Å^3	3411.3(4)	3268.5(7)
Z	4	4
ρ_{calc}g/cm^3	1.119	1.111
μ/mm^{-1}	0.103	0.069
F(000)	1248.0	1192.0
Crystal size/mm^3	0.2 × 0.17 × 0.08	0.21 × 0.17 × 0.08
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.388 to 56.692	4.63 to 56.8
Index ranges	-11 ≤ h ≤ 13, -21 ≤ k ≤ 21, -29 ≤ l ≤ 27	-14 ≤ h ≤ 14, -19 ≤ k ≤ 19, -29 ≤ l ≤ 29
Reflections collected	100908	86204
Independent reflections	8490 [R_{int} = 0.1250, R_{sigma} = 0.0729]	8174 [R_{int} = 0.0935, R_{sigma} = 0.0479]
Data/restraints/parameters	8490/0/383	8174/0/372
Goodness-of-fit on F^2	1.025	1.112
Final R indexes [I>=2σ (I)]	R_1 = 0.0633, wR_2 = 0.1185	R_1 = 0.0720, wR_2 = 0.1571
Final R indexes [all data]	R_1 = 0.1194, wR_2 = 0.1397	R_1 = 0.0994, wR_2 = 0.1707
Largest diff. peak/hole / e Å^{-3}	0.44/-0.38	0.51/-0.40

Identification code	**mo_Kb_5Sipr_ diazoester_0m_a (10)**	**mo_KB_5Idipp _ester_0m_a (11)**
CCDC Number	2347315	2347321
Empirical formula	$C_{33}H_{48}N_4O_2$	$C_{40}H_{54}N_4O_2$
Formula weight	532.75	622.87
Temperature/K	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	11.1953(7)	12.6958(10)
b/Å	13.1685(9)	17.2563(11)
c/Å	21.7390(15)	18.3270(13)

α/°	90	90
β/°	99.457(2)	107.659(2)
γ/°	90	90
Volume/Å^3	3161.3(4)	3825.9(5)
Z	4	4
ρ_{calc}g/cm^3	1.119	1.081
μ/mm^{-1}	0.070	0.067
F(000)	1160.0	1352.0
Crystal size/mm^3	0.13 × 0.1 × 0.09	0.25 × 0.22 × 0.16
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.948 to 56.65	4.194 to 56.676
Index ranges	-14 ≤ h ≤ 13, -17 ≤ k ≤ 17, -28 ≤ l ≤ 29	-16 ≤ h ≤ 16, -23 ≤ k ≤ 22, -24 ≤ l ≤ 24
Reflections collected	58847	95864
Independent reflections	7854 [R_{int} = 0.0897, R_{sigma} = 0.0555]	9522 [R_{int} = 0.1131, R_{sigma} = 0.0613]
Data/restraints/parameters	7854/0/363	9522/180/577
Goodness-of-fit on F^2	1.063	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0578, wR_2 = 0.1171	R_1 = 0.0705, wR_2 = 0.1334
Final R indexes [all data]	R_1 = 0.0882, wR_2 = 0.1298	R_1 = 0.1226, wR_2 = 0.1556
Largest diff. peak/hole / e Å^{-3}	0.24/-0.24	0.21/-0.26

Identification code	**14_mo_KB_19012024_0m_a (13)**	**mo_Kb_ltBuester_0m_a (14)**
CCDC Number	2375811	2363384
Empirical formula	$C_{23}H_{40}N_6O_4$	$C_{17}H_{30}N_4O_2$
Formula weight	464.61	322.45
Temperature/K	224(2)	100(2)
Crystal system	monoclinic	orthorhombic
Space group	$P2_1/c$	Pbca
a/Å	13.505(3)	11.4307(12)

b/Å	12.601(2)	11.4548(13)
c/Å	17.615(3)	28.925(3)
α/°	90	90
β/°	110.277(6)	90
γ/°	90	90
Volume/$Å^3$	2811.9(9)	3787.3(7)
Z	4	8
$\rho_{calc}g/cm^3$	1.097	1.131
μ/mm^{-1}	0.076	0.076
F(000)	1008.0	1408.0
Crystal size/mm^3	0.19 × 0.16 × 0.1	0.29 × 0.25 × 0.11
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.93 to 50.99	5.228 to 55.998
Index ranges	-16 ≤ h ≤ 16, -15 ≤ k ≤ 15, -21 ≤ l ≤ 21	-15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -38 ≤ l ≤ 38
Reflections collected	81214	109842
Independent reflections	5224 [R_{int} =0.0961, R_{sigma} = 0.0338]	4567 [R_{int} = 0.1792, R_{sigma} = 0.0553]
Data/restraints/ parameters	5224/135/412	4567/0/218
Goodness-of-fit on F^2	1.031	1.103
Final R indexes [I>=2σ (I)]	R_1 = 0.0683, wR_2 = 0.1766	R_1 = 0.0608, wR_2 = 0.1184
Final R indexes [all data]	R_1 = 0.0895, wR_2 = 0.1929	R_1 = 0.1040, wR_2 = 0.1396
Largest diff. peak/hole / e $Å^{-3}$	0.35/-0.29	0.24/-0.24

Table S1 and S2: Compound **6** Tau value

5-Membered Ring (1)	**N1**	**C1**	**N2**	**C2**	**C3**
	sp^2	sp^2	sp^2	sp^2	sp^2
Dev (A) from CPplane	0.0053(11)	-0.0038(12)	0.0009(11)	0.0024(13)	-0.0048(13)
Cs(I)-Asym-Par (Deg)	0.18(13)	0.87(13)	1.22(13)	1.11(13)	0.58(13)
C2(I)-Asym-Par (Deg)	1.58(13)	1.15(12)	0.27(13)	0.71(13)	1.42(13)
Ring Bond Angle (Deg)	108.55(9)	107.94(9)	108.22(9)	108.07(10)	107.22(10)

No C & P - Puckering analysis since <Tau> = 0.6 < 5.0 Deg.

5-Membered Ring (2)	**N3**	**C12**	**N5**	**N4**	**C13**
	sp^2	sp^2	sp^2	sp^2	sp^2
Dev (A) from CPplane	-0.0048(11)	0.0032(12)	-0.0004(12)	-0.0025(13)	0.0045(13)
Cs(I)-Asym-Par (Deg)	0.28(15)	0.85(14)	1.18(15)	1.03(15)	0.44(14)
C2(I)-Asym-Par (Deg)	1.47(15)	0.99(14)	0.14(14)	0.78(15)	1.39(15)
Ring Bond Angle (Deg)	99.53(9)	115.30(10)	104.38(10)	105.43(10)	115.35(11)

No C & P - Puckering analysis since <Tau> = 0.6 < 5.0 Deg.

5. DFT calculations

Quantum chemical calculations were performed using density functional theory (DFT) with the Turbomole 7.5 suite of programs.[6] The geometries of all species, including reactants, products, and transition states, were optimized using the PBE functional[7] and the def-TZVP basis set.[8] To account for long-range interactions, Grimme's dispersion correction (D3) was applied.[9] The efficiency and accuracy of the electronic Coulomb term in the DFT calculations were enhanced by employing the resolution of identity (RI) approximation[10] and the multipole accelerated resolution of identity (marij) approximations.[11] Solvent effects were included by performing optimizations using the COSMO model [12], with toluene (ε = 2.374) specified as the solvent. To confirm whether the stationary points corresponded to local minima or transition states, harmonic frequency calculations were conducted at 298.15 K. The reported ΔG values include corrections for zero-point energy, as well as internal energy and entropy contributions derived from frequency calculations on the optimized minima. The absence of imaginary frequencies confirmed that the structures were either reactants or products, while the presence of a single imaginary frequency indicated a transition state. Additionally, intrinsic reaction coordinate (IRC)[13] calculations were performed for all transition states to ensure their validity and to confirm the correct identification of reactant and product structures. Translational entropy values were corrected using the free volume correction introduced by Mammen et al.,[14] which is based on the Sackur-Tetrode equation. This correction provides a physically intuitive adjustment for the translational entropy of molecules in solution.

Finally, to refine the calculations further, single-point energy calculations were performed using the hybrid PBE0 functional[15] with a higher basis set, def2-TZVP, on the geometries optimized at the PBE-D3/defTZVP + COSMO (ε = 2.38) level of theory. Solvent effects were again considered, using toluene (ε = 2.38) *via* the COSMO solvation model. Consequently, all kinetic and thermodynamic results are reported based on the PBE0-D3/def2TZVP + COSMO (ε = 2.38)//PBE-D3/defTZVP + COSMO (ε = 2.38) level of theory.

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7. Optimized Cartesian Coordinates of all Stationary Points at the PBE0-D3/def2TZVP//PBE-D3/defTZVP level of theory

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Diazoalkane Energy = -557.1052335856

Si	-0.9562619	0.0452544	-0.0001350
N	1.8036442	-0.3951725	0.0013664
N	2.8001611	0.1764171	-0.0004892
C	-1.0160930	1.1395163	-1.5471400
C	-2.3576801	-1.2265102	0.0005475
C	-1.0196988	1.1447183	1.5430647
C	0.6413771	-0.9702731	0.0031572
H	-0.1550810	1.8245253	-1.5777314
H	-1.0008254	0.5310475	-2.4628240
H	-1.9322137	1.7501677	-1.5516631
H	-3.3327703	-0.7168178	-0.0014558
H	-2.3072219	-1.8694291	-0.8904136
H	-2.3092483	-1.8662819	0.8938874
H	-0.1590234	1.8301701	1.5730688
H	-1.9360859	1.7549947	1.5436178
H	-1.0060686	0.5394040	2.4608637
H	0.6666910	-2.0618311	0.0069785

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Diazoester Energy = -494.2147131556

O	0.3427618	18.7835957	2.1807286
O	-0.9435509	16.9751853	2.8157473
N	0.3576803	15.6411871	5.5393300
N	0.6322854	16.5253113	4.8735300
C	0.9204516	17.5323491	4.0909883
H	1.7976191	18.1231697	4.3397796
C	0.0922955	17.8456547	2.9277203
C	-1.9288066	17.0831005	1.7023827
C	-2.6666844	18.4198453	1.7864555
H	-3.4803203	18.4291320	1.0461787
H	-1.9951877	19.2609732	1.5796592
H	-3.1110788	18.5501000	2.7836103
C	-2.8741541	15.9191033	1.9943520
H	-3.6700171	15.8885618	1.2369185
H	-3.3376592	16.0357871	2.9838875
H	-2.3319423	14.9635410	1.9707487
C	-1.2205854	16.8888145	0.3611499
H	-1.9740215	16.8200341	-0.4373013
H	-0.6422387	15.9537605	0.3660825
H	-0.5482916	17.7254069	0.1386022

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5-SIPr Energy = -1160.295798220

N	-0.5051902	-0.0564544	-1.0697104

N	-0.6018991	0.0387178	1.0785204
C	0.2615226	0.0054117	0.0404140
C	-1.9758046	0.0448488	-0.8200222
H	-2.5210820	-0.7379249	-1.3654635
H	-2.3442487	1.0264206	-1.1627320
C	-2.0399714	-0.1142540	0.7006601
H	-2.6586615	0.6476490	1.1947009
H	-2.4018236	-1.1088136	1.0112080
C	-0.0061858	-0.0050254	-2.4101074
C	0.1348948	-1.2169164	-3.1239077
C	0.5962053	-1.1552576	-4.4453609
H	0.7205788	-2.0753566	-5.0185831
C	0.9047503	0.0702219	-5.0401679
H	1.2630405	0.0995885	-6.0714689
C	0.7613200	1.2541879	-4.3191683
H	1.0132455	2.2063709	-4.7920331
C	0.3002856	1.2419035	-2.9932880
C	-0.1304909	-2.5497869	-2.4386765
H	-0.8795296	-2.3704652	-1.6511421
C	1.1508964	-3.0359135	-1.7348305
H	1.9455374	-3.2281284	-2.4721786
H	0.9600250	-3.9703045	-1.1838855
H	1.5137469	-2.2807982	-1.0229420
C	-0.6927595	-3.6262994	-3.3748571
H	0.0468375	-3.9444125	-4.1252199
H	-1.5877121	-3.2729776	-3.9083652
H	-0.9699469	-4.5191166	-2.7945570
C	0.1751824	2.5448433	-2.2177861
H	-0.2529601	2.3080973	-1.2324730
C	1.5614899	3.1623439	-1.9666466
H	2.0571683	3.4223768	-2.9148790
H	2.2071589	2.4584543	-1.4226254
H	1.4722206	4.0814476	-1.3677679
C	-0.7657944	3.5418011	-2.9137437
H	-0.3679367	3.8588332	-3.8897953
H	-0.8900577	4.4442250	-2.2962280
H	-1.7600573	3.1020275	-3.0835447
C	-0.2209304	0.0047902	2.4576027
C	-0.1864134	1.2207585	3.1776994
C	0.1589819	1.1749377	4.5346914
H	0.1992218	2.0984245	5.1143947
C	0.4578993	-0.0390827	5.1574066
H	0.7249552	-0.0561156	6.2162840
C	0.4214400	-1.2270011	4.4296440
H	0.6655800	-2.1697353	4.9250111
C	0.0779840	-1.2305241	3.0686652
C	-0.4366334	2.5433243	2.4674886
H	-1.1103112	2.3390616	1.6197270
C	-1.1101983	3.6021117	3.3487003
H	-1.3655463	4.4848047	2.7436466
H	-0.4468450	3.9451627	4.1575105
H	-2.0351336	3.2206882	3.8060876
C	0.8837171	3.0705212	1.8731527
H	1.3297756	2.3274503	1.1963506
H	1.6068135	3.2872976	2.6745887
H	0.7101906	3.9982012	1.3057767
C	0.0713844	-2.5362461	2.2875279
H	-0.2865937	-2.3161358	1.2709577
C	1.4994306	-3.0915740	2.1488037
H	1.4982962	-4.0125383	1.5463213
H	1.9285090	-3.3303819	3.1342160
H	2.1543178	-2.3588029	1.6565340
C	-0.8778162	-3.5747976	2.9069440
H	-1.9004873	-3.1789061	2.9960558
H	-0.5458820	-3.8769506	3.9119288
H	-0.9128219	-4.4803748	2.2825801

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6-SIPr Energy = -1199.575387597

N	7.5013853	7.7048051	14.8454788
N	7.3017557	8.9043480	12.9130548
C	6.7079381	8.1049846	13.8274879
C	8.9309271	8.0557562	15.0270074
H	9.4284505	7.2189217	15.5372609
H	9.0152883	8.9393148	15.6837010
C	9.5664252	8.3309076	13.6710844
H	9.6259228	7.3928262	13.0962468
H	10.5900630	8.7101469	13.7985451
C	8.7182017	9.3422823	12.9116780
H	8.7975631	10.3459004	13.3673591
H	9.0480144	9.4326977	11.8661681
C	6.4949594	9.4282445	11.8385588
C	5.7717605	10.6211966	12.0391875
C	5.0099097	11.1188355	10.9704174
H	4.4300233	12.0348020	11.1024225
C	4.9793749	10.4589866	9.7427243
H	4.3821736	10.8612777	8.9213942
C	5.7086451	9.2821164	9.5617355
H	5.6697856	8.7703276	8.5982917
C	6.4811680	8.7472182	10.6015058
C	7.2159859	7.4252187	10.4338944
H	8.0328453	7.4050408	11.1722075
C	7.8446321	7.2401397	9.0466500
H	8.4501320	6.3217462	9.0286813
H	8.4963695	8.0860971	8.7817801
H	7.0815370	7.1401624	8.2597950
C	6.2701758	6.2603654	10.7827910
H	6.8015847	5.2976231	10.7265460
H	5.4230182	6.2283207	10.0802039
H	5.8719659	6.3823226	11.8008894
C	5.7566895	11.3254613	13.3875067
H	6.5707706	10.8991778	13.9932523
C	6.0029895	12.8369896	13.2734599
H	6.0698545	13.2868771	14.2756283
H	5.1852642	13.3451384	12.7403556
H	6.9396101	13.0508094	12.7370587
C	4.4408936	11.0208722	14.1250423
H	4.4333053	11.4969140	15.1173865
H	4.3206746	9.9360559	14.2571114
H	3.5770085	11.4002270	13.5570020
C	6.9386919	6.8561789	15.8662059
C	6.3959177	7.4436620	17.0294397
C	5.9247248	6.5949775	18.0422831
H	5.5015338	7.0270439	18.9519978
C	5.9861499	5.2086914	17.9061185
H	5.6173535	4.5636720	18.7065831
C	6.5101411	4.6471358	16.7421125
H	6.5431838	3.5601672	16.6378709
C	6.9947380	5.4544850	15.7033208
C	7.5629936	4.8121874	14.4460154
H	7.7785173	5.6201379	13.7324936
C	6.5421844	3.8777951	13.7773061
H	6.9454860	3.4851449	12.8316650
H	5.6076182	4.4121052	13.5550016
H	6.2996142	3.0175417	14.4199125
C	8.8801732	4.0739508	14.7417435
H	9.3069427	3.6581410	13.8161554
H	8.7184478	3.2404909	15.4428768
H	9.6269455	4.7464831	15.1902621
C	6.3171883	8.9530018	17.2054955
H	6.6000949	9.4106478	16.2458103
C	4.8872258	9.4162388	17.5282973

H	4.8416015	10.5153537	17.5646307
H	4.5518977	9.0373745	18.5056161
H	4.1771668	9.0691555	16.7648362
C	7.3061999	9.4399107	18.2798026
H	7.2839996	10.5377049	18.3578117
H	8.3368283	9.1323167	18.0485342
H	7.0486254	9.0253388	19.2670223

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5-IPr Energy = -1159.095156084

N	-1.0625745	-0.5628909	0.0452108
N	1.0617404	-0.5135945	-0.0451353
C	-0.0209141	0.3336094	-0.0103044
C	-0.6484393	-1.8969409	0.0426468
H	-1.3453956	-2.7271297	0.0800162
C	0.7112810	-1.8652360	-0.0121986
H	1.4467698	-2.6621495	-0.0315187
C	2.4246731	-0.0549041	-0.1016446
C	3.0274888	0.1127971	-1.3659973
C	4.3576306	0.5536574	-1.3967892
H	4.8554832	0.6982635	-2.3569227
C	5.0556990	0.8139514	-0.2159409
H	6.0917702	1.1562312	-0.2612334
C	4.4342197	0.6414827	1.0196600
H	4.9886359	0.8538432	1.9365326
C	3.1037905	0.2027334	1.1040826
C	2.4341867	0.0420266	2.4610011
H	1.4156505	-0.3364781	2.2907771
C	3.1705166	-0.9819903	3.3402256
H	2.6347372	-1.1236913	4.2910047
H	4.1919258	-0.6479564	3.5789093
H	3.2434440	-1.9584868	2.8387486
C	2.3009181	1.4008581	3.1691897
H	1.7702496	1.2846112	4.1265005
H	1.7368421	2.1109978	2.5481985
H	3.2885663	1.8385745	3.3812979
C	2.2375147	-0.1061905	-2.6485013
H	1.4185982	-0.8056140	-2.4184449
C	3.0671360	-0.7306850	-3.7778114
H	2.4155622	-0.9645076	-4.6327462
H	3.5553761	-1.6618863	-3.4543309
H	3.8475618	-0.0454711	-4.1423996
C	1.5930487	1.2197731	-3.0964798
H	0.9799505	1.0643479	-3.9977668
H	2.3677719	1.9657873	-3.3317725
H	0.9479055	1.6237996	-2.3031902
C	-2.4456924	-0.1682338	0.0972523
C	-3.1364502	0.0438699	-1.1106941
C	-4.4863685	0.4195308	-1.0300587
H	-5.0504341	0.5954236	-1.9486478
C	-5.1154333	0.5736934	0.2039894
H	-6.1670937	0.8650662	0.2465943
C	-4.4056375	0.3592119	1.3872523
H	-4.9105515	0.4874861	2.3458965
C	-3.0556406	-0.0162863	1.3605032
C	-2.2543087	-0.1837548	2.6441174
H	-1.4231002	-0.8737098	2.4285725
C	-3.0645937	-0.7908067	3.7965873
H	-2.4022562	-0.9931500	4.6511896
H	-3.5430524	-1.7366913	3.5022592
H	-3.8508429	-0.1066564	4.1508653
C	-1.6332602	1.1665909	3.0518457
H	-1.0107916	1.0472929	3.9522038
H	-2.4217019	1.9022486	3.2739413
H	-1.0024936	1.5636513	2.2434498
C	-2.4575372	-0.0921207	-2.4656951

H	-1.4347583	-0.4584703	-2.2939741
C	-3.1717756	-1.1131412	-3.3656163
H	-2.6222636	-1.2366749	-4.3110282
H	-4.1934757	-0.7881573	-3.6148475
H	-3.2397748	-2.0965810	-2.8772354
C	-2.3394625	1.2792393	-3.1527724
H	-1.8045607	1.1846075	-4.1101149
H	-1.7864832	1.9862319	-2.5185748
H	-3.3328299	1.7062686	-3.3601226

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5-I^{t}Bu Energy = -540.2459832739

N	8.7356836	4.6541078	7.4681248
N	7.9302184	4.4371757	9.4383392
C	7.7351090	4.0143964	8.1501645
C	9.0129619	5.3058840	9.5555873
H	9.3406713	5.7494237	10.4877793
C	9.5200794	5.4523904	8.2983220
H	10.3584078	6.0476939	7.9575637
C	8.8571643	4.5694465	5.9803892
C	8.6918969	3.1026664	5.5605507
H	8.7389258	3.0245702	4.4642050
H	7.7291776	2.7143921	5.9140883
H	9.4916010	2.4832828	5.9926193
C	7.7446387	5.4320219	5.3626589
H	7.7934094	5.3902054	4.2644527
H	7.8479815	6.4815964	5.6763099
H	6.7626151	5.0651877	5.6911128
C	10.2318344	5.0824028	5.5350843
H	10.3276979	4.9391479	4.4500358
H	11.0449608	4.5275561	6.0254983
H	10.3600732	6.1557070	5.7381805
C	7.1070048	3.9118852	10.5707333
C	7.5036083	2.4452631	10.8058140
H	6.9082915	2.0147000	11.6246859
H	8.5686697	2.3703271	11.0714297
H	7.3306373	1.8616473	9.8915107
C	5.6261558	4.0097361	10.1793000
H	5.0017819	3.5867832	10.9799958
H	5.4464084	3.4601869	9.2470914
H	5.3350052	5.0588888	10.0225567
C	7.3643645	4.7364928	11.8366321
H	6.7022802	4.3736531	12.6345917
H	7.1472066	5.8023786	11.6742741
H	8.3995488	4.6332646	12.1937609

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TS_1 Energy = -1717.395922268

N	-1.1977120	-1.0288500	0.2109637
N	0.9706380	-1.1300498	0.5619315
N	0.4309904	-0.1466044	-3.6369685
N	0.2919791	0.6548095	-2.7925744
C	-0.0580417	-0.3273514	0.2666439
C	-0.9699593	-2.4786361	0.4642980
H	-1.6103789	-2.8244007	1.2869126
C	0.5341363	-2.5303804	0.7983436
H	0.7335209	-2.8075698	1.8443493
C	2.2978171	-0.6911046	0.9023803
C	3.3166744	-0.7500104	-0.0714262
C	4.6111803	-0.3755674	0.3180637
H	5.4189417	-0.4094610	-0.4154910
C	4.8822550	0.0461328	1.6180889
H	5.8974744	0.3354338	1.8977805
C	3.8562369	0.1076541	2.5597816
H	4.0752206	0.4483492	3.5740577
C	2.5466241	-0.2629836	2.2259918

C	1.4528549	-0.1811609	3.2798597
H	0.5186287	-0.5463106	2.8313593
C	1.7568304	-1.0766226	4.4922078
H	0.9175084	-1.0540830	5.2038187
H	2.6577028	-0.7388195	5.0264525
H	1.9203127	-2.1212036	4.1880178
C	1.2106189	1.2759483	3.7086956
H	0.3849180	1.3317804	4.4347214
H	0.9548566	1.9082048	2.8456655
H	2.1053297	1.7029187	4.1856276
C	3.0554943	-1.1900914	-1.5013063
H	1.9686443	-1.2858792	-1.6366473
C	3.6900999	-2.5636831	-1.7824783
H	3.4459571	-2.8916192	-2.8036938
H	3.3302644	-3.3307894	-1.0795542
H	4.7866491	-2.5177749	-1.6934180
C	3.5407311	-0.1377770	-2.5112839
H	3.2467692	-0.4344073	-3.5272345
H	4.6354172	-0.0260082	-2.4852526
H	3.0813787	0.8386853	-2.3000105
C	-2.5074721	-0.4604775	0.0499816
C	-3.2438291	-0.7481079	-1.1190413
C	-4.5585132	-0.2653830	-1.2024184
H	-5.1495394	-0.4801144	-2.0945015
C	-5.1091663	0.5060654	-0.1841906
H	-6.1308155	0.8812902	-0.2724414
C	-4.3461705	0.8226431	0.9399937
H	-4.7798172	1.4500359	1.7190721
C	-3.0373226	0.3475391	1.0883085
C	-2.2428015	0.6715540	2.3475331
H	-1.1832315	0.7477486	2.0576546
C	-2.3668601	-0.4640954	3.3803808
H	-1.7672228	-0.2409734	4.2760385
H	-2.0244224	-1.4268499	2.9760216
H	-3.4151915	-0.5857377	3.6929920
C	-2.6233285	2.0145761	2.9843909
H	-1.9111309	2.2595278	3.7853783
H	-3.6260926	1.9868656	3.4371780
H	-2.6018155	2.8325473	2.2499749
C	-2.6577046	-1.5192036	-2.2913366
H	-1.5732693	-1.6158126	-2.1305036
C	-3.2712700	-2.9275138	-2.3991530
H	-2.7961198	-3.4911352	-3.2159017
H	-4.3491569	-2.8639849	-2.6146073
H	-3.1556476	-3.5040391	-1.4692146
C	-2.8357902	-0.7519654	-3.6124910
H	-2.2745416	-1.2524140	-4.4133178
H	-2.4512876	0.2722571	-3.5257772
H	-3.8940695	-0.7048372	-3.9113908
C	0.1896238	1.4326806	-1.7993386
H	0.0812468	0.6764110	-0.4249818
Si	-0.4519799	3.1537613	-1.6846857
C	0.4558625	4.3378631	-2.8692848
H	0.3277410	4.0123925	-3.9128332
H	0.0686007	5.3652819	-2.7815329
H	1.5334696	4.3518626	-2.6489380
C	-2.3235159	3.2492938	-2.0463160
H	-2.8791634	2.5780456	-1.3739944
H	-2.7065183	4.2736823	-1.9117022
H	-2.5364009	2.9390328	-3.0807730
C	-0.1613024	3.7066434	0.1133834
H	-0.6779577	3.0315827	0.8123403
H	0.9116901	3.6873559	0.3553204
H	-0.5385548	4.7257940	0.2874220
H	-1.2137349	-3.0605303	-0.4343449
H	1.0906622	-3.2147815	0.1439007

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Comp 1 Energy = -1717.445557754

Si	7.8658587	5.1974404	14.3705032
N	5.2746359	2.2085771	13.4056442
N	5.5994723	2.0848314	15.6658799
N	5.1168013	4.9610312	14.4194794
N	4.1333147	5.5595354	14.3793318
C	6.1356844	2.7347335	14.4714368
H	7.1951788	2.4349476	14.3405429
C	4.4154505	1.1400014	13.9215825
H	4.8679059	0.1327499	13.8260772
H	3.4495713	1.1366507	13.3934843
C	4.2767419	1.5287080	15.3916473
H	3.4426817	2.2447203	15.5236402
H	4.0864404	0.6620251	16.0416475
C	5.7966238	2.1187483	12.0707640
C	6.8647503	1.2426514	11.7433130
C	7.3570671	1.2345316	10.4304345
H	8.1836997	0.5678512	10.1728413
C	6.8021711	2.0478793	9.4443519
H	7.1999347	2.0274356	8.4272428
C	5.7293850	2.8764948	9.7627327
H	5.2834597	3.5006434	8.9846889
C	5.2089291	2.9256580	11.0642742
C	7.4799773	0.2817216	12.7514870
H	6.9862335	0.4385098	13.7193894
C	8.9847089	0.5340565	12.9425228
H	9.5377012	0.3823329	12.0038765
H	9.4007010	-0.1563694	13.6909125
H	9.1833390	1.5621802	13.2817851
C	7.2191894	-1.1820967	12.3533368
H	7.7133803	-1.4314593	11.4019980
H	6.1432106	-1.3752187	12.2334064
H	7.6072099	-1.8643437	13.1251638
C	4.0213958	3.8277247	11.3509014
H	3.8176910	3.7490664	12.4269973
C	4.3311501	5.2979802	11.0279984
H	4.4980660	5.4468723	9.9496800
H	5.2327518	5.6383794	11.5581682
H	3.4943644	5.9428050	11.3338042
C	2.7660475	3.3503656	10.5998343
H	2.9032441	3.4109176	9.5087077
H	1.8999028	3.9754891	10.8656434
H	2.5254366	2.3064003	10.8500640
C	6.1042042	2.3318530	16.9787477
C	5.4683095	3.2304077	17.8719234
C	5.9905679	3.3858158	19.1665070
H	5.4966326	4.0687265	19.8614534
C	7.1316071	2.7048038	19.5741077
H	7.5297277	2.8487760	20.5809728
C	7.7658917	1.8349992	18.6866008
H	8.6585777	1.3006013	19.0140791
C	7.2648508	1.6211489	17.3974451
C	4.2386175	4.0411006	17.4948073
H	4.0629357	3.9075672	16.4222267
C	2.9873828	3.5376845	18.2365808
H	2.0972182	4.1016040	17.9187914
H	3.0982276	3.6637878	19.3247523
H	2.8068900	2.4706268	18.0398489
C	4.4486800	5.5458992	17.7304210
H	5.3558552	5.9008697	17.2196675
H	4.5503869	5.7794377	18.8006835
H	3.5926553	6.1145064	17.3396996
C	7.9229186	0.5934136	16.4877077
H	7.8627783	0.9783360	15.4610618

C	9.4067981	0.3488367	16.7874464
H	9.8399496	-0.3036378	16.0152506
H	9.5550808	-0.1557889	17.7544976
H	9.9793518	1.2877063	16.8000766
C	7.1419750	-0.7338967	16.5201522
H	6.0917554	-0.5829587	16.2359123
H	7.1669582	-1.1713216	17.5301998
H	7.5844028	-1.4615592	15.8215849
C	6.2139503	4.2805028	14.4722143
C	7.5342722	7.0320031	14.6957850
H	8.4686351	7.6075074	14.6184465
H	7.1207697	7.1870149	15.7033532
H	6.8221237	7.4450038	13.9659298
C	9.0289599	4.4626001	15.6753769
H	9.2289489	3.3983867	15.4808430
H	8.5923937	4.5419164	16.6810869
H	9.9937907	4.9924781	15.6630132
C	8.5934957	4.9377365	12.6363364
H	7.9545486	5.4101050	11.8757244
H	8.6583221	3.8671285	12.3905687
H	9.6034722	5.3701414	12.5628288

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$TS_{1'}$ Energy = -1717.383847685

Si	-2.8447002	0.6083914	1.9135387
N	1.5734483	0.0266411	0.1118929
N	0.8182263	0.6129818	-1.8585405
N	-0.7639979	-0.9955185	-0.6731172
N	-1.6481997	-1.2739403	0.0931393
C	0.4387839	0.2743140	-0.5986001
C	2.8070619	0.1922926	-0.6973139
H	3.3593876	1.0879463	-0.3678898
C	2.2518031	0.3371175	-2.1192131
H	2.7137505	1.1563473	-2.6855756
C	-0.0831503	1.0262228	-2.8913491
C	-0.5039091	2.3798444	-2.9160640
C	-1.3355001	2.7906262	-3.9659495
H	-1.6780820	3.8254846	-4.0083794
C	-1.7338010	1.8978912	-4.9629284
H	-2.3786928	2.2404988	-5.7751215
C	-1.3210755	0.5688706	-4.9132035
H	-1.6525998	-0.1277221	-5.6865009
C	-0.4994415	0.1041453	-3.8748012
C	-0.0958602	-1.3624101	-3.8313731
H	0.4269700	-1.5327223	-2.8798539
C	0.8515241	-1.7163561	-4.9914033
H	1.1798950	-2.7642681	-4.9158291
H	1.7457859	-1.0752182	-4.9956086
H	0.3484788	-1.5910625	-5.9629093
C	-1.3244757	-2.2864916	-3.8188344
H	-1.0068022	-3.3353313	-3.7153232
H	-1.9054373	-2.2040236	-4.7500465
H	-1.9801399	-2.0415990	-2.9726939
C	-0.0457817	3.3681429	-1.8508059
H	0.0643173	2.7984702	-0.9158123
C	1.3341839	3.9593623	-2.1960427
H	1.6730444	4.6364551	-1.3962762
H	1.2868440	4.5343036	-3.1337857
H	2.0951588	3.1765647	-2.3207653
C	-1.0512976	4.4948004	-1.5816012
H	-0.7343755	5.0710691	-0.6994957
H	-2.0564437	4.0983258	-1.3827670
H	-1.1167601	5.1991578	-2.4253824
C	1.6641754	-0.0347080	1.5410307
C	1.8479942	1.1627062	2.2720954
C	2.0024643	1.0690767	3.6622601

H	2.1391691	1.9798715	4.2494824
C	1.9728582	-0.1664832	4.3076854
H	2.0864118	-0.2179051	5.3926292
C	1.7929094	-1.3354702	3.5692788
H	1.7717640	-2.2984662	4.0836734
C	1.6461701	-1.2954638	2.1753775
C	1.5121678	-2.5839255	1.3787967
H	1.2287189	-2.3041172	0.3534184
C	0.4051533	-3.4966522	1.9281268
H	0.2647364	-4.3615716	1.2627408
H	-0.5502153	-2.9584274	1.9984331
H	0.6581890	-3.8848484	2.9271318
C	2.8603487	-3.3258405	1.3208395
H	2.7777485	-4.2283745	0.6961310
H	3.1806236	-3.6382539	2.3271196
H	3.6542163	-2.6901207	0.9006611
C	1.8942560	2.5277444	1.5991771
H	1.7086280	2.3782326	0.5258971
C	0.7920755	3.4656092	2.1183920
H	0.8229604	4.4232213	1.5765547
H	0.9203748	3.6819699	3.1898704
H	-0.2035802	3.0257358	1.9796437
C	3.2804481	3.1790505	1.7517204
H	3.3218625	4.1272867	1.1947017
H	4.0798835	2.5237746	1.3751784
H	3.5001989	3.3981953	2.8079931
C	-2.4860328	-1.0382726	1.0649939
H	-3.1210739	-1.8974578	1.3157852
C	-2.5866008	2.0253566	0.6801841
H	-2.7666574	3.0064366	1.1453555
H	-3.2666412	1.9161747	-0.1777512
H	-1.5598751	1.9983509	0.2911028
C	-4.6688594	0.5277721	2.4464364
H	-4.9532883	1.4420224	2.9900914
H	-4.8471558	-0.3292762	3.1138469
H	-5.3312316	0.4254394	1.5742398
C	-1.7867888	0.8603746	3.4717093
H	-2.0013762	1.8314802	3.9460129
H	-0.7144905	0.8177390	3.2403419
H	-2.0021650	0.0669986	4.2031397
H	2.3686924	-0.5933898	-2.6987203
H	3.4662052	-0.6802234	-0.5852980

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Comp 1' Energy = -1717.475976580

Si	4.7332026	0.2713837	12.7919705
N	0.2181113	-3.7113317	10.8368723
N	0.9007946	-3.5522838	12.9626901
N	2.7759425	-1.6098535	12.1268068
N	1.9019894	-2.1462502	11.2019242
C	1.0920400	-3.0580867	11.6865851
H	3.3248314	-0.2912054	10.6347139
C	-0.4200892	-4.8416551	11.5165668
H	0.1087468	-5.7859283	11.2905585
H	-1.4693886	-4.9482695	11.2077006
C	-0.2703986	-4.4461144	12.9867988
H	-1.1583841	-3.9032264	13.3566793
H	-0.0886467	-5.3054834	13.6470922
C	0.3763823	-3.7050582	9.4128498
C	1.4531333	-4.3912655	8.8133114
C	1.5424998	-4.3733106	7.4132466
H	2.3704210	-4.8891787	6.9215391
C	0.5938715	-3.7052099	6.6407923
H	0.6792513	-3.7062174	5.5518796
C	-0.4641321	-3.0313318	7.2546005
H	-1.1949026	-2.5062654	6.6374317

C	-0.5914918	-3.0155082	8.6494454
C	2.5144146	-5.1136401	9.6315266
H	2.2404736	-5.0363692	10.6939987
C	3.8859441	-4.4346835	9.4771349
H	4.2479479	-4.5023791	8.4393405
H	4.6287388	-4.9213107	10.1278630
H	3.8206998	-3.3745768	9.7569436
C	2.5845786	-6.6094310	9.2817598
H	2.8977545	-6.7630931	8.2378753
H	1.6080806	-7.0992658	9.4136131
H	3.3155361	-7.1186207	9.9281144
C	-1.6849068	-2.2158613	9.3435928
H	-1.8948383	-2.7171499	10.3023392
C	-1.1632165	-0.8041825	9.6796623
H	-0.9728752	-0.2371792	8.7546714
H	-0.2213835	-0.8536987	10.2449091
H	-1.9052889	-0.2490637	10.2749322
C	-2.9986767	-2.1470480	8.5558940
H	-2.8920963	-1.5605561	7.6304348
H	-3.7734156	-1.6552644	9.1626957
H	-3.3617015	-3.1490867	8.2831161
C	1.3003084	-2.9506329	14.2021246
C	0.6570991	-1.7837726	14.6668797
C	1.0223359	-1.2931817	15.9288022
H	0.5498311	-0.3839659	16.3078530
C	1.9721912	-1.9499429	16.7101974
H	2.2401745	-1.5532891	17.6917891
C	2.5846378	-3.1119154	16.2372748
H	3.3313822	-3.6138907	16.8549538
C	2.2591097	-3.6363513	14.9808240
C	-0.3912624	-1.0492336	13.8428100
H	-0.5229620	-1.5897623	12.8938172
C	-1.7550617	-1.0268909	14.5551063
H	-2.5132180	-0.5489178	13.9161209
H	-1.7029681	-0.4595613	15.4967540
H	-2.0995724	-2.0437355	14.7963278
C	0.0693981	0.3743240	13.4853868
H	1.0338793	0.3528311	12.9611026
H	0.1820705	0.9931056	14.3889845
H	-0.6700773	0.8622915	12.8322757
C	2.9648422	-4.8685063	14.4321454
H	2.3146862	-5.2921705	13.6510091
C	4.2815255	-4.4640031	13.7434791
H	4.7409565	-5.3325204	13.2461468
H	4.9991195	-4.0769210	14.4841569
H	4.1061946	-3.6761923	12.9976404
C	3.1993518	-5.9591287	15.4862885
H	2.2635901	-6.2397775	15.9927837
H	3.9181230	-5.6379632	16.2554528
H	3.6151011	-6.8594532	15.0096976
C	3.4872286	-0.6213602	11.6819722
C	4.1642795	2.0798633	12.9620683
H	4.8941030	2.6660239	13.5414622
H	3.1936780	2.1329643	13.4773553
H	4.0533056	2.5545394	11.9754192
C	4.8143998	-0.5558304	14.4895406
H	5.1935321	-1.5837923	14.4051786
H	3.8145503	-0.6114535	14.9420586
H	5.4776472	0.0069969	15.1638972
C	6.4327734	0.2366980	11.9382450
H	6.3781728	0.6821708	10.9334340
H	6.7944543	-0.7969987	11.8333208
H	7.1753757	0.8031291	12.5211286

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TS 3 Energy = -1756.674471630

Si	-4.1061190	-0.0656236	1.7308066
N	1.3831558	0.2584845	0.3836766
N	0.8156743	0.7900356	-1.7817977
N	-1.1308899	-1.2945347	-0.6599539
N	-2.0325281	-0.9043783	-0.0112317
C	0.4593931	0.3041225	-0.5866400
C	2.7851554	0.7155985	0.2261396
H	3.4201379	0.0996505	0.8772552
H	2.8707196	1.7602270	0.5713899
C	3.2012999	0.5970047	-1.2338968
H	3.2730166	-0.4660232	-1.5137360
H	4.1921407	1.0482303	-1.3828198
C	2.1704336	1.2909060	-2.1153789
H	2.2008085	2.3851182	-1.9738407
H	2.3551684	1.0907566	-3.1796287
C	-0.1752884	0.8520909	-2.8303904
C	-1.0773216	1.9352886	-2.8664952
C	-1.9962166	1.9849199	-3.9251813
H	-2.7076932	2.8119405	-3.9791909
C	-2.0174516	0.9974710	-4.9087696
H	-2.7414607	1.0548344	-5.7245391
C	-1.1215736	-0.0693303	-4.8452795
H	-1.1566338	-0.8476103	-5.6114748
C	-0.1853379	-0.1659986	-3.8073898
C	0.7662720	-1.3520673	-3.7486432
H	1.3639647	-1.2522279	-2.8308176
C	1.7305579	-1.3619672	-4.9475283
H	2.4483087	-2.1915212	-4.8565298
H	2.3003083	-0.4229232	-5.0207311
H	1.1840030	-1.4932472	-5.8940450
C	0.0042304	-2.6837195	-3.6396133
H	0.7133466	-3.5181445	-3.5248847
H	-0.5966268	-2.8760934	-4.5419523
H	-0.6629390	-2.6711709	-2.7677457
C	-1.0587967	3.0406934	-1.8212691
H	-0.4052180	2.7094715	-1.0007629
C	-0.4662038	4.3359872	-2.4069045
H	-0.4040703	5.1173830	-1.6337371
H	-1.0950718	4.7188087	-3.2258178
H	0.5439323	4.1710374	-2.8106637
C	-2.4489828	3.2941027	-1.2165919
H	-2.3770367	4.0211105	-0.3926971
H	-2.8787226	2.3648719	-0.8166934
H	-3.1470253	3.7063754	-1.9612944
C	1.0162262	-0.3045553	1.6637491
C	0.5948946	0.5575126	2.6985850
C	0.2733079	-0.0113939	3.9389708
H	-0.0590185	0.6324153	4.7558190
C	0.3586986	-1.3874548	4.1409624
H	0.0944539	-1.8137831	5.1110904
C	0.7737457	-2.2213676	3.1031698
H	0.8333793	-3.2985128	3.2716817
C	1.1144958	-1.7016070	1.8463744
C	1.6060028	-2.6288321	0.7423961
H	1.5596884	-2.0689629	-0.2018808
C	0.7165885	-3.8677495	0.5663348
H	1.0542651	-4.4504452	-0.3045178
H	-0.3259187	-3.5702479	0.3939199
H	0.7579106	-4.5311175	1.4436931
C	3.0704385	-3.0395821	0.9883847
H	3.4394269	-3.6649468	0.1607805
H	3.1623643	-3.6201142	1.9193532
H	3.7326075	-2.1650937	1.0757286
C	0.5214973	2.0666492	2.5079877
H	0.5865762	2.2652889	1.4270604
C	-0.8022698	2.6695641	3.0043429

H	-0.8525475	3.7381756	2.7463429
H	-0.9007780	2.5893823	4.0976742
H	-1.6658648	2.1656399	2.5503769
C	1.7142385	2.7582923	3.1958315
H	1.7017500	3.8415182	2.9994557
H	2.6758485	2.3553183	2.8461884
H	1.6696573	2.6102895	4.2861482
C	-2.5607442	0.0573434	0.7004870
H	-1.8482197	0.9051509	0.7464021
C	-5.2624326	-1.3716389	0.9814090
H	-6.1641495	-1.4976555	1.5996164
H	-4.7560373	-2.3464011	0.9149789
H	-5.5750634	-1.0812371	-0.0323583
C	-3.7002398	-0.5460959	3.5305566
H	-4.6106908	-0.6116775	4.1469702
H	-3.0271313	0.1966315	3.9849888
H	-3.1844032	-1.5175963	3.5608952
C	-4.9384137	1.6456711	1.7504376
H	-5.8142040	1.6541929	2.4172614
H	-5.2667779	1.9328311	0.7408262
H	-4.2369138	2.4159759	2.1071586

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Comp 3 Energy = -1756.750083722

Si	-2.8318637	-1.5665896	2.7079481
N	1.3195823	0.9529281	0.3086678
N	0.8522977	0.4961475	-1.9495620
N	-0.4545386	-0.5449677	-0.3996287
N	-1.0167172	-0.5067043	0.8511794
C	0.5499186	0.2903570	-0.6189909
C	2.3093553	1.9413067	-0.1559489
H	2.9743780	2.1545967	0.6892808
H	1.8085657	2.8868189	-0.4352925
C	3.0739660	1.3806865	-1.3469038
H	3.5874196	0.4535663	-1.0482884
H	3.8373557	2.0916410	-1.6939740
C	2.0768600	1.1158647	-2.4642404
H	1.8071809	2.0655578	-2.9622164
H	2.5091796	0.4601719	-3.2386058
C	-0.1410543	0.1646348	-2.9380580
C	-1.1564999	1.1037692	-3.2220853
C	-2.0805610	0.7892197	-4.2282890
H	-2.8826430	1.4926647	-4.4621806
C	-1.9910340	-0.4105444	-4.9357971
H	-2.7177258	-0.6365524	-5.7192185
C	-0.9786859	-1.3241522	-4.6392184
H	-0.9279908	-2.2678283	-5.1871081
C	-0.0386672	-1.0567395	-3.6341563
C	1.0089986	-2.0958706	-3.2629748
H	1.6826632	-1.6352613	-2.5240543
C	1.8542599	-2.5330013	-4.4688736
H	2.6406584	-3.2346900	-4.1517978
H	2.3369365	-1.6721685	-4.9556392
H	1.2408173	-3.0452599	-5.2259689
C	0.3446511	-3.2994642	-2.5704858
H	1.1075464	-4.0185132	-2.2334168
H	-0.3360419	-3.8242651	-3.2591651
H	-0.2301353	-2.9584809	-1.6982089
C	-1.2903430	2.3953707	-2.4278457
H	-0.3655915	2.5199876	-1.8438461
C	-1.4339303	3.6324672	-3.3274857
H	-1.4440627	4.5477575	-2.7163300
H	-2.3725171	3.6102890	-3.9017152
H	-0.6018564	3.7073237	-4.0438719
C	-2.4521656	2.2966633	-1.4215048
H	-2.4972856	3.2014967	-0.7953304

H	-2.3296188	1.4263148	-0.7625382
H	-3.4145168	2.1986185	-1.9476908
C	1.3901142	0.5980867	1.7025102
C	0.9158655	1.5361265	2.6456758
C	1.1398224	1.2822483	4.0036259
H	0.7794955	1.9941685	4.7502499
C	1.7930840	0.1207278	4.4187918
H	1.9530362	-0.0668371	5.4826814
C	2.2227418	-0.8086672	3.4733282
H	2.7209959	-1.7219709	3.8066517
C	2.0451533	-0.5870619	2.0995530
C	2.5499541	-1.6176564	1.1005727
H	2.3093340	-1.2575796	0.0908295
C	1.8296502	-2.9650060	1.2756590
H	2.1548598	-3.6764711	0.5012914
H	0.7419055	-2.8374701	1.1923295
H	2.0508751	-3.4110705	2.2579899
C	4.0771333	-1.7811999	1.1805382
H	4.4294949	-2.4862479	0.4120052
H	4.3871937	-2.1719410	2.1617311
H	4.5909068	-0.8199646	1.0280570
C	0.1147143	2.7556195	2.2145404
H	0.0855301	2.7571537	1.1151502
C	-1.3418944	2.6325258	2.6906362
H	-1.9429921	3.4762735	2.3177110
H	-1.4066373	2.6283601	3.7899287
H	-1.7764957	1.6977365	2.3111966
C	0.7546630	4.0733817	2.6766405
H	0.1738413	4.9328281	2.3081825
H	1.7861685	4.1720378	2.3057591
H	0.7865522	4.1395976	3.7750471
C	-1.8690924	-1.4608266	1.0819772
H	-2.0363540	-2.2106239	0.2812708
C	-4.2722008	-0.3209187	2.6984175
H	-4.8580690	-0.3946343	3.6278401
H	-4.9463860	-0.5108025	1.8501247
H	-3.8970247	0.7090854	2.6096080
C	-3.5414176	-3.3271537	2.8101479
H	-4.1439008	-3.4555242	3.7219928
H	-2.7356507	-4.0767917	2.8262698
H	-4.1873658	-3.5416319	1.9450382
C	-1.6926947	-1.2241826	4.1817533
H	-2.2525342	-1.2543146	5.1290179
H	-1.2203338	-0.2376407	4.0816624
H	-0.8842049	-1.9684964	4.2283845

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TS 3' Energy = -1756.680423758

Si	-3.2058507	-1.0181221	0.8910823
N	1.6268231	-0.2104388	0.4452614
N	0.5998300	0.2434848	-1.5909764
N	-0.8640753	-3.8228320	-0.5263451
N	-1.2591161	-2.7915208	-0.1411460
C	0.5114369	0.0101871	-0.2702444
C	2.9794914	-0.2669400	-0.1480084
H	3.5691288	-0.9919081	0.4284479
H	3.4688368	0.7164287	-0.0411815
C	2.8767234	-0.6664202	-1.6122206
H	2.5340051	-1.7099975	-1.6916414
H	3.8629402	-0.5982713	-2.0912595
C	1.8906776	0.2545300	-2.3154313
H	2.2810484	1.2851019	-2.3581417
H	1.7059962	-0.0660662	-3.3469068
C	-0.5810144	0.6082278	-2.3508433
C	-1.1885298	1.8703266	-2.1345905
C	-2.2507398	2.2387611	-2.9716095

H	-2.7377934	3.2033975	-2.8251485
C	-2.6973243	1.4017443	-3.9922615
H	-3.5204617	1.7160841	-4.6373858
C	-2.1077565	0.1547052	-4.1668665
H	-2.4840481	-0.5139294	-4.9434427
C	-1.0553262	-0.2758730	-3.3460295
C	-0.5210883	-1.6889423	-3.5320122
H	0.1587812	-1.9105672	-2.6956239
C	0.2518883	-1.8505346	-4.8547524
H	0.6522005	-2.8718050	-4.9390088
H	1.0932900	-1.1473933	-4.9444046
H	-0.4132671	-1.6770388	-5.7145601
C	-1.6673829	-2.7152407	-3.4717249
H	-1.2611692	-3.7341173	-3.4143829
H	-2.3039440	-2.6484039	-4.3669737
H	-2.2948714	-2.5522420	-2.5866591
C	-0.7102652	2.8367317	-1.0584595
H	-0.3401922	2.2282559	-0.2193173
C	0.4566954	3.7015249	-1.5701282
H	0.8180772	4.3728548	-0.7763757
H	0.1325081	4.3220194	-2.4197532
H	1.3045946	3.0899132	-1.9076170
C	-1.8281075	3.7310552	-0.5064312
H	-1.4646643	4.2828915	0.3714819
H	-2.7044472	3.1425465	-0.1994895
H	-2.1585267	4.4775812	-1.2442550
C	1.5674692	-0.2346568	1.8944422
C	1.6241084	0.9953594	2.5886742
C	1.6367474	0.9647481	3.9903097
H	1.6776153	1.9036863	4.5458747
C	1.6111574	-0.2427053	4.6835504
H	1.6240415	-0.2479376	5.7755065
C	1.5681049	-1.4440704	3.9799921
H	1.5472326	-2.3863836	4.5296753
C	1.5493092	-1.4710870	2.5777112
C	1.5250423	-2.8134745	1.8636807
H	1.2709154	-2.6345209	0.8089557
C	0.4521312	-3.7498020	2.4419304
H	0.3616563	-4.6459418	1.8140312
H	-0.5263419	-3.2501473	2.4633544
H	0.7052823	-4.0718674	3.4635241
C	2.9070442	-3.4936520	1.9150521
H	2.8846589	-4.4405153	1.3553675
H	3.1904456	-3.7191267	2.9549704
H	3.6990580	-2.8625824	1.4853247
C	1.7085889	2.3407367	1.8823803
H	1.5772948	2.1697924	0.8044482
C	0.5907993	3.2919342	2.3386169
H	0.6250322	4.2276172	1.7610426
H	0.6982386	3.5566683	3.4009603
H	-2.1648594	0.3277341	2.7347385
C	3.0916843	2.9864155	2.0841995
H	3.1633593	3.9267455	1.5167147
H	3.9008761	2.3202323	1.7506280
H	3.2672169	3.2173588	3.1461366
C	-1.5801855	-1.6353447	0.2703150
H	-0.5997689	-0.6221933	0.1152415
C	-4.0605157	-2.2961358	2.0132213
H	-5.0350768	-1.9260468	2.3680620
H	-3.4343699	-2.5190854	2.8900065
H	-4.2305945	-3.2385013	1.4703582
C	-2.8141082	0.5601092	1.8775297
H	-3.7288231	1.0459802	2.2496378
H	-2.2791658	1.2808823	1.2417140
H	-0.3999829	2.8353010	2.2054525
C	-4.3714909	-0.5720193	-0.5497296

H -5.3127935 -0.1278715 -0.1887780

H -4.6180605 -1.4693034 -1.1378783

H -3.8809693 0.1450104 -1.2255527

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Comp 3' Energy = -1756.717937642

Si -3.3543099 -0.4403207 1.9124712

N 0.4548387 0.2124537 0.9201064

N -0.6161144 0.1545175 -1.2129012

N -1.7677008 -3.1132522 0.2006499

N -1.7513270 -1.9869498 0.4265472

C -0.8701614 0.2700934 0.2295319

C 1.3638347 1.2734627 0.4776102

H 2.3082812 1.1652289 1.0291759

H 0.9679470 2.2893173 0.7032653

C 1.5928587 1.1899346 -1.0289390

H 2.1221346 0.2583304 -1.2803361

H 2.2095880 2.0425538 -1.3568204

C 0.2371528 1.2196034 -1.7297280

H -0.2286634 2.2191186 -1.5629229

H 0.3396255 1.0900624 -2.8151575

C -1.4733361 -0.5222098 -2.1421083

C -2.7430964 -0.0107714 -2.5156548

C -3.5098438 -0.7201647 -3.4512103

H -4.4920599 -0.3417269 -3.7406122

C -3.0311365 -1.8898286 -4.0407078

H -3.6428402 -2.4252926 -4.7703100

C -1.7645151 -2.3630534 -3.7065801

H -1.3870489 -3.2702152 -4.1831315

C -0.9698163 -1.6983353 -2.7621972

C 0.4292318 -2.2135917 -2.4579883

H 0.7394043 -1.7263375 -1.5218610

C 1.4189221 -1.7807382 -3.5564459

H 2.4414365 -2.1011239 -3.3021334

H 1.4280133 -0.6899258 -3.6917036

H 1.1507220 -2.2354465 -4.5232875

C 0.4936994 -3.7347366 -2.2598231

H 1.5016038 -4.0267330 -1.9276066

H 0.2887724 -4.2787970 -3.1949059

H -0.2274740 -4.0734004 -1.5037574

C -3.2411532 1.3369586 -2.0106941

H -2.7094271 1.5623821 -1.0742650

C -2.8928017 2.4445620 -3.0266515

H -3.1864395 3.4320461 -2.6380595

H -3.4298122 2.2769801 -3.9733723

H -1.8182324 2.4685683 -3.2511602

C -4.7482565 1.3651927 -1.7180705

H -5.0257234 2.3188301 -1.2439974

H -5.0503993 0.5468899 -1.0504794

H -5.3409275 1.2814332 -2.6409460

C 0.5621961 -0.1843529 2.2999222

C 0.3274524 0.6960506 3.3889417

C 0.5489995 0.2318386 4.6963303

H 0.3763533 0.9047011 5.5388109

C 0.9754700 -1.0695867 4.9422957

H 1.1282252 -1.4135009 5.9676904

C 1.2142725 -1.9283145 3.8704815

H 1.5660028 -2.9428279 4.0661671

C 1.0357211 -1.5026826 2.5481041

C 1.4344129 -2.4164139 1.3984748

H 0.8344460 -2.1185844 0.5296973

C 1.1923895 -3.9055024 1.6705594

H 1.3750351 -4.4852194 0.7540636

H 0.1569216 -4.0947037 1.9855812

H 1.8686563 -4.2999990 2.4453671

C 2.9062750 -2.1686691 1.0172768

H	3.1900950	-2.7901422	0.1532125
H	3.5749543	-2.4203958	1.8553888
H	3.0757586	-1.1161124	0.7495529
C	-0.1159265	2.1450962	3.2111970
H	-0.4899861	2.2593690	2.1826573
C	-1.2522738	2.5505586	4.1668370
H	-1.6432440	3.5409919	3.8890864
H	-0.8972472	2.6199122	5.2056904
H	-2.9343262	2.0497390	2.0026346
C	1.0719092	3.1096343	3.4014652
H	0.7619256	4.1491008	3.2122524
H	1.9076069	2.8720532	2.7302295
H	1.4456200	3.0505452	4.4354635
C	-1.8706600	-0.7321193	0.7473387
H	-1.3121522	1.2785156	0.4356744
C	-2.9256775	-1.0386488	3.6578884
H	-3.7769904	-0.8838448	4.3388359
H	-2.0451104	-0.5254494	4.0651825
H	-2.7004119	-2.1157019	3.6347834
C	-3.8076788	1.3981087	1.8735150
H	-4.5120297	1.6126752	2.6915112
H	-4.2950858	1.6592722	0.9257167
H	-2.0858330	1.8367893	4.1459864
C	-4.7920252	-1.4964575	1.2676917
H	-5.6942968	-1.3098208	1.8696163
H	-4.5607516	-2.5696718	1.3397725
H	-5.0218960	-1.2706250	0.2169996

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TS 4 Energy = -1716.189826684

Si	-3.2732813	-0.5888037	2.6068614
N	1.5781502	0.3797626	0.2149558
N	0.9656434	0.7221053	-1.8098800
N	-0.9797584	-1.1889081	-0.6501081
N	-1.7068493	-1.0223049	0.2712671
C	0.4741889	0.3700262	-0.5889940
C	2.7281180	0.7530860	-0.4829785
H	3.6972155	0.8342541	-0.0038666
C	2.3384639	0.9721371	-1.7702010
H	2.8973566	1.2832890	-2.6454230
C	0.1500960	0.7995997	-2.9939299
C	-0.7316054	1.8895262	-3.1382139
C	-1.5164605	1.9321648	-4.2994335
H	-2.2169437	2.7571649	-4.4426401
C	-1.4214027	0.9364460	-5.2712833
H	-2.0411241	0.9905758	-6.1688838
C	-0.5457122	-0.1337802	-5.0944688
H	-0.4933643	-0.9186481	-5.8521015
C	0.2527517	-0.2329136	-3.9465513
C	1.1456304	-1.4485533	-3.7418497
H	1.6780628	-1.3252567	-2.7878868
C	2.2042730	-1.5690563	-4.8505146
H	2.8659763	-2.4260026	-4.6550508
H	2.8251110	-0.6626572	-4.9137196
H	1.7371791	-1.7247810	-5.8350454
C	0.3043117	-2.7311698	-3.6218954
H	0.9566696	-3.5938170	-3.4172020
H	-0.2456673	-2.9378577	-4.5529908
H	-0.4193069	-2.6387893	-2.8006019
C	-0.8825631	2.9609738	-2.0685967
H	-0.0501352	2.8477273	-1.3581873
C	-0.8065452	4.3837579	-2.6438363
H	-0.8413359	5.1209211	-1.8272919
H	-1.6512338	4.5985291	-3.3153951
H	0.1241824	4.5401090	-3.2085334
C	-2.1876637	2.7453531	-1.2795082

H	-2.2758382	3.4898379	-0.4728236
H	-2.2151671	1.7454179	-0.8253403
H	-3.0636790	2.8519062	-1.9381561
C	1.5395702	0.0924808	1.6275793
C	1.3743034	1.1656612	2.5255686
C	1.3636337	0.8673080	3.8950700
H	1.2358410	1.6741323	4.6195415
C	1.4968806	-0.4456403	4.3450378
H	1.4818501	-0.6579677	5.4162328
C	1.6332043	-1.4896149	3.4310388
H	1.7199406	-2.5151706	3.7949957
C	1.6514796	-1.2461206	2.0501900
C	1.8005588	-2.3971316	1.0669279
H	1.5660720	-2.0141442	0.0634719
C	0.8031466	-3.5304670	1.3511233
H	0.8659288	-4.2921245	0.5595837
H	-0.2264428	-3.1486056	1.3762965
H	1.0124654	-4.0300015	2.3095413
C	3.2489573	-2.9179974	1.0542911
H	3.3612417	-3.7240600	0.3131187
H	3.5303159	-3.3209525	2.0396784
H	3.9612217	-2.1186301	0.8010038
C	1.2084616	2.6027810	2.0524974
H	1.1099376	2.5880755	0.9570350
C	-0.0707436	3.2470799	2.6121727
H	-0.1948228	4.2608558	2.2024965
H	-0.0363111	3.3319973	3.7086516
H	-0.9609677	2.6601099	2.3458019
C	2.4504912	3.4426401	2.3984162
H	2.3400718	4.4693452	2.0178897
H	3.3605105	3.0092296	1.9582453
H	2.5976382	3.4984405	3.4880550
C	-2.0199649	-0.2474040	1.2747476
H	-1.3601952	0.6450324	1.2700410
C	-3.6077108	-2.4567431	2.6751450
H	-4.3922714	-2.6981012	3.4079245
H	-2.6922005	-2.9987415	2.9561765
H	-3.9325759	-2.8272982	1.6912850
C	-2.5300207	0.0342335	4.2425585
H	-3.2264309	-0.1081003	5.0827432
H	-2.2951885	1.1078761	4.1740508
H	-1.5920336	-0.4953262	4.4646365
C	-4.8993952	0.3519452	2.2916294
H	-5.6241676	0.1980924	3.1063259
H	-5.3616146	0.0225761	1.3489700
H	-4.7022094	1.4320322	2.2080462

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Comp 4 Energy = -1716.264366216

Si	-1.3962715	2.6935453	9.5628605
N	1.0070017	7.4040382	8.4632693
N	1.7332678	8.1346103	10.4108886
N	0.6461498	6.0457461	10.5230788
N	-0.0808756	5.1284789	9.8051948
C	1.0597627	7.0794921	9.8147092
C	2.0866458	9.0847262	9.4517836
H	2.6190393	9.9876382	9.7241829
C	1.6417211	8.6352658	8.2524688
H	1.7120582	9.0617521	7.2590179
C	0.4400529	6.6203973	7.4001434
C	1.2466788	5.6497439	6.7758820
C	0.6721896	4.9027327	5.7387350
H	1.2626549	4.1294086	5.2421924
C	-0.6432463	5.1301797	5.3335002
H	-1.0759742	4.5327933	4.5281714
C	-1.4073158	6.1226478	5.9498921

H	-2.4340745	6.2936274	5.6197999
C	-0.8805092	6.8947341	6.9931336
C	-1.7306165	7.9424564	7.6973460
H	-1.0616116	8.5411187	8.3333724
C	-2.7613858	7.2742701	8.6241947
H	-3.3090734	8.0360660	9.2001718
H	-2.2687834	6.5871907	9.3261626
H	-3.4936050	6.6942152	8.0418744
C	-2.4057991	8.9077382	6.7115959
H	-2.9457747	9.6936057	7.2607226
H	-3.1373845	8.3895929	6.0730657
H	-1.6680205	9.3927795	6.0550870
C	2.6794266	5.3892400	7.2170395
H	2.9220729	6.1089283	8.0133037
C	1.9793459	8.2348740	11.8212033
C	0.9753625	8.7847322	12.6419493
C	1.2386979	8.8704638	14.0166179
H	0.4809393	9.2847341	14.6847199
C	2.4515174	8.4265622	14.5429829
H	2.6378628	8.5013082	15.6165277
C	3.4279724	7.8846858	13.7057396
H	4.3690083	7.5355367	14.1342976
C	3.2126206	7.7733951	12.3252836
C	4.2393937	7.1113853	11.4177233
H	4.0288413	7.4337031	10.3861728
C	5.6835266	7.5225095	11.7379647
H	6.3689632	7.0932063	10.9922394
H	6.0039135	7.1553004	12.7245104
H	5.8045693	8.6158871	11.7260170
C	4.0702963	5.5796825	11.4631762
H	4.7531842	5.0964215	10.7474798
H	3.0383721	5.2922778	11.2150296
H	4.3013446	5.1964581	12.4695475
C	-0.3684920	9.2248260	12.0799991
H	-0.2877462	9.2283850	10.9824920
C	-1.4638020	8.2097534	12.4556632
H	-2.4217582	8.4901438	11.9909265
H	-1.6102535	8.1781735	13.5464562
H	-1.1899387	7.2019769	12.1120259
C	-0.7472648	10.6492692	12.5140876
H	-1.6849980	10.9560201	12.0267780
H	0.0343974	11.3732722	12.2402837
H	-0.9038667	10.7142494	13.6014398
C	-0.4050320	4.0453564	10.4460135
H	-0.0698100	3.9320095	11.4974217
C	-2.8333192	3.4563936	8.5881369
H	-3.3874756	2.6791102	8.0396861
H	-2.4436930	4.1847231	7.8625040
H	-3.5345780	3.9798886	9.2540645
C	-0.2804156	1.7472687	8.3469428
H	-0.8350473	0.9234403	7.8716047
H	0.6004716	1.3248035	8.8525256
H	0.0721028	2.4295280	7.5596139
C	-2.0403855	1.5044849	10.8979797
H	-2.6120943	0.6784993	10.4484942
H	-2.6987924	2.0277712	11.6079349
H	-1.2067124	1.0673880	11.4686951
C	2.8364787	3.9809317	7.8141359
H	2.6370678	3.2041130	7.0603382
H	3.8627382	3.8370238	8.1855591
H	2.1397079	3.8297331	8.6493728
C	3.6729784	5.6262859	6.0677015
H	3.5822525	6.6461058	5.6650927
H	4.7061661	5.4866202	6.4204871
H	3.5034888	4.9203890	5.2401587

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TS 4' Energy = -1716.195664332

N	-1.2516352	-1.0322213	0.6213296
N	0.9118296	-1.2369647	0.3937100
N	-0.4793765	-0.3141319	-3.6372913
N	-0.1918294	0.4707995	-2.8043286
C	-0.1020672	-0.3420807	0.4524789
C	-0.9650327	-2.3963098	0.6425572
H	-1.7456691	-3.1375012	0.7619006
C	0.3841997	-2.5231104	0.5011852
H	1.0184158	-3.4000347	0.4729455
C	2.3140594	-0.8944600	0.3030044
C	3.0028134	-1.1704394	-0.8944693
C	4.3707538	-0.8566782	-0.9286810
H	4.9373277	-1.0542158	-1.8396403
C	5.0075275	-0.2759845	0.1636512
H	6.0696065	-0.0290553	0.1073224
C	4.2915125	0.0028594	1.3282420
H	4.8027835	0.4648086	2.1728134
C	2.9292759	-0.3035980	1.4313574
C	2.1740226	-0.0589684	2.7330382
H	1.1388557	0.2118713	2.4769398
C	2.1177661	-1.3487335	3.5749685
H	1.5306520	-1.1845596	4.4915768
H	3.1317857	-1.6592035	3.8693155
H	1.6563623	-2.1792555	3.0218547
C	2.7347688	1.1025051	3.5624194
H	2.0647163	1.3076728	4.4096294
H	2.8191065	2.0228699	2.9669879
H	3.7253919	0.8689021	3.9805733
C	2.3367768	-1.7847646	-2.1155145
H	1.2474149	-1.6776290	-2.0098870
C	2.6690112	-3.2854933	-2.2233125
H	2.1442505	-3.7268980	-3.0833857
H	2.3762544	-3.8441739	-1.3222188
H	3.7501123	-3.4346443	-2.3695607
C	2.7246589	-1.0592859	-3.4130135
H	2.0980087	-1.4246980	-4.2371772
H	3.7791289	-1.2316515	-3.6776090
H	2.5568075	0.0213183	-3.3210450
C	-2.5360846	-0.4383347	0.9244115
C	-3.4742329	-0.2733777	-0.1121268
C	-4.7187527	0.2704478	0.2396544
H	-5.4741760	0.4115650	-0.5349819
C	-5.0015853	0.6430277	1.5524587
H	-5.9761172	1.0694826	1.7989046
C	-4.0434232	0.4784353	2.5518561
H	-4.2735745	0.7801437	3.5755446
C	-2.7875839	-0.0723843	2.2630264
C	-1.7572357	-0.2370108	3.3709829
H	-0.8916707	-0.7772509	2.9606413
C	-2.2963644	-1.0835426	4.5358308
H	-1.5068189	-1.2432450	5.2855287
H	-2.6420576	-2.0671224	4.1865337
H	-3.1389354	-0.5870504	5.0393186
C	-1.2595936	1.1344248	3.8608338
H	-0.4867396	1.0091512	4.6339330
H	-2.0828375	1.7185336	4.2987501
H	-0.8306454	1.7258929	3.0381705
C	-3.1856782	-0.6671309	-1.5489067
H	-2.1084587	-0.8564043	-1.6485246
C	-3.9243719	-1.9663739	-1.9181256
H	-3.6623494	-2.2652653	-2.9434021
H	-5.0158059	-1.8293339	-1.8678918
H	-3.6576519	-2.7928723	-1.2418720
C	-3.5245525	0.4630286	-2.5323628

H	-3.1960915	0.1753336	-3.5402747
H	-2.9907055	1.3839578	-2.2578457
H	-4.6048114	0.6716203	-2.5636583
C	0.0590046	1.2282964	-1.8346911
H	-0.0218217	0.7280985	0.3027956
Si	0.9411695	2.8073765	-1.6124044
C	2.7463906	2.7791168	-2.2393005
H	2.7829022	2.5907433	-3.3232142
H	3.2517313	3.7388289	-2.0438272
H	3.3120186	1.9803100	-1.7362488
C	0.0510226	4.2762043	-2.4452171
H	-0.9761163	4.3707509	-2.0620854
H	0.5804210	5.2249914	-2.2610113
H	-0.0080211	4.1219287	-3.5332639
C	1.0217228	3.1636885	0.2654911
H	0.0193393	3.1655335	0.7228282
H	1.6427049	2.4165196	0.7848261
H	1.4738214	4.1503019	0.4504691

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Comp 4' Energy = -1716.227678941

N	-0.8069954	0.6543913	0.0243103
N	1.4055952	0.7908359	-0.5343865
N	-0.0018779	2.3683178	-3.4982526
N	-0.0346210	2.5918064	-2.3672151
C	0.2818571	1.6429994	-0.1327866
C	-0.3755846	-0.5867442	-0.4786813
H	-1.0660743	-1.4161144	-0.5828567
C	0.9417546	-0.5215927	-0.7636338
H	1.6102607	-1.2857024	-1.1441268
C	2.7472956	1.0885936	-0.1236563
C	3.6782614	1.5358810	-1.0910602
C	4.9819274	1.8451770	-0.6747123
H	5.7084746	2.1959658	-1.4109557
C	5.3646865	1.7095183	0.6580416
H	6.3836509	1.9563038	0.9642057
C	4.4453991	1.2455187	1.5980132
H	4.7569914	1.1216571	2.6377975
C	3.1317760	0.9222894	1.2299289
C	2.1801626	0.3740043	2.2832276
H	1.1923251	0.2462767	1.8193347
C	2.6267566	-1.0208692	2.7555925
H	1.9037510	-1.4294414	3.4783361
H	3.6115478	-0.9798841	3.2458219
H	2.6960426	-1.7186343	1.9085638
C	2.0338869	1.3378511	3.4722902
H	1.3028052	0.9495572	4.1965098
H	1.6970666	2.3333347	3.1458935
H	2.9888195	1.4669404	4.0036174
C	3.3099038	1.6765965	-2.5574529
H	2.2708144	1.3409264	-2.6623236
C	4.1776999	0.7728606	-3.4494330
H	3.8435364	0.8394776	-4.4958139
H	4.1108859	-0.2792053	-3.1347859
H	5.2378955	1.0678476	-3.4163345
C	3.3804984	3.1422397	-3.0149302
H	3.0393361	3.2367020	-4.0563605
H	4.4092861	3.5312673	-2.9561457
H	2.7413219	3.7794760	-2.3869181
C	-2.1595867	1.0177443	0.2820809
C	-3.1329534	0.9835959	-0.7476345
C	-4.4522601	1.3427497	-0.4309397
H	-5.2131402	1.3165938	-1.2140276
C	-4.8055265	1.7572696	0.8492861
H	-5.8341540	2.0522364	1.0674419
C	-3.8391006	1.7889819	1.8559157

H	-4.1272545	2.0961960	2.8621300
C	-2.5179371	1.4029910	1.6020737
C	-1.5192414	1.2885069	2.7442527
H	-0.5233573	1.5390195	2.3540817
C	-1.4596917	-0.1743002	3.2266992
H	-0.7238899	-0.2884811	4.0376883
H	-1.1745916	-0.8496837	2.4077898
H	-2.4416039	-0.4913160	3.6099365
C	-1.7910417	2.2386927	3.9162078
H	-0.9559009	2.1968716	4.6306085
H	-2.7034707	1.9645595	4.4674160
H	-1.8981316	3.2804188	3.5789747
C	-2.8109596	0.5758612	-2.1771966
H	-1.7208856	0.4772259	-2.2670640
C	-3.4281159	-0.7942298	-2.5134751
H	-3.1503618	-1.1011333	-3.5329693
H	-4.5269773	-0.7535675	-2.4579544
H	-3.0883913	-1.5743353	-1.8163881
C	-3.2675866	1.6356815	-3.1936460
H	-2.9094748	1.3750901	-4.2000099
H	-2.8711099	2.6285327	-2.9399587
H	-4.3648198	1.7097567	-3.2348963
C	-0.0307110	2.8258319	-1.0960533
H	0.5033670	2.1489579	0.8243736
Si	-0.4660869	4.5705745	-0.4981438
C	0.3352858	4.7810241	1.2092511
H	1.4119451	4.5571377	1.1805818
H	0.2121064	5.8240393	1.5389850
H	-0.1346449	4.1385802	1.9684550
C	0.2463865	5.8148258	-1.7367298
H	-0.0455324	6.8390301	-1.4595400
H	1.3445247	5.7640359	-1.7632227
H	-0.1277269	5.6231748	-2.7537725
C	-2.3430619	4.7968907	-0.3648058
H	-2.8220254	4.6766797	-1.3478817
H	-2.7803316	4.0508320	0.3142484
H	-2.5862867	5.8021561	0.0133693

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TS_7 Energy = -1097.338570492

N	-0.3379499	1.3418831	1.8290607
N	0.5725767	-0.5700994	2.2650641
C	0.5932462	0.1616633	3.4472331
H	1.0303666	-0.2002044	4.3689769
C	0.0195246	1.3661165	3.1725805
H	-0.1247359	2.2245542	3.8158999
C	-1.0776117	2.4491794	1.1388700
C	-2.5842983	2.1904695	1.3006475
H	-3.1564842	2.9895001	0.8072252
H	-2.8619541	2.1725692	2.3649131
H	-2.8532204	1.2259585	0.8497772
C	-0.6965221	3.7900218	1.7844298
H	-1.1678201	4.6006399	1.2120431
H	0.3917591	3.9463813	1.7688316
H	-1.0545048	3.8747716	2.8202519
C	-0.6826054	2.4769276	-0.3409644
H	-1.1967590	3.3178713	-0.8277609
H	-0.9611965	1.5552151	-0.8621264
H	0.4016485	2.6199160	-0.4535502
C	1.0358207	-1.9920982	2.1521875
C	1.5650793	-2.2422688	0.7366052
H	1.9407194	-3.2738614	0.6767622
H	2.3916050	-1.5565465	0.5019626
H	0.7884315	-2.1147219	-0.0245128
C	-0.1584562	-2.9089440	2.4610846
H	0.1502085	-3.9621866	2.3916615

H	-0.9711999	-2.7249078	1.7457391
H	-0.5355279	-2.7258616	3.4783428
C	2.1684437	-2.2361582	3.1607585
H	2.5647647	-3.2486871	3.0041435
H	1.8225360	-2.1811365	4.2025343
H	2.9914047	-1.5204782	3.0192923
C	-0.0124744	0.1440344	1.2574668
N	-1.4857510	-0.7941424	0.2022071
N	-1.2430936	-0.9487936	-0.9585534
C	-0.3724234	-0.7511055	-1.9176239
H	0.5399435	-0.2405057	-1.5494489
Si	-0.6151259	-1.3142654	-3.6816683
C	0.1234236	0.0038692	-4.8367416
H	1.1867841	0.1716277	-4.6053060
H	0.0533505	-0.3074664	-5.8902584
H	-0.4034967	0.9628289	-4.7230745
C	-2.4713374	-1.5387322	-4.0123738
H	-2.6454432	-1.9166113	-5.0313079
H	-2.9071311	-2.2576823	-3.3024282
H	-3.0073908	-0.5848696	-3.9005581
C	0.2800963	-2.9633701	-4.0169651
H	-0.1253346	-3.7602378	-3.3753264
H	0.1669845	-3.2750888	-5.0673823
H	1.3556703	-2.8721202	-3.8017778

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Comp 7 Energy = -1097.398411305

N	-0.0112142	1.5332339	1.4188708
N	-0.0319472	-0.3519335	2.6125497
C	-0.0634873	0.7155016	3.4987022
H	-0.0927205	0.5869530	4.5709724
C	-0.0537919	1.8599146	2.7765435
H	-0.0744121	2.8803085	3.1291115
C	0.0420207	2.5779893	0.3360358
C	-1.2344160	2.4959428	-0.5151748
H	-1.2107429	3.2777241	-1.2892724
H	-2.1211234	2.6588679	0.1152034
H	-1.2994339	1.5189591	-1.0069859
C	0.1019990	3.9736909	0.9794428
H	0.1532265	4.7108451	0.1669882
H	0.9961856	4.1068635	1.6053636
H	-0.7959841	4.2002191	1.5723719
C	1.3190997	2.3871927	-0.4985941
H	1.3798442	3.1832446	-1.2555437
H	1.3073399	1.4201308	-1.0127284
H	2.2083136	2.4549070	0.1455096
C	-0.0367623	-1.7993226	3.0050334
C	1.2622367	-2.4639134	2.5171984
H	1.2672299	-3.5212180	2.8194651
H	2.1371852	-1.9710420	2.9669256
H	1.3347616	-2.4004709	1.4253290
C	-1.2770616	-2.4867447	2.4078747
H	-1.2940144	-3.5412324	2.7193381
H	-1.2524259	-2.4344886	1.3135465
H	-2.1957528	-2.0033746	2.7722365
C	-0.1022622	-1.9044421	4.5352890
H	-0.1069582	-2.9698774	4.8010092
H	-1.0201131	-1.4557925	4.9424661
H	0.7716044	-1.4451637	5.0199952
C	-0.0001191	0.1324216	1.3030348
N	0.0529095	-0.7504190	0.3108228
N	-0.0348608	-0.3156682	-0.9753222
C	0.0833134	-1.2439229	-1.8847528
H	0.2521876	-2.2870810	-1.5465610
Si	0.0026571	-0.8343924	-3.7246105
C	-1.2708039	-1.9814319	-4.5515261

H	-2.2789045	-1.8052711	-4.1477143
H	-1.3013387	-1.8132385	-5.6391145
H	-1.0162279	-3.0382798	-4.3791659
C	1.7065559	-1.1652825	-4.5080833
H	1.6772894	-0.9984269	-5.5961426
H	2.4701016	-0.4997208	-4.0783437
H	2.0243559	-2.2041265	-4.3321812
C	-0.4792174	0.9807844	-3.9867519
H	0.2366727	1.6499260	-3.4884485
H	-0.4907970	1.2217372	-5.0605804
H	-1.4771320	1.1888855	-3.5749429

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$TS_{7'}$ Energy = -1097.341440323

N	8.2316775	4.8958211	7.6430019
N	7.0930733	4.1913024	9.3463435
C	6.8826572	5.5600503	9.2626230
H	6.2585068	6.1074643	9.9585461
C	7.5968542	6.0025891	8.1914781
H	7.7018150	7.0035449	7.7916628
C	9.3195091	5.0173966	6.6129152
C	8.7477441	5.6523191	5.3394983
H	9.5536043	5.7685392	4.6013673
H	8.3316915	6.6509418	5.5374293
H	7.9637759	5.0170083	4.9051569
C	10.4128309	5.9150413	7.2244803
H	11.2555120	5.9955631	6.5242574
H	10.7823229	5.4856770	8.1669544
H	10.0438598	6.9311597	7.4250214
C	9.9092456	3.6362098	6.3173486
H	10.7364105	3.7614945	5.6039310
H	9.1759310	2.9563591	5.8703605
H	10.3054950	3.1715724	7.2314269
C	6.6426477	3.3625439	10.5078707
C	7.0902767	1.9163972	10.2976376
H	6.7564950	1.3135797	11.1530005
H	8.1833719	1.8413168	10.2211663
H	6.6505672	1.4974580	9.3867789
C	5.1135027	3.4409595	10.6164144
H	4.7725575	2.8195290	11.4570380
H	4.6380095	3.0729972	9.6973972
H	4.7709304	4.4694389	10.8005898
C	7.3142540	3.9323695	11.7700393
H	7.0389249	3.3227269	12.6416131
H	7.0028029	4.9678015	11.9664488
H	8.4079437	3.9121338	11.6620792
C	7.9110204	3.7650486	8.3386436
N	6.6386024	3.0601391	4.7131632
N	6.7394894	2.3987280	5.6705083
C	6.9319108	1.7407505	6.7481655
H	7.6436858	2.6328930	7.6947623
Si	5.9684283	0.1530527	6.9570319
C	5.5775625	-0.5803831	5.2452053
H	6.5009432	-0.8592665	4.7163805
H	4.9496801	-1.4797996	5.3405238
H	5.0372414	0.1477494	4.6214408
C	4.3034455	0.4684911	7.8398655
H	3.6837324	-0.4420110	7.8446829
H	4.4437204	0.7861037	8.8835203
H	3.7454504	1.2604264	7.3174453
C	6.9540766	-1.1219720	7.9660912
H	7.2370498	-0.7388950	8.9570580
H	6.3463092	-2.0283314	8.1153118
H	7.8746017	-1.4087692	7.4369348

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Comp 7' Energy = -1097.370555239

N	-0.6937940	1.0774649	-1.0381119
N	-0.5389590	0.1992160	1.1330509
C	-1.6511879	1.0583579	1.0192519
H	-2.3897168	1.1213239	1.8121789
C	-1.7396539	1.5628819	-0.2269970
H	-2.5653958	2.1204168	-0.6575510
C	-0.0073160	1.9993619	-1.9868719
C	-1.0796079	2.7741648	-2.7687898
H	-0.5980570	3.3560528	-3.5670267
H	-1.6260889	3.4801037	-2.1279038
H	-1.7997719	2.0813889	-3.2282868
C	0.9024259	2.9960448	-1.2402919
H	1.3413359	3.7226577	-1.9400749
H	1.7343849	2.4838978	-0.7332879
H	0.3224350	3.5446407	-0.4832460
C	0.8140409	1.1690179	-2.9820368
H	1.2839269	1.8299749	-3.7247757
H	0.1720180	0.4447810	-3.5029507
H	1.6158329	0.6139300	-2.4785058
C	0.3033280	0.2449760	2.3618038
C	1.2032359	-0.9967719	2.3956698
H	1.7933799	-1.0068739	3.3236198
H	1.9085529	-1.0086639	1.5545009
H	0.5989630	-1.9132369	2.3459328
C	-0.6250780	0.2041650	3.5854567
H	-0.0216320	0.0972720	4.4976947
H	-1.3128959	-0.6515590	3.5203037
H	-1.2148349	1.1261749	3.6849827
C	1.1568129	1.5277719	2.4092418
H	1.7138139	1.5897569	3.3557948
H	0.5126260	2.4154628	2.3224588
H	1.8928199	1.5565009	1.5910859
C	0.1125120	0.1568070	-0.1991430
N	-2.0020409	-2.3398138	-1.0874119
N	-0.9699689	-1.8489219	-0.9494429
C	0.1795480	-1.2740739	-0.7853539
H	1.1619379	0.4956510	-0.1365990
Si	1.6986379	-2.2895238	-1.2898539
C	1.5675669	-2.7461268	-3.1267648
H	1.5874419	-1.8463439	-3.7585357
H	2.4017158	-3.3993708	-3.4255918
H	0.6283860	-3.2827508	-3.3296528
C	1.7594569	-3.8836947	-0.2630430
H	2.5900768	-4.5277677	-0.5904900
H	1.8940209	-3.6601667	0.8049609
H	0.8245899	-4.4527757	-0.3757260
C	3.2720378	-1.2676059	-0.9934419
H	3.4115068	-0.9937459	0.0617200
H	4.1355397	-1.8833609	-1.2900569
H	3.2998438	-0.3486590	-1.5950009

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TS_{14} Energy = -1034.459009204

N	-0.2917298	1.3931519	1.9619184
N	0.6059347	-0.5160276	2.4039217
C	0.5196839	0.1705472	3.6109627
H	0.8835130	-0.2198655	4.5529411
C	-0.0477451	1.3771263	3.3317982
H	-0.2587251	2.2099313	3.9906405
C	-0.9806967	2.5137335	1.2437442
C	-2.4933313	2.2420298	1.2703701
H	-3.0302799	3.0511497	0.7546206
H	-2.8605837	2.1888395	2.3059206
H	-2.7198805	1.2917027	0.7688098
C	-0.6659824	3.8398585	1.9515024
H	-1.0966865	4.6632655	1.3655687

H	0.4186295	4.0038843	2.0278645
H	-1.1062942	3.8922909	2.9570451
C	-0.4655998	2.5812839	-0.1979152
H	-0.9380130	3.4344049	-0.7049652
H	-0.7056465	1.6731281	-0.7596615
H	0.6244166	2.7210516	-0.2183645
C	1.1033758	-1.9236298	2.2715834
C	1.7375310	-2.1074089	0.8886453
H	2.1376591	-3.1285184	0.8133823
H	2.5615397	-1.3960137	0.7379586
H	1.0094895	-1.9642024	0.0840880
C	-0.0912245	-2.8734213	2.4550982
H	0.2424889	-3.9180326	2.3731349
H	-0.8522463	-2.6834648	1.6866321
H	-0.5502758	-2.7342951	3.4452544
C	2.1645934	-2.1909609	3.3493844
H	2.5900100	-3.1902626	3.1845047
H	1.7425490	-2.1808140	4.3639776
H	2.9822862	-1.4574025	3.2958543
C	0.0964419	0.2230168	1.3743764
N	-1.4242724	-0.8152485	-0.0039724
N	-1.0509481	-0.8960931	-1.1049807
C	-0.1737596	-0.7041877	-2.0648127
H	0.7471602	-0.1923845	-1.7684266
C	-0.4486147	-1.1593605	-3.4109375
O	-1.4628205	-1.7447990	-3.7849653
O	0.6162716	-0.8300862	-4.2119454
C	0.6253965	-1.1812215	-5.6499693
C	0.5760192	-2.7014700	-5.8240315
H	-0.3892627	-3.1062567	-5.4992009
H	0.7275239	-2.9512874	-6.8846333
H	1.3783712	-3.1776034	-5.2416981
C	1.9734007	-0.6296012	-6.1158860
H	2.1097238	-0.8292246	-7.1883021
H	2.0234037	0.4563846	-5.9528551
H	2.7968256	-1.1047456	-5.5639664
C	-0.5240477	-0.4774493	-6.3758676
H	-0.4948277	0.6036971	-6.1758444
H	-0.4163511	-0.6284185	-7.4603528
H	-1.4952903	-0.8728408	-6.0576410

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Comp 14 Energy = -1034.517239759

O	6.5623812	5.9813016	9.3341681
O	8.1093353	6.1103459	11.0390188
N	2.2428572	8.6853307	10.2655285
N	2.3440331	9.6561425	12.2702315
N	4.2752508	8.4361955	11.7663779
N	4.9462168	7.6490878	10.9230061
C	3.0571785	8.8518734	11.3904825
C	1.1207313	9.9759547	11.7052146
H	0.3872480	10.5933086	12.2032033
C	1.0584805	9.3859551	10.4866066
H	0.2567444	9.4157198	9.7641594
C	2.5021520	7.9174771	8.9846197
C	2.6757838	6.4245550	9.3031667
H	2.7767750	5.8683112	8.3603413
H	1.7933155	6.0428505	9.8379298
H	3.5801194	6.2558780	9.8972329
C	3.7252838	8.5105375	8.2690137
H	3.8557148	8.0016311	7.3031110
H	4.6348287	8.3566006	8.8592370
H	3.5737528	9.5834390	8.0784914
C	1.2844962	8.0706516	8.0575949
H	1.4995123	7.5086370	7.1393538
H	1.1052989	9.1166635	7.7693660

H	0.3682575	7.6483999	8.4946683
C	2.8144598	10.1081186	13.6255225
C	1.7282470	10.9846865	14.2642027
H	2.0916644	11.3064690	15.2489340
H	0.7889072	10.4346293	14.4202063
H	1.5251172	11.8892492	13.6729792
C	3.0489959	8.8767216	14.5162530
H	3.3674894	9.2077260	15.5152583
H	3.8268353	8.2341200	14.0878312
H	2.1202571	8.2969934	14.6227897
C	4.0963751	10.9426659	13.4665496
H	4.4216210	11.2979150	14.4549960
H	3.9082472	11.8188435	12.8286226
H	4.8954585	10.3392775	13.0215144
C	6.1301744	7.2658781	11.3222774
H	6.5509787	7.5712140	12.2896399
C	6.9088117	6.3966762	10.4364339
C	9.1055214	5.2354472	10.3811438
C	10.2433693	5.1993391	11.4020163
H	11.0629853	4.5692171	11.0282254
H	9.8913415	4.7858895	12.3576315
H	10.6336724	6.2111349	11.5814101
C	9.5793931	5.8653127	9.0683681
H	10.4163787	5.2769134	8.6639864
H	9.9342136	6.8911563	9.2449427
H	8.7730053	5.8901189	8.3264476
C	8.5242933	3.8341768	10.1734104
H	9.3180070	3.1604034	9.8180221
H	7.7131841	3.8457375	9.4361637
H	8.1376661	3.4377967	11.1235038

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$TS_{Int1'}$ Energy = -1528.648750409

O	-2.5253568	-0.4429627	-2.6722660
O	-1.9346751	1.3876733	-1.3942534
O	0.0360549	0.1220380	3.2941312
N	-0.2516150	-0.7367153	0.1414296
N	0.2226876	0.5088613	0.2831289
N	-2.6440262	-0.1310277	0.8233644
N	-2.0686017	0.8204845	1.4522049
C	-2.0710536	-0.6945887	-0.3412457
C	-2.1948330	0.0667034	-1.5924263
C	-2.4531648	2.4364981	-2.3090887
C	-1.8218679	2.3449493	-3.6994626
H	-2.1731876	3.1936107	-4.3053331
H	-2.1018891	1.4110934	-4.1996003
H	-0.7273800	2.4034264	-3.6352662
C	-3.9766863	2.3190601	-2.3672220
H	-4.3887344	3.1689003	-2.9303758
H	-4.3981838	2.3356967	-1.3521332
H	-4.2820577	1.3899924	-2.8652906
C	-2.0257042	3.7221936	-1.6027251
H	-2.3578123	4.5967977	-2.1798383
H	-0.9311477	3.7611243	-1.5073706
H	-2.4676223	3.7736125	-0.5980781
C	-0.6749431	1.1903454	1.2062866
H	-0.7116542	2.2490754	0.9093445
C	0.0605592	1.0930294	2.5548115
O	0.8052174	2.2110101	2.7314491
N	1.1058170	-1.6352096	-1.8499131
N	0.4469047	-2.9616692	-0.1965292
C	0.4348234	-1.6538429	-0.6343569
C	1.0574141	-3.7491128	-1.1481587
H	1.1747554	-4.8175998	-1.0435024
C	1.4555686	-2.9375355	-2.1608558
H	1.9552211	-3.1974700	-3.0836695

C	1.7918921	2.3066606	3.8430641
C	1.0660086	2.2760718	5.1888143
H	0.6034589	1.2988742	5.3688493
H	1.7863760	2.4822278	5.9940206
H	0.2857591	3.0505329	5.2194774
C	2.4272596	3.6743818	3.5973217
H	3.1824375	3.8795900	4.3690235
H	2.9141629	3.7031194	2.6123969
H	1.6656782	4.4661122	3.6346581
C	2.8322512	1.1930067	3.7118237
H	3.2525365	1.1840820	2.6956970
H	3.6506281	1.3768383	4.4232789
H	2.3945244	0.2106046	3.9238044
C	0.1623734	-3.4537208	1.2207879
C	1.4503202	-0.5517807	-2.8718656
C	0.3751318	-4.9740104	1.2561755
H	1.4155456	-5.2608075	1.0476011
H	0.1406977	-5.3137445	2.2730382
H	-0.2981240	-5.5047110	0.5669742
C	1.1775670	-2.7720348	2.1486027
H	1.0178526	-1.6889004	2.1808081
H	1.0445841	-3.1581255	3.1692164
H	2.2060656	-2.9920632	1.8258646
C	-1.2784096	-3.1539106	1.6456961
H	-1.9979518	-3.5738001	0.9284150
H	-1.4537245	-3.6338844	2.6191164
H	-1.4565666	-2.0820700	1.7624139
C	1.3377425	0.8592459	-2.3088619
H	1.6035385	1.5521458	-3.1206650
H	0.3357527	1.0991930	-1.9477361
H	2.0241172	1.0128846	-1.4683279
C	0.5098920	-0.7420603	-4.0717201
H	0.7538901	0.0077611	-4.8372518
H	0.6302072	-1.7377873	-4.5231619
H	-0.5397907	-0.6146914	-3.7763115
C	2.9179877	-0.7730670	-3.2891007
H	3.0759578	-1.6957763	-3.8628355
H	3.2162076	0.0627140	-3.9358677
H	3.5788608	-0.7799801	-2.4110020
H	-2.3993722	-1.7264003	-0.4904277

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Int1' Energy = -1528.669939633

O	-1.6390025	0.7112885	-3.1771479
O	-0.5602718	2.1773544	-1.7720740
O	-0.9334933	-0.2531754	2.9423961
N	-0.2432586	-0.3179439	-0.1995827
N	0.5975632	0.5918118	0.4700521
N	-2.2553057	1.1069214	0.1193969
N	-1.6312335	1.7570322	1.0028149
C	-1.4827228	0.2293265	-0.8043608
C	-1.2393688	1.0548632	-2.0677298
C	-0.4576250	3.3232446	-2.7205597
C	0.3388068	2.9439027	-3.9675989
H	0.4758715	3.8418876	-4.5882714
H	-0.1854899	2.1847017	-4.5590934
H	1.3323841	2.5657432	-3.6925275
C	-1.8688544	3.8020175	-3.0603581
H	-1.8052265	4.7330355	-3.6419836
H	-2.4339186	4.0048184	-2.1397610
H	-2.4102748	3.0557553	-3.6548720
C	0.2915848	4.3586795	-1.8844472
H	0.4238231	5.2826492	-2.4646085
H	1.2814688	3.9776798	-1.5967366
H	-0.2709725	4.5918873	-0.9699553
C	-0.2205336	1.4216723	1.2986101

H	0.2825835	2.3939030	1.4154057
C	-0.2740932	0.7453146	2.6777112
O	0.6078276	1.3535599	3.5140825
N	1.3718231	-1.6368994	-1.6047528
N	-0.3227456	-2.6854567	-0.6086409
C	0.2690274	-1.4471891	-0.7821545
C	0.3655209	-3.6115979	-1.3726634
H	0.0817797	-4.6520019	-1.4320959
C	1.4057368	-2.9760172	-1.9625302
H	2.1544114	-3.3755664	-2.6314467
C	0.9205307	0.7744866	4.8477282
C	-0.3285097	0.7835413	5.7310095
H	-1.0906561	0.0960274	5.3467835
H	-0.0543193	0.4763726	6.7513649
H	-0.7534878	1.7964514	5.7790564
C	1.9733105	1.7426353	5.3863544
H	2.2891598	1.4303802	6.3918755
H	2.8551821	1.7589036	4.7306029
H	1.5642565	2.7608181	5.4481536
C	1.5088183	-0.6285792	4.6827393
H	2.3331405	-0.6120075	3.9546366
H	1.9076668	-0.9715308	5.6485276
H	0.7483430	-1.3406122	4.3423153
C	-1.1747767	-3.1548738	0.5765158
C	2.2954830	-0.6820021	-2.3590992
C	-1.6615829	-4.5826648	0.2824004
H	-0.8476057	-5.3206076	0.2761119
H	-2.3488922	-4.8698515	1.0881626
H	-2.2156549	-4.6389234	-0.6659560
C	-0.2405117	-3.1541455	1.7944710
H	0.1068532	-2.1381440	2.0147846
H	-0.7888174	-3.5172795	2.6751872
H	0.6209948	-3.8157549	1.6205046
C	-2.4049036	-2.2775881	0.8133611
H	-3.0440255	-2.2335047	-0.0794689
H	-2.9916258	-2.7422716	1.6184330
H	-2.1435085	-1.2727043	1.1550774
C	2.5004269	0.6510037	-1.6487273
H	3.1396806	1.2683638	-2.2969477
H	1.5694167	1.1842187	-1.4381111
H	3.0039671	0.5111950	-0.6841960
C	1.6751537	-0.4863783	-3.7524709
H	2.3224173	0.1730333	-4.3474836
H	1.5835939	-1.4454507	-4.2820945
H	0.6802090	-0.0292875	-3.6891420
C	3.6749935	-1.3593265	-2.4785777
H	3.6847077	-2.2235440	-3.1564741
H	4.3764533	-0.6226691	-2.8919240
H	4.0487648	-1.6699482	-1.4931770
H	-2.1409969	-0.5927179	-1.0974554

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$TS_{14'}$ Energy = -1034.463158091

N	8.7342448	4.6839546	7.9688178
N	7.1182139	4.3206601	9.3591310
C	7.8152639	5.4222324	9.8358681
H	7.5512127	5.9508279	10.7424664
C	8.8324290	5.6550190	8.9558311
H	9.5972674	6.4203983	8.9689285
C	9.6273557	4.5386235	6.7694567
C	8.8308271	4.9564503	5.5245159
H	9.4681360	4.8771719	4.6324523
H	8.4842300	5.9963820	5.6126519
H	7.9588937	4.3065713	5.3793897
C	10.8541831	5.4416162	6.9362096
H	11.5201969	5.2819636	6.0784327

H	11.4161449	5.1987361	7.8497405
H	10.5851580	6.5079338	6.9509105
C	10.0672691	3.0707281	6.6756383
H	10.7359529	2.9469478	5.8121103
H	9.2043886	2.4041348	6.5425821
H	10.6093284	2.7686796	7.5832388
C	5.9525594	3.6453794	10.0282754
C	6.4017188	2.2378118	10.4469278
H	5.5675351	1.7173063	10.9391342
H	7.2399838	2.2968813	11.1571726
H	6.7185375	1.6413833	9.5794054
C	4.7918606	3.5802272	9.0260119
H	3.9239417	3.1046371	9.5038997
H	5.0651130	2.9856150	8.1434435
H	4.5002612	4.5888791	8.6988424
C	5.5310981	4.4536963	11.2594280
H	4.6696395	3.9526981	11.7202468
H	5.2229368	5.4757995	10.9946940
H	6.3289781	4.5015831	12.0151533
C	7.6799797	3.8627348	8.2104609
N	5.4566687	2.9226788	4.5322549
N	5.9820775	2.3930572	5.4140588
C	6.6269673	1.9635181	6.4429152
H	7.1623945	2.8833949	7.3103326
C	6.6265228	0.5720271	6.8194337
O	7.2174240	0.1373812	7.8141383
O	5.8891492	-0.2111519	5.9584777
C	5.6949465	-1.6558344	6.2057853
C	4.8107145	-2.0728145	5.0295782
H	5.3214985	-1.8773496	4.0761298
H	4.5821798	-3.1464547	5.0918369
H	3.8662871	-1.5109152	5.0400275
C	4.9615729	-1.8713158	7.5327669
H	5.5889805	-1.5771453	8.3820571
H	4.0330295	-1.2822950	7.5519181
H	4.6962852	-2.9340972	7.6371832
C	7.0352202	-2.3947807	6.1596144
H	7.5598061	-2.1713296	5.2189507
H	7.6744036	-2.1050277	7.0012644
H	6.8556131	-3.4792733	6.2030166

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Comp 14' Energy = -1034.480475694

N	8.4496201	4.1329996	7.5909851
N	6.8370506	3.9831476	9.1454451
C	6.7929136	5.2687506	8.5819852
H	6.1244719	6.0406098	8.9436382
C	7.7668359	5.3592523	7.6420987
H	8.0748438	6.2217752	7.0636769
C	9.4855906	3.8018305	6.5883139
C	8.8949145	3.6408612	5.1697820
H	9.7049345	3.5143524	4.4364116
H	8.3118133	4.5298918	4.8880429
H	8.2404106	2.7617076	5.1045914
C	10.5156997	4.9461383	6.5813937
H	11.3513947	4.6828171	5.9178216
H	10.9096221	5.1171044	7.5933038
H	10.0847823	5.8867842	6.2108299
C	10.1918230	2.5066697	7.0156823
H	11.0056397	2.2882750	6.3104574
H	9.5118209	1.6436829	7.0217673
H	10.6253063	2.6132373	8.0213260
C	5.8373735	3.4641935	10.1043892
C	6.3537228	2.1424902	10.6918548
H	5.6475359	1.7846580	11.4541294
H	7.3342572	2.2848500	11.1701619

H	6.4517458	1.3574731	9.9295454
C	4.4554788	3.2483252	9.4490361
H	3.7145467	2.9746609	10.2142232
H	4.4863700	2.4420597	8.7040201
H	4.1118700	4.1675341	8.9523937
C	5.7030246	4.4913095	11.2435667
H	5.0336095	4.0942071	12.0197545
H	5.2745334	5.4407174	10.8929281
H	6.6840021	4.6971511	11.6949366
C	7.5885123	3.1532890	8.2239977
N	5.1018698	3.4152326	5.6857732
N	5.8413126	2.8932182	6.3979054
C	6.6796253	2.3168013	7.2044672
H	8.1484324	2.3549337	8.7271588
C	6.8033224	0.8675457	7.1936802
O	7.5890365	0.2521278	7.9179231
O	5.9521787	0.2979357	6.2984275
C	5.9081612	-1.1752958	6.1037469
C	4.8302548	-1.3263778	5.0314600
H	5.1175095	-0.7907364	4.1157500
H	4.6934838	-2.3893370	4.7877955
H	3.8722951	-0.9216444	5.3868320
C	5.4841370	-1.8647155	7.4021133
H	6.2546475	-1.7675145	8.1756840
H	4.5448969	-1.4311063	7.7747044
H	5.3134798	-2.9336195	7.2058626
C	7.2601471	-1.6747585	5.5913704
H	7.5636573	-1.1059482	4.7003082
H	8.0371717	-1.5789989	6.3585842
H	7.1716322	-2.7336405	5.3074780

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TS_{Int1} Energy = -1528.681832189

N	3.5122379	-0.5268333	-1.2491729
N	3.4100767	-1.8797080	0.4639039
C	4.3147172	-2.4214009	-0.4344159
H	4.8441601	-3.3456725	-0.2445011
C	4.3787341	-1.5751625	-1.5046170
H	4.9747368	-1.6354477	-2.4049129
C	3.1786360	0.6192661	-2.1782778
C	3.1836346	1.9130973	-1.3554631
H	2.9190102	2.7522935	-2.0121547
H	4.1787726	2.1008693	-0.9269179
H	2.4401031	1.8852674	-0.5474448
C	4.2449057	0.6892403	-3.2751635
H	4.0302994	1.5652457	-3.9002584
H	4.2245274	-0.1928929	-3.9311448
H	5.2555420	0.8108867	-2.8585416
C	1.7966206	0.3333897	-2.7804944
H	1.5426240	1.1288395	-3.4941828
H	1.0174443	0.3306240	-2.0062084
H	1.7993074	-0.6286179	-3.3135952
C	2.9721573	-2.5373202	1.7500363
C	1.9512473	-3.6247709	1.3814072
H	1.6144442	-4.1318583	2.2959656
H	2.3943457	-4.3777073	0.7132133
H	1.0765901	-3.1771608	0.8898563
C	2.3319265	-1.4848625	2.6551081
H	2.0773658	-1.9548212	3.6140045
H	1.4034905	-1.1002631	2.2175474
H	3.0165994	-0.6490481	2.8572529
C	4.2098635	-3.1387021	2.4277254
H	3.9056468	-3.5597137	3.3949726
H	4.9738877	-2.3704259	2.6124007
H	4.6567034	-3.9548387	1.8429455
C	2.9242061	-0.7356892	-0.0547866

N	0.5204836	1.3165484	3.5038314
N	0.4531439	1.3541392	2.3485380
C	0.4576161	1.2372137	1.0700507
H	2.1583963	-0.0885681	0.3905820
C	-0.1215634	2.2442156	0.2087012
O	-0.2419131	2.1186884	-1.0117352
O	-0.5130068	3.3651299	0.9067932
C	-1.1807091	4.4950586	0.2199109
C	-1.4453245	5.4661448	1.3709274
H	-0.5017365	5.7633233	1.8502371
H	-1.9470998	6.3682762	0.9929494
H	-2.0888248	4.9975596	2.1287518
C	-2.4978872	4.0305001	-0.4064227
H	-2.3214594	3.3365172	-1.2356613
H	-3.1238354	3.5302113	0.3470681
H	-3.0512339	4.9033942	-0.7839238
C	-0.2367405	5.1238314	-0.8092442
H	0.7208538	5.3867403	-0.3352733
H	-0.0468090	4.4352739	-1.6404506
H	-0.6879770	6.0461747	-1.2042442
N	-0.1248680	-0.6642618	0.4193327
N	-1.3039963	-0.7337323	0.3048459
C	-2.4752050	-0.1497994	0.4451041
C	-3.7171804	-0.7873429	0.0765906
O	-4.8169551	-0.2473217	0.2132225
O	-3.5243508	-2.0455075	-0.4396780
C	-4.6685186	-2.8716281	-0.8733827
C	-3.9848108	-4.1507710	-1.3599437
H	-3.4159652	-4.6170445	-0.5431159
H	-4.7381095	-4.8673229	-1.7172208
H	-3.2930001	-3.9272592	-2.1842934
C	-5.4141437	-2.1912744	-2.0250193
H	-5.9162897	-1.2782877	-1.6853132
H	-4.7119701	-1.9339408	-2.8312466
H	-6.1679128	-2.8820700	-2.4321313
C	-5.5899740	-3.1742831	0.3120665
H	-5.0120819	-3.6082113	1.1412480
H	-6.0907107	-2.2654411	0.6646699
H	-6.3523105	-3.9055565	0.0049594
H	-2.4959769	0.8644095	0.8531614

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Int1 Energy = -1528.724698442

N	1.0671951	0.6774584	3.1657878
N	-0.1657995	-1.0795610	2.7696773
C	0.0975588	-1.0626058	4.1296454
H	-0.2780946	-1.8150778	4.8094299
C	0.8759667	0.0340275	4.3770165
H	1.2956851	0.3933031	5.3067854
C	1.9074463	1.9039652	2.9044395
C	1.1041991	2.8461790	1.9977700
H	1.7022634	3.7479964	1.8074064
H	0.1658630	3.1495506	2.4842384
H	0.8649504	2.3794972	1.0293145
C	2.2162593	2.5867511	4.2392624
H	2.7772686	3.5072546	4.0310777
H	2.8431927	1.9614633	4.8912669
H	1.2982035	2.8660078	4.7763443
C	3.2016169	1.4419596	2.2192828
H	3.8275820	2.3169523	1.9940852
H	2.9840180	0.9121627	1.2821470
H	3.7720426	0.7683804	2.8755706
C	-1.0500090	-2.0563619	2.0279597
C	-0.3110813	-2.5037393	0.7606663
H	-0.9455471	-3.2156160	0.2157366
H	0.6389173	-2.9962871	1.0112153

H	-0.0952935	-1.6608538	0.0936116
C	-2.3583372	-1.3310957	1.6856052
H	-3.0329742	-2.0290478	1.1701219
H	-2.1851743	-0.4788298	1.0126750
H	-2.8597607	-0.9794056	2.5998920
C	-1.3199475	-3.2613018	2.9328495
H	-1.9151415	-3.9870361	2.3635925
H	-1.9024561	-2.9891734	3.8249595
H	-0.3888765	-3.7583098	3.2427279
C	0.4304236	-0.0144220	2.2007956
N	0.8145711	1.9024545	-3.7573875
N	1.0511843	1.2514760	-2.8386001
C	1.1201945	0.5703850	-1.7161890
H	0.4175747	0.2574101	1.1244528
C	2.3236843	-0.1859811	-1.4059492
O	2.4923111	-0.7589048	-0.3285645
O	3.2151493	-0.1629236	-2.4377296
C	4.5139090	-0.8736222	-2.3480470
C	5.1515654	-0.5616072	-3.7014422
H	5.2806670	0.5226524	-3.8271184
H	6.1373158	-1.0428769	-3.7695684
H	4.5211464	-0.9348918	-4.5204866
C	4.2791171	-2.3775792	-2.1917952
H	3.8192589	-2.6082708	-1.2237245
H	3.6255453	-2.7461028	-2.9954394
H	5.2414944	-2.9051330	-2.2622697
C	5.3557777	-0.2947612	-1.2078812
H	5.4319966	0.7977311	-1.3069920
H	4.9213554	-0.5353881	-0.2309645
H	6.3710306	-0.7150040	-1.2580913
N	0.1763072	0.8311305	-0.6638449
N	-1.1091450	0.7004313	-0.8530487
C	-1.6955544	0.3470605	-1.9843061
C	-3.1319669	0.1523837	-2.0726408
O	-3.6848989	-0.2772772	-3.0911432
O	-3.8019539	0.4845707	-0.9215229
C	-5.2667030	0.3456946	-0.8326455
C	-5.5588610	0.8198658	0.5926975
H	-5.2149166	1.8546097	0.7315735
H	-6.6396448	0.7786550	0.7898000
H	-5.0435387	0.1815587	1.3243188
C	-5.6835445	-1.1188871	-1.0022980
H	-5.4855761	-1.4689579	-2.0217148
H	-5.1324552	-1.7548745	-0.2935369
H	-6.7585340	-1.2223213	-0.7904489
C	-5.9579893	1.2599647	-1.8490819
H	-5.5956094	2.2923948	-1.7371268
H	-5.7659317	0.9251961	-2.8745328
H	-7.0434774	1.2545860	-1.6683513
H	-1.1474168	0.1200236	-2.9055314

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TS_{13} Energy = -1528.718960464

N	0.9091052	1.1154245	2.8169792
N	-0.4210207	-0.6112343	2.9227197
C	-0.2539551	-0.1443035	4.2160546
H	-0.7297481	-0.6032678	5.0721457
C	0.5847929	0.9346306	4.1508199
H	0.9641613	1.5693161	4.9403010
C	1.8526242	2.1342184	2.2246267
C	1.1376029	2.8147968	1.0490519
H	1.8108344	3.5616762	0.6061158
H	0.2266589	3.3277928	1.3893541
H	0.8646902	2.0904449	0.2681444
C	2.2095495	3.1641729	3.2989928
H	2.8618978	3.9210551	2.8439941

H	2.7615499	2.7144051	4.1368381
H	1.3169797	3.6775784	3.6846301
C	3.1078295	1.3841441	1.7547715
H	3.8122870	2.1000976	1.3084010
H	2.8650640	0.6237698	0.9999872
H	3.6070854	0.8917444	2.6022026
C	-1.3039523	-1.7525814	2.4706603
C	-0.4985030	-2.6114191	1.4862559
H	-1.1286223	-3.4449295	1.1469136
H	0.3976528	-3.0259192	1.9696603
H	-0.1893675	-2.0409185	0.6010105
C	-2.5467590	-1.1477779	1.8009944
H	-3.2198798	-1.9607060	1.4928698
H	-2.2782656	-0.5691705	0.9032833
H	-3.0906953	-0.5004980	2.5049606
C	-1.6967476	-2.5839840	3.6945955
H	-2.2809778	-3.4459616	3.3472608
H	-2.3307354	-2.0195599	4.3935871
H	-0.8157209	-2.9672171	4.2298808
C	0.2906524	0.1676892	2.0862255
N	-0.1077028	1.1796851	-3.5907738
N	0.7613038	0.6985158	-2.9816782
C	1.0688651	-0.0879611	-1.9188712
H	0.3545090	0.0754415	0.9754262
C	2.4320846	-0.5293513	-1.6917575
O	2.7805652	-1.1103883	-0.6614189
O	3.2467587	-0.2385130	-2.7476555
C	4.6687824	-0.6519327	-2.7525355
C	5.1570038	-0.1351584	-4.1058179
H	5.0390588	0.9558542	-4.1678875
H	6.2198587	-0.3818195	-4.2399261
H	4.5842784	-0.5950387	-4.9232776
C	4.7780363	-2.1769267	-2.6845178
H	4.4367152	-2.5567406	-1.7147688
H	4.1757810	-2.6373301	-3.4810859
H	5.8270029	-2.4732336	-2.8333948
C	5.4207387	0.0357897	-1.6094197
H	5.2556521	1.1227234	-1.6461966
H	5.0917747	-0.3424785	-0.6348959
H	6.4994116	-0.1510624	-1.7186362
N	0.1817721	0.0188618	-0.8492528
N	-1.1175036	0.0225715	-1.0619613
C	-1.6413997	-0.3338783	-2.2412548
C	-3.0899820	-0.3583050	-2.4243852
O	-3.6319298	-0.9341678	-3.3706727
O	-3.7608667	0.3117093	-1.4400859
C	-5.2363091	0.3213483	-1.3977515
C	-5.5236675	1.1351473	-0.1344725
H	-5.0945240	2.1432111	-0.2210149
H	-6.6088364	1.2260529	0.0168513
H	-5.0853731	0.6448472	0.7464863
C	-5.7755549	-1.1042097	-1.2480131
H	-5.5818322	-1.6981477	-2.1482080
H	-5.3037199	-1.5982251	-0.3855204
H	-6.8609161	-1.0679074	-1.0719546
C	-5.8039409	1.0282411	-2.6317893
H	-5.3497568	2.0240220	-2.7399625
H	-5.6107436	0.4491548	-3.5417487
H	-6.8902845	1.1560853	-2.5129405
H	-1.0801862	-0.8772412	-3.0076472

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Comp 13 Energy = -1528.756148899

O	0.8109429	5.6153470	8.2339920
O	0.4055452	6.0231984	10.4568641
O	6.1570956	2.4205105	11.0789631

N	3.2089658	4.3837531	8.9376292
N	4.3292961	3.8777546	9.2971447
N	2.4143989	4.3023280	11.1367934
N	3.5142845	3.7834486	11.5314253
C	2.3734514	4.9067861	9.8973379
C	1.1360250	5.5345860	9.4234394
C	-0.9387691	6.6076369	10.2418391
C	-0.8377962	7.8707116	9.3832164
H	-1.8170358	8.3713453	9.3574385
H	-0.5326051	7.6307857	8.3582906
H	-0.1075126	8.5680065	9.8189243
C	-1.8767732	5.5626754	9.6316530
H	-2.9020340	5.9604669	9.6142234
H	-1.8736132	4.6482084	10.2424386
H	-1.5786744	5.3105205	8.6072316
C	-1.3746498	6.9551417	11.6651251
H	-2.3780482	7.4039701	11.6516029
H	-0.6755095	7.6727197	12.1169232
H	-1.3989353	6.0522204	12.2907051
C	4.6512157	4.2613385	10.6919192
H	4.6818497	5.3697755	10.7556123
C	5.9406059	3.6188737	11.1345766
O	6.7978367	4.5629178	11.5998559
N	2.9946812	2.4338543	6.3525266
N	1.9956182	1.3641529	7.9753465
C	2.0040959	2.5049468	7.2605598
C	3.0310803	0.5581133	7.5261660
H	3.2444057	-0.4095378	7.9613291
C	3.6537402	1.2260603	6.5148918
H	4.5096966	0.9457191	5.9147351
C	8.1386879	4.1909782	12.1284587
C	7.9834824	3.2794818	13.3469356
H	7.5765418	2.3017267	13.0648692
H	8.9678337	3.1319280	13.8152100
H	7.3165186	3.7433328	14.0880493
C	8.7209777	5.5444521	12.5332005
H	9.7283893	5.4070508	12.9511152
H	8.7914817	6.2116464	11.6625942
H	8.0892683	6.0253936	13.2931237
C	8.9765245	3.5485122	11.0209145
H	9.0029614	4.2005388	10.1359117
H	10.0075895	3.4150463	11.3802061
H	8.5735378	2.5712389	10.7320401
C	1.0395605	0.9721792	9.0711337
C	3.4056616	3.5064106	5.3799023
C	0.2761496	-0.2704470	8.5878251
H	0.9540913	-1.1119705	8.3872225
H	-0.4297496	-0.5851327	9.3682061
H	-0.2923236	-0.0511690	7.6724006
C	1.8626629	0.6700676	10.3313191
H	2.4592764	1.5399021	10.6367938
H	1.1768067	0.4156483	11.1508283
H	2.5367961	-0.1846618	10.1805748
C	0.0645131	2.1196043	9.3378445
H	-0.5055844	2.3979045	8.4393682
H	-0.6545839	1.7867169	10.0972057
H	0.5806558	3.0008719	9.7374980
C	2.4076744	4.6623165	5.4565556
H	2.7335084	5.4441161	4.7577658
H	1.3982909	4.3441309	5.1546731
H	2.3571778	5.0941585	6.4654660
C	3.4000575	2.8881853	3.9740421
H	3.6816118	3.6591618	3.2439091
H	4.1209919	2.0633455	3.8824552
H	2.4001422	2.5129111	3.7132210
C	4.8127636	3.9785569	5.7753241

H	5.5502311	3.1691415	5.6727653
H	5.1167169	4.7987787	5.1102310
H	4.8237616	4.3294119	6.8148349
H	1.3493599	3.3560902	7.4056569